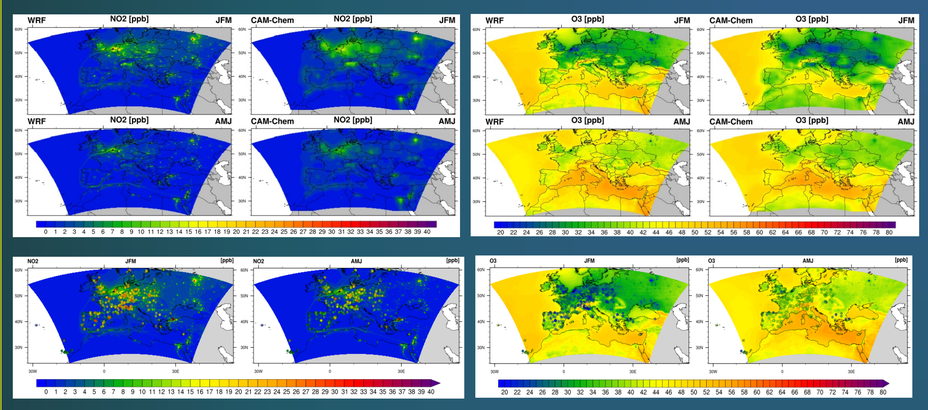
Italian National Agency for New Technologies, Energy and Sustainable Economic Development

CRESCO HPC Applications

Energy Technologies Department – ICT Division

Environments: Air quality simulations

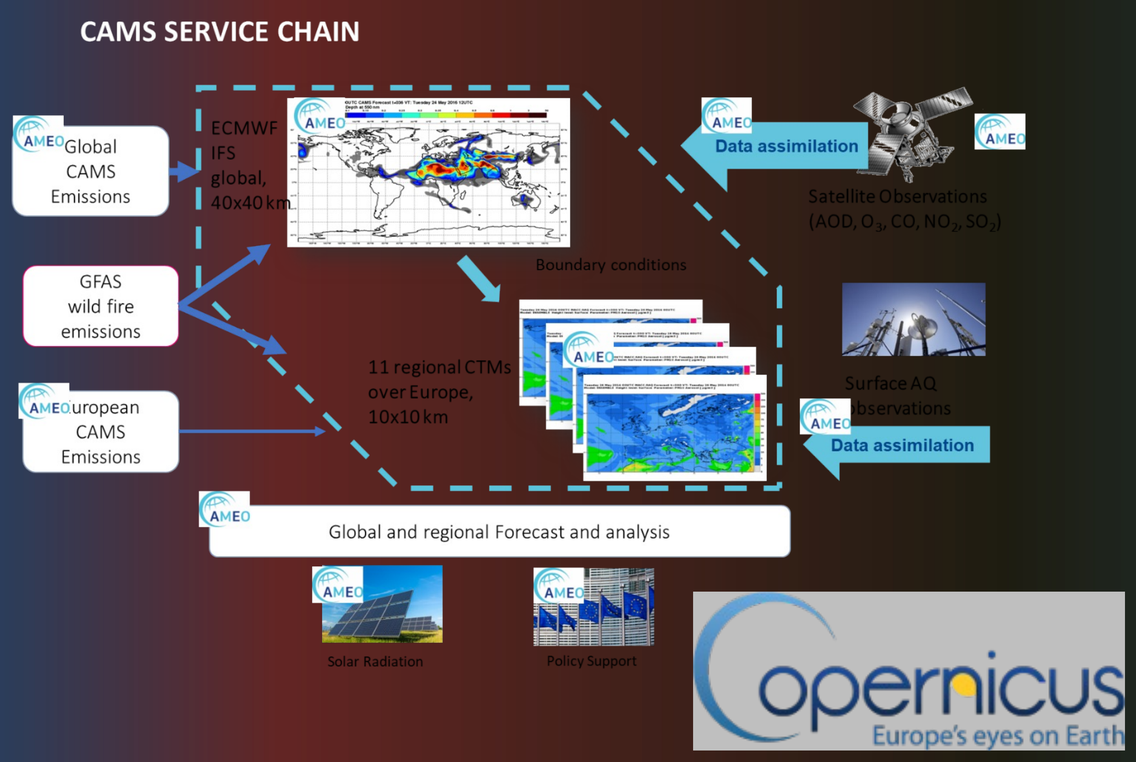
To efficiently reduce air pollution in cities, municipalities and city planners urgently need a quantitative and concrete assessment of the role of urban trees in affecting air quality. In this study, we selected two front-runner cities: Aix-en-Provence in Southeastern France and Florence in Italy, where population is regularly exposed to high particles (PM2.5, PM10), nitrogen dioxide (NO_2) and tropospheric ozone (O_3) levels, exceeding the World Health Organization Air Quality Guidelines. This study is performed within the LIFE project AIRFRESH, which aims to produce new information and recommendations to be integrated into ambitious Urban Greening Plans and Air Quality plans. We use the coupled chemistry-climate model WRF-Chem firstly over European and Mediterranean scale domains then we run the model considering different afforestation scenarios at city-levels. This allows to qualify the difference in pollutants, and the effects of tree species in air pollution removal.



