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HIGH PERFORMANCE *COMPUTING* NEWSLETTER

INSTITUTE FOR PLASMA RESEARCH, INDIA

HAPPY NEW YEAR 2023

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Installation and Initial Testing of ITER Integrated Modeling and Analysis Suite (IMAS) on ANTYA

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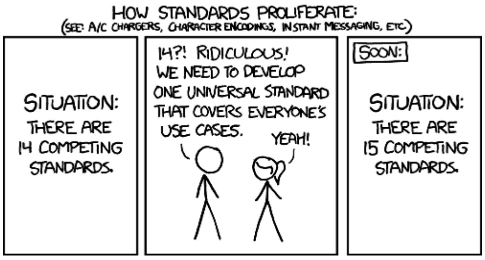
Integrated Modeling and Analysis Suite (IMAS) [1] is a critical part of the ITER Integrated modeling program whose objective is to allow researchers across the globe to predict and understand the behavior of the ITER plasma and in general fusion plasmas as well as to understand the overall performance of the fusion device. IMAS aims to deliver a unified data system and standards for code integration along with workflows for data analysis, code verification, and validation. With a number of experimental facilities and working tokamaks within ITER Members generating a lot of data and developing numerical tools to accurately model complex plasma phenomena, there is a pressing need to have a software suite that can bring all the fusion data in a common format and integrate codes across tokamaks. A cartoonist representation of the adoption of data standards in scientific simulations is shown below:


HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)
SITUATION: THERE ARE 14 COMPETING STANDARDS.
14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES.
YEAH!
SOON:
SITUATION: THERE ARE 15 COMPETING STANDARDS.

© xkcd

The actual data formats [2] used for inputs and outputs of tokamak simulation codes across Europe are shown in figure 1.

ITER has come up with a collaborative development and data exchange approach via developing IMAS for the fusion community. The backbone of the IMAS infrastructure is a standardized, machine-generic data architecture that represents simulated and experimental data with identical structures using Interface Data Structures (IDSs) described by Data Dictionary. IMAS includes a set of tools to access data and design integrated modeling workflows using the Kepler workflow engine and coupling tools as shown in figure 2. IMAS is being continuously developed and upgraded using expertise and technologies developed within the ITER Members' research programs.

> ***"IMAS is an essential part of the research and development process for ITER and adaption of indigenous codes to IMAS is critical to exploit ITER's data"***

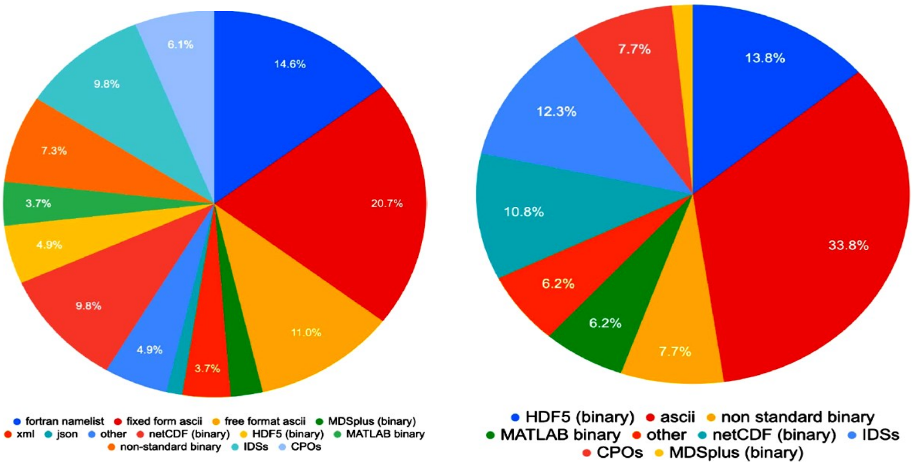


Figure 1: Characterization of code (left) input (right) output data formats [2]. These graphs represents the responses from experimental facilities and code developers.

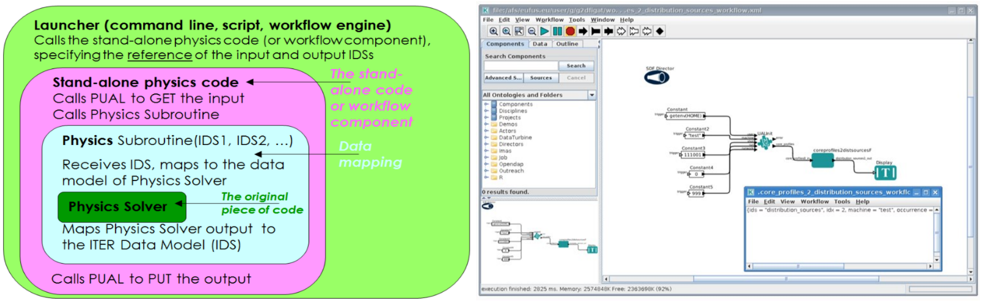

Launcher (command line, script, workflow engine)
Calls the stand-alone physics code (or workflow component), specifying the reference of the input and output IDSs
Stand-alone physics code
Calls PUAL to GET the input
Calls Physics Subroutine
The stand-alone code or workflow component
Physics Subroutine(IDS1, IDS2, ...)
Receives IDS, maps to the data model of Physics Solver
Data mapping
Physics Solver
The original piece of code
Maps Physics Solver output to the ITER Data Model (IDS)
Calls PUAL to PUT the output
File Edit View Workflow Tools Window Help
Components Data Outline
Search Components
Search
All Ontologies and Folders
0 results found.

Figure 2: (Left) IMAS structure [1], (right) Accessing IMAS IDS through Kepler workflow and executing a program.

