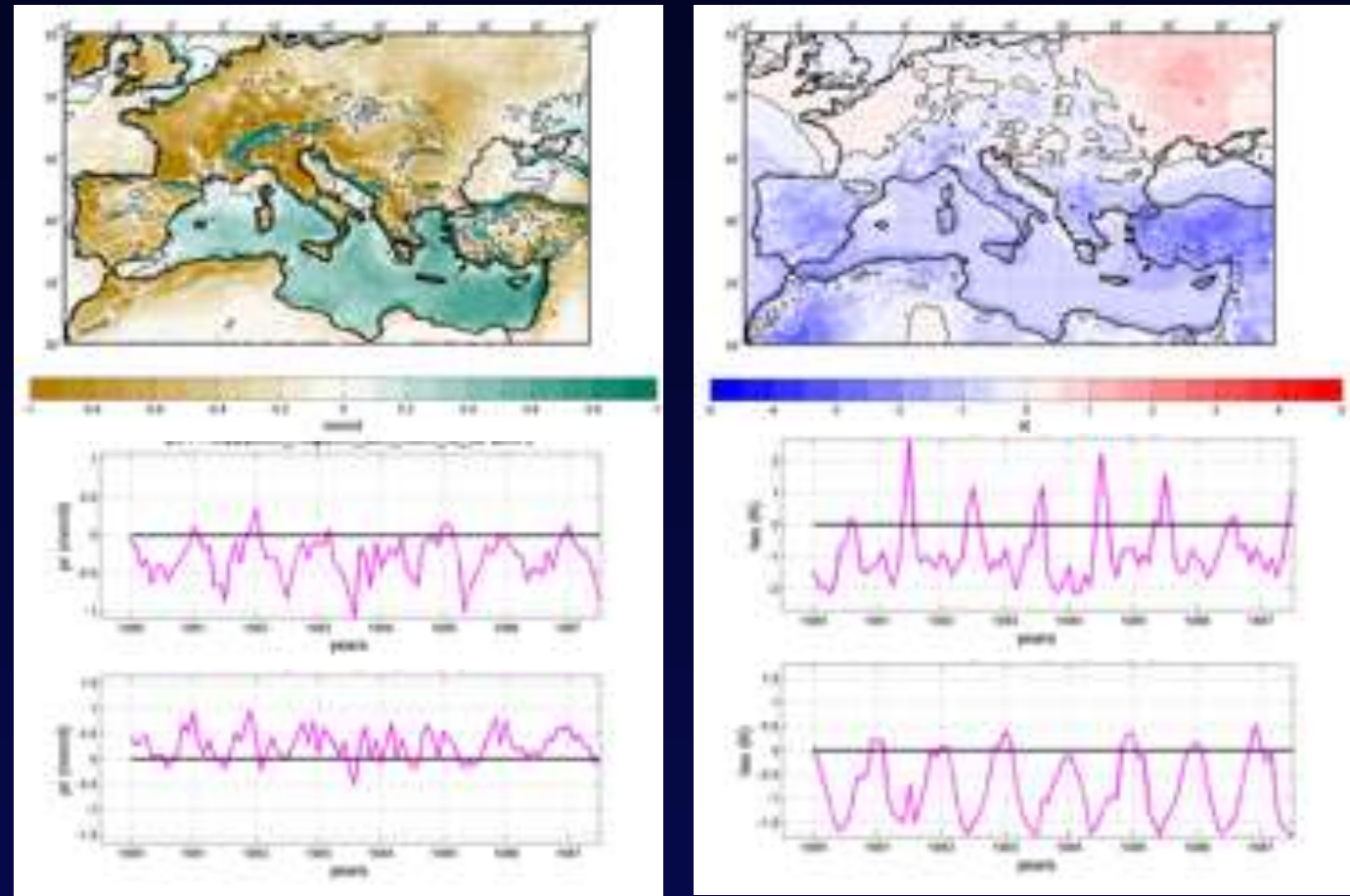


Global Climate Changes: The Regional Earth System Model (RegESM)

In the framework of global climate studies, there is an growing concern about the vulnerability of the Mediterranean region, where high population density and intense exploitation activities pose severe questions on the sustainability of terrestrial water management, both for the present and the future. ENEA CRESCO HPC provides the climate simulations performed in the framework of the Med-CORDEX initiative.

