

INSIDE THIS ISSUE

(3 Pages)

- ◆ Research Highlight: **Studies on Impurity Seeding in Tokamak Plasma**
- ◆ HPC Article Series: **Python Package Management Using Conda — Part-3: Using Different Conda Channels for Packages Installation**
- ◆ ANTYA Updates and News: **1-Day GPU Bootcamp at IPR**
- ◆ ANTYA Job Queuing System (AJQS) as on 31st August 2021
- ◆ ANTYA HPC Users' Statistics—AUGUST
- ◆ Other Recent Work on HPC (Available in IPR Library)

GANANAM (गणनम्)

HIGH PERFORMANCE COMPUTING NEWSLETTER
INSTITUTE FOR PLASMA RESEARCH, INDIA



Studies on Impurity Seeding in Tokamak Plasma

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Tokamak is an example of a low pressure gas discharge tube bent into a closed circular shape (Torus). The plasma inside a tokamak is generated with the ohmic current usually induced by transformer action. In the presence of thermal energy, plasma is lost at the walls of tokamak vessel. This is the reason why plasma-surface interaction is an unavoidable situation in all fusion grade tokamaks. This radial loss of plasma is minimized by introducing a toroidal magnetic field, but the charge particles moving parallel to this magnetic field with very high velocity can not be stopped to interact with the vessel wall. This hot plasma when interacts with wall causes serious damage to vessel [1]. To minimize these damages, things like limiter, and divertor comes into picture. These have high heat withstanding capacity and are conductors. Plasma which was earlier going to vessel wall now collected on to this limiter/divertor material which helps in substantial reduction in wall damage. These plasma-limiter/divertor interactions results in formation of two regions inside the tokamak named as Edge and Scrape-off-layer region (SOL) as shown in Figure 1. To protect these material plates from the hot plasma, impurity seeding of low Z and medium Z impurities like neon, nitrogen, or argon gases have been proposed as an effective strategy. The plasma-impurity gas interactions involve many processes such as electron impact ionization, radiative recombination, molecular dissociation (for nitrogen). Also, the flow of plasma in the edge and SOL region is turbulent because here motion is governed by non-linear dynamics. The plasma transport in the edge and SOL regions therefore, is mainly through interchange plasma turbulence [2, 3, 4, 5] and, the plasma-impurity interaction is associated with the turbulent transport process.

In this work, a two-dimensional (2D) numerical simulation of the impurity seeding for nitrogen gas has been done using BOUT++ code in the edge and SOL regions of a tokamak plasma by solving a set of 2D partial differential equations. Details of modeling can be found in [6,7]. **The runtime of**

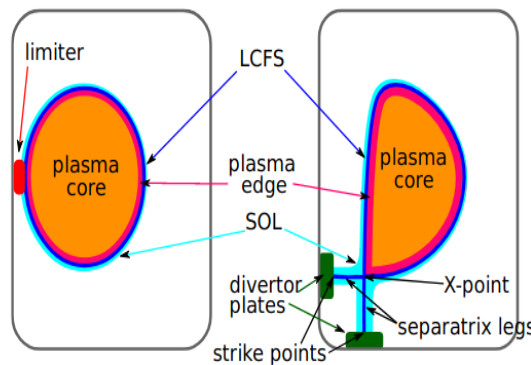


Figure 1: Sketch of a limited and diverted configuration. The confined plasma (core-edge) are separated from SOL by the LCFS (also called separatrix).

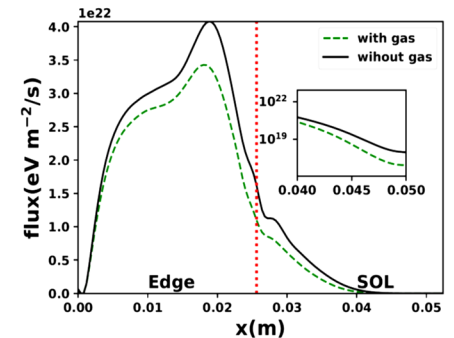


Figure 2: Poloidal and long-time averaged radial profile of radial electron energy flux based on the turbulent transport. The flux decreases in the SOL region in the presence of nitrogen seeding. The vertical dotted line indicates edge-to-SOL transition region. The inset plot indicates the magnitude of energy flux in log scale for $x = 0.04-0.05$ m.

