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(3 Pages)

ION TEMPERATURE GRADIENT MODES

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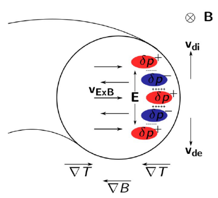


Figure 1: Schematic diagram of Ion Temperature Gradient Modes (ITGs)

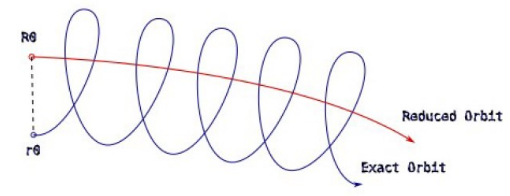


Figure 2: Orbit of the gyrokinetic particle

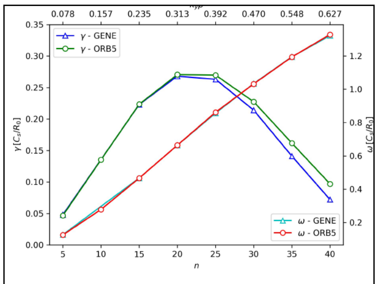


Figure 3: Linear growth rates and real frequencies for ITG modes

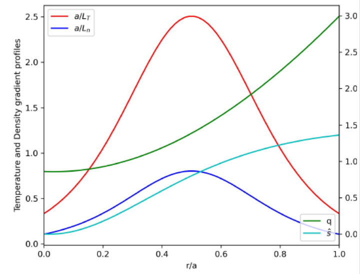


Figure 4: Equilibrium profiles of CBC

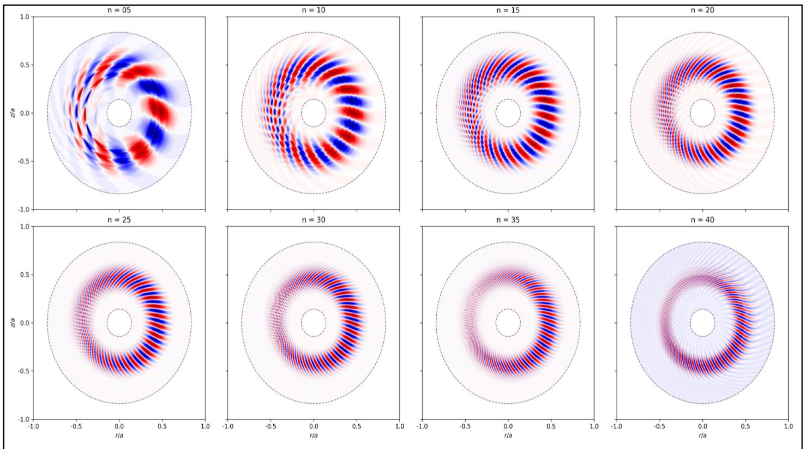


Figure 5: 2D plots of electrostatic potential

Nuclear Fusion is one of the most promising ways to meet the growing future energy needs. Many decades of research, it is found that toroidal plasma devices known as Tokamaks are the most optimum of all the possible configuations studied. These devices are still unstable at Magneto Hydrodynamic (MHD) scales. Even if we come to a point where the device is stable at MHD instabilities, there exists instabilities whose length scales and time scales are of the range ion larmour radius and gyrofrequencies respectively, which are collectively know as microinstabilities [1,2]. One of this kind are Ion Temperature Gradient Modes (ITGs), which are drift waves driven by gradient in ion temprature. ITGs are extensively studied, because these are responsible for the anamalous heat transport in Tokamkas, and are characterized by the short perpendicular wavelengths and long parallel wavelengths compared to the ion Larmor radius.

Due to curvature and gradient in background magnetic field, there is a vertical charge separation, which generates an electric field ***E*** between the opposite charges, which in turn induces charge independent ***E x B*** drift. Toroidal-ITGs tends to be unstable where ∇T_i is parallel to ∇B (bad curvature) and otherwise stable if ∇T_i is anti-parallel to ∇B (good curvature). A schematic diagram of ITG instability is given in **Fig 1**.

Since length scales are shorter and time scales are larger, for a microinstability as compared to MHD scales, kinetic simulations are required in order to study ITGs. The simulations presented here are performed using nonlinear global electromagnetic gyrokinetic [3] particle-in-cell (PIC) code, ORB5 [4], which solves the gyrokinetic Vlasov equation, gyrokinetic poisson equation and equations of motion. **Fig 2.** is schematic diagram of reduced particle orbit following its guiding center/gyro center (red), whereas exact orbit gyrates (blue) around the field line, the former one is compuationally less expensive than the latter, while preserving the finite larmour radius effects.