NO_3 O_3

Left boxes show the seasonal averages for O3, in the upper box from January to March, in the lower box from April to June, the right boxes show the CAM-chem NCAR reanalyses for the same periods. The data of the measurement stations are shown in the two boxes at the bottom

Environments: CAMS Service Evolution (CAMEO)



The CAMS Service Evolution project (CAMEO) will enhance the quality and efficiency of the CAMS service, addressing the needs for monitoring air pollutants and greenhouse gases, achieving sustainable development goals, and promoting the use of sustainable and clean energy. Specifically, CAMEO will help prepare CAMS for the acquisition of next-generation air quality satellite data, including Sentinel-4, -5, and 3MI. It will improve data assimilation methods for aerosols and gases, as well as enhance the capability of global and regional production systems for data inversion. CAMEO will develop methods to provide uncertainty information for CAMS product users (emissions, solar radiation, deposition, policy).

ENEA activities outlined in the CAMEO project are a natural continuation of the CAMS50 project (led by Meteo France), carried out in collaboration with nine other European institutes, as well as the CAMS2_40 project, including the deployment and maintenance of the ENEA MINNI model running in High Availability on HPC CRESCO clusters, like the other partnering institutes.

Energy: HYDROGEN PRODUCTION

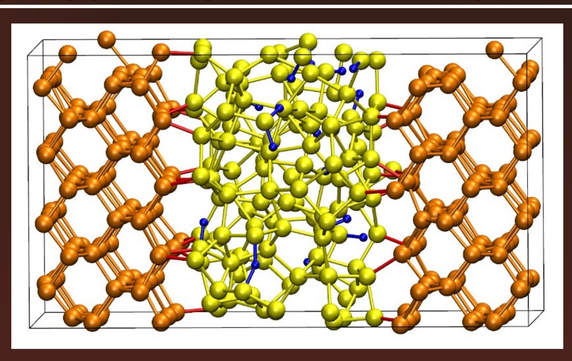
modeling and simulation activities of a Dual Fluidized Bed (DFB) for hydrogen production and CO_2 capture, using a bifunctional catalyst/sorbents solid. The activities carried out were mainly focused on the study of a continuous process for hydrogen production from steam methane reforming (SMR), intensified by CO_2 capture through a $CaO/CaCO_3$ cycle (i.e. Sorption Enhanced Steam Methane Reforming SE-SMR). The double fluidized bed system consists of a carbonation reactor, where CO_2 capture is integrated in a single circuit with a calcination reactor in which the exhausted catalyst/sorbent is regenerated at high temperature. In this model, both the chemical kinetics of the SMR and CO_2 capture reactions were implemented. The main result is the confirmation of the solid material flow rate to be recirculated from the carbonator to the calciner (2.8 g/s) and the production of a gas flow at the exit of the carbonator with a fairly high purity in H_2, about 87.7%. The residual CH_4 is less than 2.5%, a sign that methane reforming and CO_2 capture take place effectively. Conversely, the methane conversion is around 90% .

The computational grid is made of approximately 1.5 million cells. The simulations were carried out on the ENEA CRESCO platform equipped with a TESLA V100-PCIE-32GB GPU .

Instantaneous particle volume fraction in DFB

This work addresses the kinetic and fluid dynamics aspects of the SE-SMR process, using the CPFD (Computational Particles Fluid Dynamics) Barracuda software. It is based on the MP-PIC (multiphase particle-in-cell method) model with a Lagrangian-Eulerian approach. The gaseous phase is treated as a continuous fluid with its own density, temperature and velocity, whereas the solid phase is modelled as a discrete Lagrangian phase.