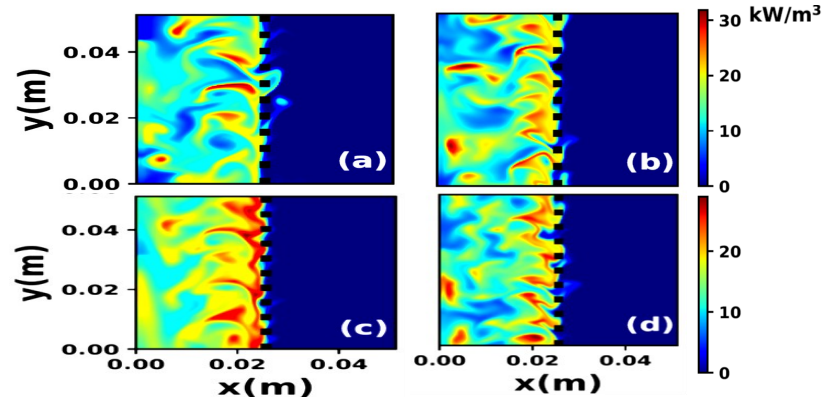


Figure 3: Radiation cooling front from nitrogen ions obtained from 2D simulation for non-coronal equilibrium state [8]. (a), (b), (c), and (d) are taken at 0.55 ms, 0.60 ms, 0.65 ms, and 0.70 ms, after the gas puff, respectively. The magnitude of the color bar is in kW/m^3 . The vertical dotted line indicates the edge-to-SOL transition region.

simulation is approximately 10 hours for 16 cores of ANTYA HPC Cluster. All the parameter used in the simulation belongs to ADITYA-U tokamak.

“As our model is independent of tokamak geometry or magnetic equilibrium, we believe our results should be useful for interpretation and/or predictive purposes in most experimental situations of neutral seeding in the edge and SOL regions.”

The energy flux with and without nitrogen gas is shown in Figure 2. It has been

found that there is about a 30% reduction in the energy flux after the nitrogen gas is introduced. Also, the Nitrogen gas is found to radiate locally about 20-30 kW/m^3 of incoming power near LCFS as shown in Figure 3. This local radiative tendency of nitrogen indicates that nitrogen seeding does not contaminate the tokamak core plasma much. A comparative study of Nitrogen, Neon and Ar-

gon is planned to be performed next to get the best suitable candidate for seeding in Aditya tokamak.

References:

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2. Nirmal Bisai, Amita Das, Shishir Deshpande, Rameshwar Jha, Pradhiman Kaw, Abhijit Sen, and Raghvendra Singh. Simulation of plasma transport by coherent structures in scrape-off-layer tokamak plasmas. *Physics of Plasmas*, 11(8):4018-4024, August 2004.
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8. A. A. Mavrin, *J. Fusion Energy* 36, 161-172 (2017).

Python Package Management Using Conda – Part-3 Using Different Conda Channels for Packages Installation

If you find yourself in need to install a Python package that is not available through the default Conda channels, you would wonder from where you should install the package in the newly created Conda environment (Creating Conda environment was discussed in part-2, issue8). In this part-3 of the Conda article series, we will cover how you can use different Conda channels for the Python package installation as well as the default Python package manager Pip to install packages from PyPI (Python Package Index) repository.

What are Conda Channels?

When we try to install the packages using Conda, the Conda command searches a default set of channels from Anaconda Cloud. Collectively, the Anaconda managed channels are referred to as the default channels. There are other channels also namely conda-forge, bioconda, etc. which should be used when the package is not available in the default channels.

When to use Pip instead of Conda?

If a Python package that you need is not available in any of the Conda channels, then you can use Pip to install the package. The important thing to remember when you are using pip inside a conda environment for package installation is to first install the pip package using conda inside the environment and then use that pip to install the required package.

Example Project: Implementation in ANTYA

Suppose we need to create a machine-learning environment which require the packages, scipy-1.7 and combo. We will see that scipy version 1.7 is not available in the default channels and we have to use other conda channel to install it. Also the other package, combo, could be successfully installed only using the pip package manager.

Create the project name with Conda

```
[user@login1 ~]$ conda create --name machine-learning
```

Now activate the created environment

```
[user@login1 ~]$ conda activate machine-learning
```

This will activate the environment and your shell would show you are inside the environment. Now check the available packages in environment

```
(machine-learning) [user@login1 ~]$ conda list
```

Since there are no packages installed, this will not list any packages. Now install the required packages

```
(machine-learning) [user@login1 ~]$ conda install scipy=1.7
```

PackagesNotFoundError: The following packages are not available from current channels: - scipy=1.7

scipy version 1.7 is not available in the default conda channels. Now let us explore the other channel viz conda-forge. This successfully installs the package

```
(machine-learning) **$ conda install scipy=1.7 --channel conda-forge
```

Successful

To install combo package, first try with conda default and forge channels

```
(machine-learning) [user@login1 ~]$ conda install combo
```

PackagesNotFoundError

```
(machine-learning) **$ conda install combo --channel conda-forge
```

PackagesNotFoundError

To install combo using pip (First install pip)

```
(machine-learning) [user@login1 ~]$ conda install pip
```

```
(machine-learning) [user@login1 ~]$ pip install combo
```

Successful

ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

⇒ **LAMMPS 2020 module**

lammps-2020/intel/03MAR2020

⇒ **Miniconda module**

miniconda/3

⇒ **Update hpc_sdk**

module

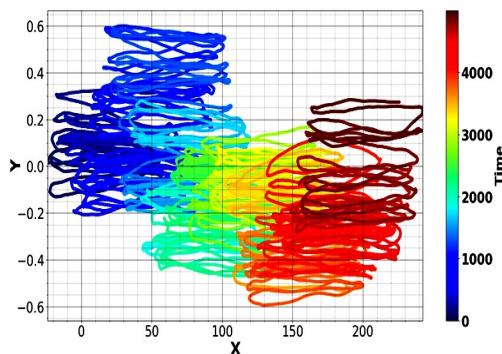
nvhpc modules

1-Day GPU Bootcamp

Tentative Date: 16th Sept.