A circular concentric "adhoc" magnetic equilibirum is used in the present simulations based on the Cyclone Base Case (CBC) [5]. CBC is a set of parameters derived from the H-Mode of the DIII-D Tokamak (**Fig 3.**). In this simulation, the ions are treated as gyrokinetic, whereas the electrons are treated as adiabatic and the temperature and density profiles of the CBC case satisfy $L_n/L_T > 1$ (gradient length scales for *n* and *T)* in order to destablize ITGs. The linear growthrates (**Fig 4.**) and frequencies (**Fig 4.**) calculated from the electric field are plotted for various toroidal mode numbers *n and benchmarked against GENE code [6]*. The maxima of linear growthrates is at *n ~ 20* and the magnitude of frequency increases with *n*. ITG modes rotates in ion diamagnetic direction, which is counter clockwise in ORB5 convention.

Fig 5. is a 2D plot of electrostatic potential. The blues and reds in the figure indicate the positive and negative values of perturbed electrostatic potential. The number of red or blue structures are proportional to *m ~ nq* calculated at the reference point *s ~ 0.5.* One can observe that, the eigenmode structure balloons in the outboard side where as it is smaller in inboard side, due to bad and good curvature respectivley.

These simulations were performed on a grid size of 512 x 256 x 128 for 5 < *n* < *30* and 512 x 512 x 256 otherwise. Each point in the plots is one simulation, which ran for 10000 time steps with dt = $40\Omega^{-1}$. It took ~ 3 hrs each with 512 CPU cores. All the simulations are performed in the state of the art HPC machine, ANTYA available at Institute for Plasma Research (IPR).

References:

1. W. Horton, "Drift waves and transport," Rev.Mod.Phys., 1999
2. Jan Weiland, "Collectives Modes in Inhomogeneous Plasma", IOP Publishing, 1999
3. A. J. Brizard and T. S. Hahm, "Foundations of Nonlinear Gyrokinetic Theory,"Rev.Mod.Phys., 2007
4. E. Lanti et al., "Orb5: A global electromagnetic gyrokinetic code using the PIC approach in toroidal geometry," Computer Physics Communications, 2020
5. A. M. Dimits et al., "Comparisons and physics basis of tokamak transport models and turbulence simulations," Physics of Plasmas, 2000T. Görler et al., "Intercode comparison of gyrokinetic global electromagnetic modes," Physics of Plasmas, 2016

Efficient HPC Workflow Management with PBS Scheduler

High-Performance Computing (HPC) plays a crucial role in solving computational problems in fields like science, engineering, and artificial intelligence. Efficiently managing HPC workflows is essential to utilize available resources effectively and reduce processing time. The Portable Batch System (PBS) Scheduler is a powerful job scheduling system used in ANTYA. This article provides a detailed guide on optimizing workflows using PBS Scheduler, ensuring resource efficiency and smooth job execution.

PBS Scheduler provides several features that make it an excellent choice for HPC workload management like **Resource Management** using which users can define the exact computational resources required, such as CPU cores, memory, GPUs, and wall time and **Scalability** using which PBS can manage systems ranging from small clusters to massive supercomputers.

Below are the best practices for Efficient Workflow Management using PBS.

A) Understand Resource Requirements

Efficient scheduling begins with accurately estimating the resources required for the job. Specifying the number of CPUs, memory, GPUs, and runtime ensures that the job is allocated appropriate resources without wastage.

```
#!/bin/bash
#PBS -N simulation_job
#PBS -l select=1:ncpus=8:mem=32gb:ngpus=1
#PBS -l walltime=02:00:00
```

In this example, a job requests 8 CPU cores, 32 GB memory, and 1 GPU, ensuring resources match the workload needs.

B) Use Job Arrays for Parametric Studies

If user needs to run a program multiple times with different input parameters, job arrays are an excellent choice. They allow user to submit multiple jobs with a single command, reducing overhead. The below mentioned script runs the simulation for 4 different input files, specified by the job array index.

```
#!/bin/bash
#PBS –J 1-4
#PBS -l select=1:ncpus=1:ngpus=1
mpirun –np 1 lmp –sf gpu –pk gpu 1 –in  in${PBS_ARRAY_INDEX}.nemd > out${PBS_ARRAY_INDEX}
```

C) Optimize Queue Selection

PBS environment on ANTYA offer multiple queues, such as regularq, mediumq, debugq, longq, etc. catering to jobs of varying durations and core requirements. Submitting a job to the appropriate queue reduces wait times. Jobs requiring more cores should use the mediumq queue, while for debugging purpose, debugq can be used..

```
#!/bin/bash
#PBS –q longq
```

D) Monitor Jobs Effectively

Monitoring job's progress helps user identify potential issues early. PBS provides several commands:

qstat –answ1 -u username : Shows the status of jobs for user.

pbsnodes -aSj : Displays information about available and occupied nodes.