Materials Science: SILICON BASED MATERIALS HETEROINTERFACE

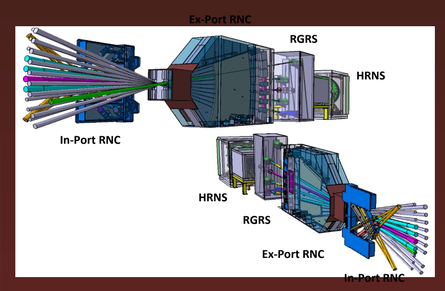


Snapshot of the c-Si/a-Si:H heterointerface in the simulation cell. Hydrogen atoms are in blue, Silicon atoms are in orange in the c-Si side and are in yellow in the a-Si:H side

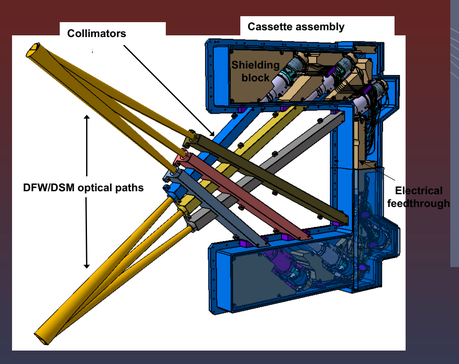
Benchmark results for PWscf code (Quantum Espresso suite) to perform ad-initio study of a crystalline Silicon/hydrogenated amorphous Silicon heterointerface system. The ab initio characterization of the c-Si/a-Si:H/c-Si heterointerface, giving the electronic properties, can provide useful indications in the understanding of the transport mechanisms underlying photovoltaic devices based on silicon heterojunction technology .

Nuclear Fusion: THE ITER RADIAL NEUTRON CAMERA IN-PORT SYSTEM

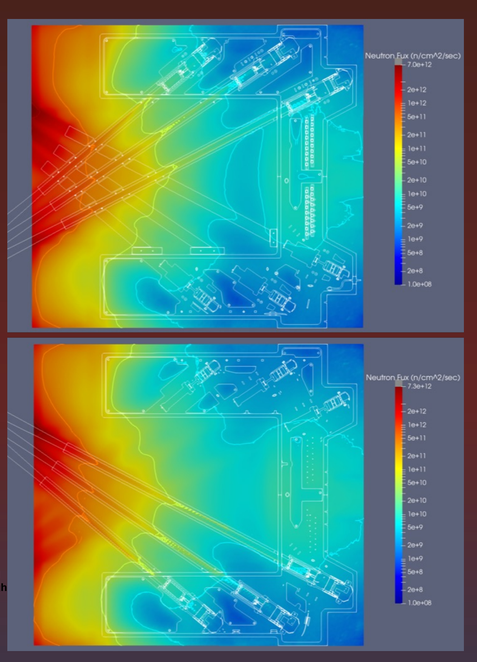
The Radial Neutron Camera (RNC) is a key ITER diagnostic system designed to measure the uncollided 14 MeV and 2.5 MeV neutrons from deuterium-tritium (DT) and deuterium-deuterium (DD) fusion reactions, through an array of detectors covering a full poloidal plasma section along collimated Lines of Sight (LoS). Its main objective is the assessment of the neutron emissivity/α source profile and the total neutron source strength, providing spatial resolved measurements of several parameters needed for fusion power estimation, plasma control and plasma physics studies. The present RNC layout is composed by two fan-shaped collimating structures viewing the plasma radially through vertical slots in the Diagnostic Shielding Module (DSM) of ITER Equatorial Port 1 (EP01): the ex-port sub-system and the in-port one. The in-port system consists of a cassette, integrated inside the port plug DSM, containing two detectors per each of the of six LoS looking at the plasma edges. A neutronic analysis of the in-port system and port plug has been performed by means of the Monte Carlo MCNP code and making use of the ENEA CRESCO HPC cluster.



Overall layout of RNC



In-port RNC subsystem



Sections of the total neutron flux ($n/cm^2/s$) map across the upper LoS (top panel) and lower LoS (bottom panel