Installation and Initial Testing of IMAS on ANTYA

IMAS is a complex software platform that integrates data from multiple sources and models, and it requires a lot of dependencies to install and configure correctly on any HPC platform. As the source code of IMAS is available on a private ITER GitHub repository, an IDM account is required to get the code and related packages. On ANTYA, IMAS has been installed in a group account with all its dependencies. The workflow engine Kepler and coupling software FC2K have also been installed. The integrated testing of IMAS for FORTRAN and Python codes has been successfully completed on ANTYA with the IMAS data model where both the test codes could communicate with IDS of IMAS. A team of 3 members (see Acknowledgement) is currently involved in the ongoing testing of Kepler workflow and FC2K with IMAS using the test codes. As a next step after the full testing, the work will be started on integrating an indigenous code developed at IPR on IMAS platform. Interested people are encouraged to join in this effort for other codes adaptation to IMAS.

The Way Forward

To interpret, understand, and exploit ITER's data, it is necessary that the indigenous modeling and analysis codes shall be made compatible to integrate with IMAS. This will allow us to fully participate in the simulation and analysis of ITER plasmas over the next decade and beyond when ITER becomes operational. With the knowledge and expertise attained by playing a proactive role in the IMAS integrated modeling activities, our domestic programs would get a huge push.

With the installation of IMAS on ANTYA, we have begun the journey where a strong collaborative effort is required to seize this opportunity to develop/integrate/validate our codes towards a whole device modeling capability on the IMAS platform.

Acknowledgement: ***Amit Singh*** **and** ***Anil Tyagi*** from ITER-India are helping in installation & testing of IMAS.

Disclaimer: The views and opinions expressed herein do not necessarily reflect those of the ITER Organization.

References:

1. *F. Imbeaux et al. 2015 Nucl. Fusion 55 123006.*
2. *P Strand et al 2022 Plasma Phys. Control. Fusion 64 104001 .*

Running GPU Container Workloads on GPU Nodes of ANTYA

This article is to show how a container with GPU code inside can be launched on ANTYA GPU nodes. The source code inside a directory in the container can be compiled on the system based on the GPU compute capability. This is done so that the same container image can be used on different GPU architectures.

How to Implement in ANTYA?

Example-1: As an example here to run GPU workload on a single node, we will use an existing container image (gpu.sif) which is having a gpu burn source code and execution script inside the container directory /opt/gpu-burn/.

```
# Copy the paraview container image available on ANTYA to your home or working directory.
[user@login1 ~]$ cp /home/application/singularity_images/
singularity_3.4.1/gpu.sif .

# Here is the PBS job script for submitting paraview container job.
[user@login1 ~]$ cat jobscript_gpu_container.sh

#!/bin/bash
#PBS -q serialq
#PBS -N gpu_container
#PBS -l select=1:ncpus=1:ngpus=1
#PBS -l walltime=00:10:00
#PBS -j oe
cd $PBS_O_WORKDIR

# Load the singularity module
module load singularity/3.4.1/3.4.1
export COMPUTE=60
#  Run the following command to execute the container image on a GPU node.

singularity exec --nv gpu.sif /opt/gpu-burn/gpu_burn.sh
```

ANTYA HPC USERS' STATISTICS— DECEMBER 2022

♦ **Total Successful Jobs — 5069**

♦ **Top Users (Cumulative Resources):**

CPU Cores	Amit Singh
GPU Cards	Shishir Biswas
Walltime	Anjan Paul
Jobs	Someswar Dutta

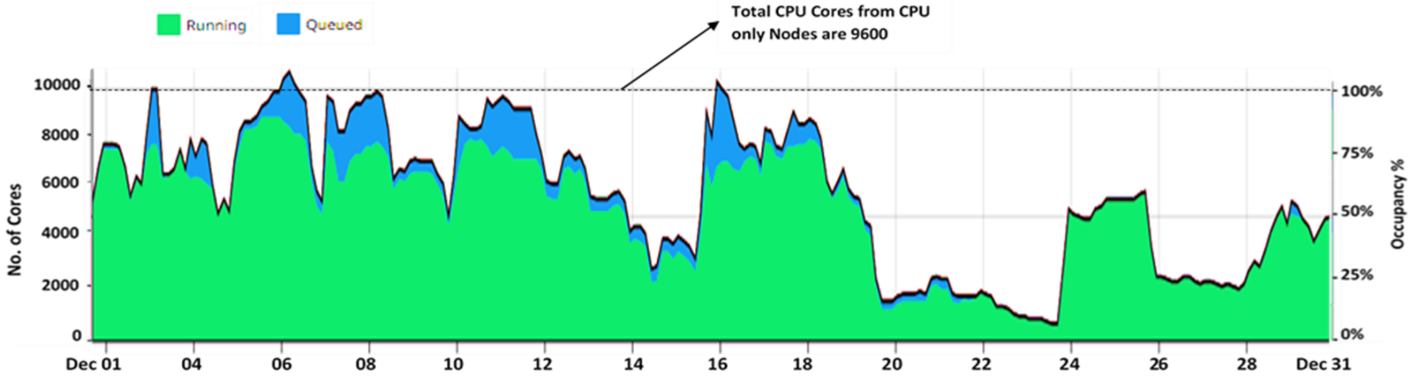
Other Recent Work on HPC

(Available in IPR Library)

Off-target flows and shoulder formation in 3D simulations of inboard limited scrape-off-layer plasma transport of ADITYA-U tokamak	ARZOO MALWAL

ANTYA Utilization: DECEMBER 2022

ANTYA Daily Observed Workload



Acknowledgement

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

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