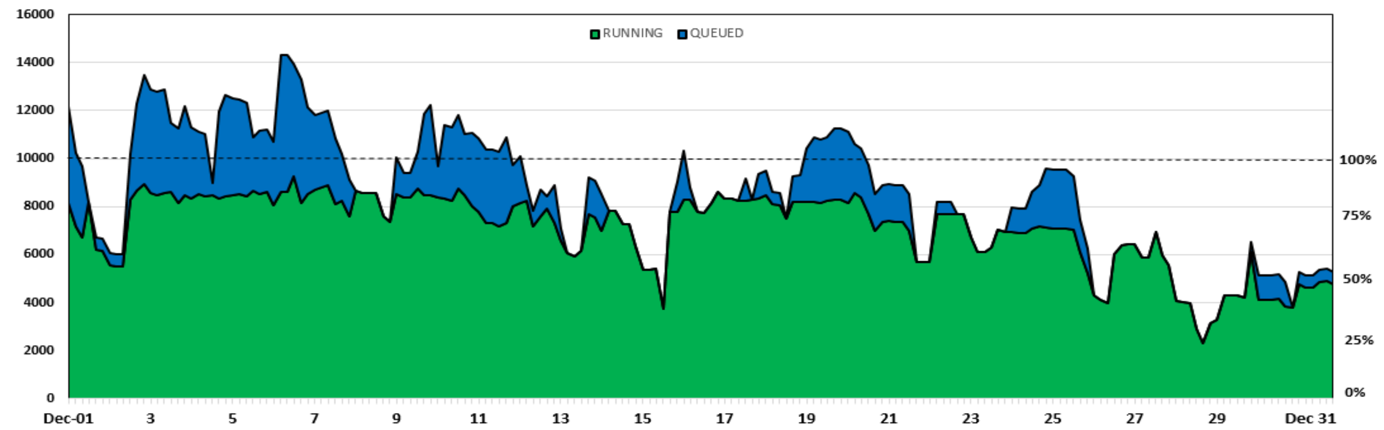
E) Automate Dependencies with Job Dependencies

For workflows with multiple stages or for inter dependent jobs, job dependencies ensure that a subsequent task begins only after the preceding one completes successfully. Here, the job waits until job ID 339639 finishes successfully before starting.

```
#!/bin/bash
#PBS –W depend=afterok:339639
```

Efficient management of HPC workflows with PBS Scheduler requires understanding workload, optimizing resource requests, and leveraging advanced features like job arrays, automate jobs dependencies. By implementing these practices, one can reduce job wait times, minimize resource wastage, and improve overall productivity in HPC environment.

ANTYA Utilization: DECEMBER 2024



ANTYA Daily Observed Workload

Other Recent Work on HPC

Conceptual design of a fusion pilot and its role in fusion electricity roadmap	**Shishir P. Deshpande**
3D Computational Fluid Dynamics Analysis of Prototype Ion Extractor Grid-1 using ANSYS	**Tejendrakumar Bhanabhai Patel**
Development of a sensitive flowmeter for electrically conducting liquids and its calibration using first principles in a novel high temperature set up	**Srikanta Sahu**
Dynamic Analysis of Soft Catch for Electromagnetic Launcher System using ANSYS	**Vishal Verma**
Benchmarking of spherical tokamak power plant design in PROCESS and SARAS	**Shishir P. Deshpande**
Impact of ion-neutral collision on edge biasing	**Vijay Shankar**
Development of a Novel High Temperature Superconducting Compact D-shaped magnet for Tokamak	**Mahesh M Ghate**
Two-Phase Flow Studies on Subcooled Nucleate Boiling in HyperVapotron Elements for the Neutral Beam Flux Loads of 10 MW/M² in the Fusion Devices.	**M. Venkata Nagaraju**
Design and Analysis of the Cryogenic Extruder of Solid Hydrogen for Fusion Reactor	**Vishal Gupta**

ANTYA UPDATES AND NEWS

1. New Packages/ Applications Installed

=> New modules have been installed in ANTYA

To check the list of available modules
$ module avail –l

ANTYA HPC USERS' STATISTICS— DECEMBER 2024

Total Successful Jobs~ 1133

♦ **Top Users** (Cumulative Resources)

● **CPU Cores**	**Amit Singh**
● **GPU Cards**	**Abhishek Agraj**
● **Walltime**	**Tulchhi Ram**
● **Jobs**	**Souvik Mondal**

Acknowledgement

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

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