Energy-oriented Center of Excellence (EoCoE) Summer School

lundi 6 juin 2022

Opening: Opening (09:00 - 09:30)

Welcome general presentation agenda Q&A

-Présidents de session: Celino, Massimo (ENEA)

SaaS portal presentation: SaaS portal presentation (09:30 - 10:15)

GCQ presentation Q&A

-Présidents de session: Wolniewicz, Paweł (PSNC)

[11] SaaS Portal presentation (09:30, 35 minutes)

Orateur: WOLNIEWICZ, Paweł (PSNC)
EoCoE Saas Portal is a portal to access software solutions for the energy sector. It showcases simple and clear use cases (with a limited number of parameters) that users can run as example jobs with limited resources. The presentation covers the functionality of the portal that includes: - Submit jobs using a click-through interface - Monitor status of the submitted jobs - Manage input and output data - Flexible application template with predefined examples - Integration with SLURM resource management system

[12] Conclusion (10:05, 10 minutes)

Orateur: WOLNIEWICZ, Paweł (PSNC)
Time for summary, QA, ideas.

Setup: Technical environment (10:15 - 10:45)

Preliminary unified session on the school's technical environment, so the target audience should already be versed in Linux environment. SaaS portal individual accounts setup.

Break (10:45 - 11:15)

WEATHER FORECASTING: Large ensemble simulation for short-term weather forecasting using ESIAS-met (11:15 - 15:05)

The weather simulation is an essential tool for weather forecasting and prediction. The powerful supercomputers now can enhance the simulation capability of weather simulation for large ensembles to provide probabilistic simulation. In EoCoE project, we have create a large ensemble simulation system, ESIAS-met, to enhance the power of the codes of Weather Research and Forecasting to perform probabilistic simulation. However, the atmospheric simulation require a good knowledge of atmospheric science and basic understanding of how weather forecasting be performed by large ensemble. This course will cover basic theory of atmospheric science to handle the science behind the weather model, basic knowledge of WRF for installing this software, and the basic analysis technics to produce meaningful results for comparison.

[1] Crash course in weather forecasting (11:15, 1 heure)

Orateur: Dr LU, Yen-Sen (Forschungszentrum Jülich GmbH, Germany)
In this course we will have a crash course in weather forecasting for non-professionals. We will learn what is weather forecasting is and how we do the weather forecasting and climate simulation. Prerequisite: Basic mathematics, basic knowledge to the Earth system. Outline: 1) Introduction to weather forecasting for non-professionals 2) The basic theory of computational fluid dynamic without equations 3) Weather forecasting and how we do it.

[2] Tutorial of weather forecasting application(s) (12:15, 1 heure)

Orateur: Dr LU, Yen-Sen (Forschungszentrum Jülich GmbH, Germany)
In this tutorial we will learn what ESIAS-met/WRF is, how to install and utilise the weather forecasting prorgram, how to run the system, and how to analyze the results. Prerequisite: Basic computation concept, basic programming skill. 1) Introduction to the structure of ESIAS-met/WRF. 2) The installation of ESIAS-met/WRF. 3) Introduction to the tools for weather data analysis.

[3] ESIAS-met hands on with SaaS Portal (13:45, 1 heure)

Orateur: Dr LU, Yen-Sen (Forschungszentrum Jülich GmbH, Germany)
In this course we will try to use the SaaS Portal to submit your weather forecasting simulation, and try to do some analysis. 1) Let's do weather simulation with ESIAS-met using SaaS Portal 2) Hands on the SaaS portal and create your first weather forecasting/hindcasting.

[10] Conclusion for weather forecasting (14:45, 20 minutes)

Orateur: Dr LU, Yen-Sen (Forschungszentrum Jülich GmbH, Germany)
Summary, QA, Ideas

time	[id] title	presenter
13:15	Break (30 minutes)	

mardi 7 juin 2022

MATERIALS: Use of dftb+ and transport calculations (09:00 - 12:35)

[4] Introduction (09:00, 45 minutes)

Orateur: Dr PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Introduction to the density functional tight-binding approach (DFTB) and transport calculations

[5] Graphene electronic bands (09:45, 30 minutes)

Orateur: PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Calculation of the electronic bands in graphene

[6] Graphene nanoribbons (10:15, 30 minutes)

Orateur: PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Graphene nanoribbons with a vacancy defect

[7] Setup and transport (11:00, 45 minutes)

Orateur: PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Setup and transport calculations

[8] Si/aSi/Si (11:45, 30 minutes)

Orateur: PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Another example: Si/aSi/Si interface

[9] Conclusion (12:15, 20 minutes)

Orateur: PECCHIA, Alessandro (Consiglio Nazionale delle Ricerche)
Time for summary, QA, ideas.

time	[id] title	presenter
10:45	Break (15 minutes)	

mercredi 8 juin 2022

Mathematical Software: PSCToolkit Session (09:00 - 12:30)

-Présidents de session: Pasqua, D'Ambra (IAC-CNR); Durastante, Fabio (Università di Pisa); Filippone, Salvatore (University Rome Tor Vergata)

[14] PSBLAS: A Toolkit for Parallel Sparse Computations (09:00, 1 heure)

Orateur: FILIPPONE, Salvatore (University Rome Tor Vergata)

We provide a description of the architecture of PSBLAS and its usage in the solution of large and sparse linear systems arising in applications. We will describe the data setup process, the available facilities, and the plugin architecture that enables us to support multiple extensions, e.g. running on NVIDIA GPUs.

[13] AMG4PSBLAS: a Package of Parallel AMG Preconditioners for Scalable Linear Solvers (10:00, 1 heure)

Orateur: Dr PASQUA, D'Ambra (IAC-CNR)

Current applications in Computational and Data Science often require the solution of large and sparse linear systems. The notion of "large" is qualitative and there is a clear tendency to increase it; currently, it is not unusual the need to solve systems with millions or even billions of unknowns. The methods of choice to efficiently solve the above systems on high-end massively parallel computers are the Krylov methods, whose convergence and scalability properties are related to the choice of suitable preconditioning techniques. In this tutorial, we will present AMG4PSBLAS (Algebraic MultiGrid Preconditioners for PSBLAS) which provides efficient and easy-to-use preconditioners in the context of the PSBLAS (Parallel Sparse Basic Linear Algebra Subprograms) computational framework. The package, whose features are constantly updated within the EoCoE project, includes multilevel cycles and smoothers widely used in multigrid methods. A purely algebraic approach is applied to generate coarse-level corrections so that no geometric background is needed concerning the matrix to be preconditioned. We will present the main features of the package and example of usage of the main APIs needed to setup the preconditioner, together with its application within the Krylov solvers available from PSBLAS. Some results on test cases relative to the EoCoE application areas highlight how the PSBLAS/AMG4PSBLAS software framework can be used to obtain highly scalable linear solvers.

[15] PSCToolkit: hands-on (11:20, 1 heure)

Orateur: Dr DURASTANTE, Fabio (Università di Pisa)

time	[id] title	presenter
11:00	Break (20 minutes)	

Closing: Closing (14:00 - 15:00)

Awards, Summary