Registration link will be shared soon

Run-time Trajectories in a 2D Yukawa System (HPC Picture of the Month)



Pic Credit: **Anshika Chugh**

The figure shows particles information about their mean position by color coding particles' trajectories in a box having 1024 particles. The Particles' trajectories obtained can be used in tracking the drift velocity of the system.

The figure is generated using in-house developed multicore MPMD-2D (Multi Potential Molecular Dynamics) code using a total of 1024 cores simulation run on ANTYA.

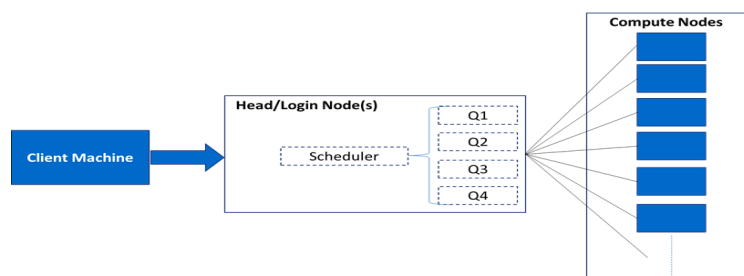
Tip of the month

TO SEE THE LIST OF ALL THE AVAILABLE MODULES

\$ module avail

ANTYA Job Queuing System (AJQS) as on 31st August 2021

HPC Users access to the compute nodes of ANTYA is managed by a software called the Scheduler. The scheduler manages occupied and free available compute resources according to the queues that the Users can access. Just like the lanes on a highway with each lane dedicated to the different type of vehicles based on their load capacity to manage the traffic in a better way, every HPC cluster has queues which are made and managed so that the HPC resources are fairly allocated to all the Users. The Schematic below shows how a job can be submitted from a client machine (User) through the head/login node on the cluster compute nodes.



In ANTYA, we have PBS Pro scheduler for job submission and monitoring. A unique queue policy has been made based on Users feedback and their usage characteristics for ANTYA cluster given in the table below. Once the job is submitted, the scheduler allocates the resources (compute nodes) in one of the queues based on resources limits and availability of free nodes. The job is then computed on the compute nodes. The queues have been designed to ensure all Users have a fair and reasonable opportunity to submit and complete their jobs.

Queue Name	Nodes (cores) allocation/queue	Max. Walltime	Max. Cores/job	Min. Cores/job	Max. Running jobs/User	Max Queued jobs/User	Max Queued jobs/Queue	Node Sharing
debugq	3 (120)	30 min	120	1	2	1	5	Yes
serialq	13 (520)	360 hours	10	1	154	40	200	Yes
regularq	53 (2120)	96 hours	40	20	25	5	30	No
mediumq	150 (6000)	48 hours	1600 (2100 user limit)	80	10	2	20	No
longq	60 (2400)	120 hours	600 (1600 user limit)	80	10	2	10	No

AJQS is reviewed every 3-4 months and minor changes are done on Users' requests and/or usage pattern on a regular basis. If Users do not indicate the queue name in their job scripts, then their jobs will automatically go to the "default" queue which is regularq. For **Advance Reservations (asking for computational resources for a specific duration beyond the limit of the queues available in the cluster but not more than 30-40% of the available HPC resources)**, a separate queue "rq" is being used for which an additional request should be made 1-2 weeks in advance to HPC Team. For external Users, separate queues (**extq1 and extq2**) are maintained and they are allowed to submit jobs in these queues only.

Other Recent Work on HPC (Available in IPR Library)

Impurity Seeding in a Tokamak Plasma and Comparison with Experiments	SHRISH RAJ
Effects of transmutations in material damage for plasma facing materials in fusion systems	AKASH GARG
Toroidal field coil for an electron plasma experiment: SMARTEX-C	LAVKESH TEKCHAND LACHHVANI
Theory of Plasma Blob Formation and its Experimental Validation	NIRMAL K BISAI

Acknowledgement

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

ANTYA HPC USERS'

STATISTICS—AUGUST

- ◆ Total Successful Jobs — **2932**
- ◆ Top Users (Cumulative Resources):
 - ⇒ CPU Cores — **Anshika Chugh**
 - ⇒ GPU Cards — **Suruj Kalita**
 - ⇒ Walltime — **Promit Moitra**
 - ⇒ Jobs — **Vijay Shankar**

On Demand Online Tutorial Session on HPC Environment for New Users Available
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