The Mediterranean Coordinated Regional Downscaling Experiment (Med-CORDEX) initiative aims at coordinating the Mediterranean climate modeling community toward the development of fully coupled regional climate simulations, improving all relevant components of the system from atmosphere and ocean dynamics to land surface, hydrology, and biogeochemical processes.

The figure shows systematic bias for rainfall (left column) and temperature (right column) in the calibrated configuration. The panels show the mean annual bias (a,b); the seasonal bias over land (c,d) and over sea (e,f).

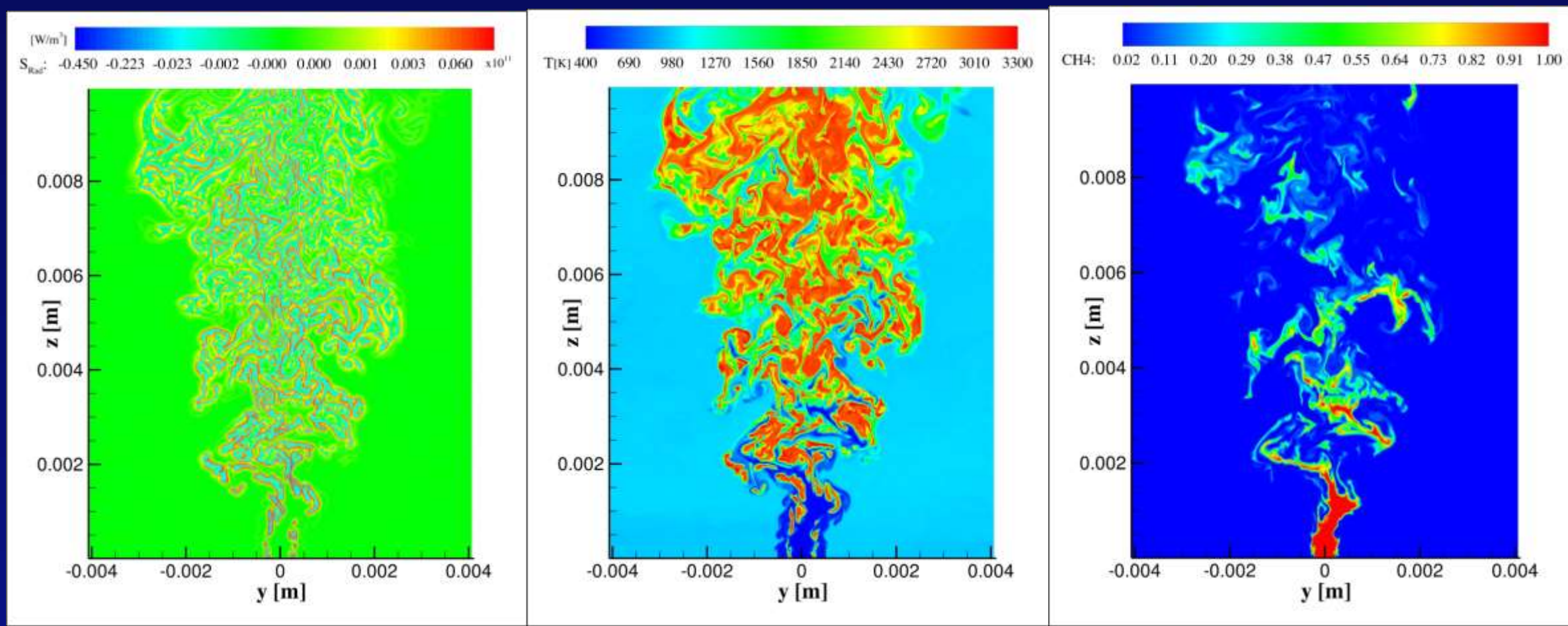


CFD Combustion: The Role of Radiant Transfer of Energy and the Flame Structure

High-pressure combustion in super-critical CO₂ gas turbine cycles, liquid rocket engines, diesel engines exhibit real gas behavior: different fluid properties has to be accounted for by means of real gas equations of state and specific models for molecular transport.

Numerical Set-Up of the ENEA HeaRT Code

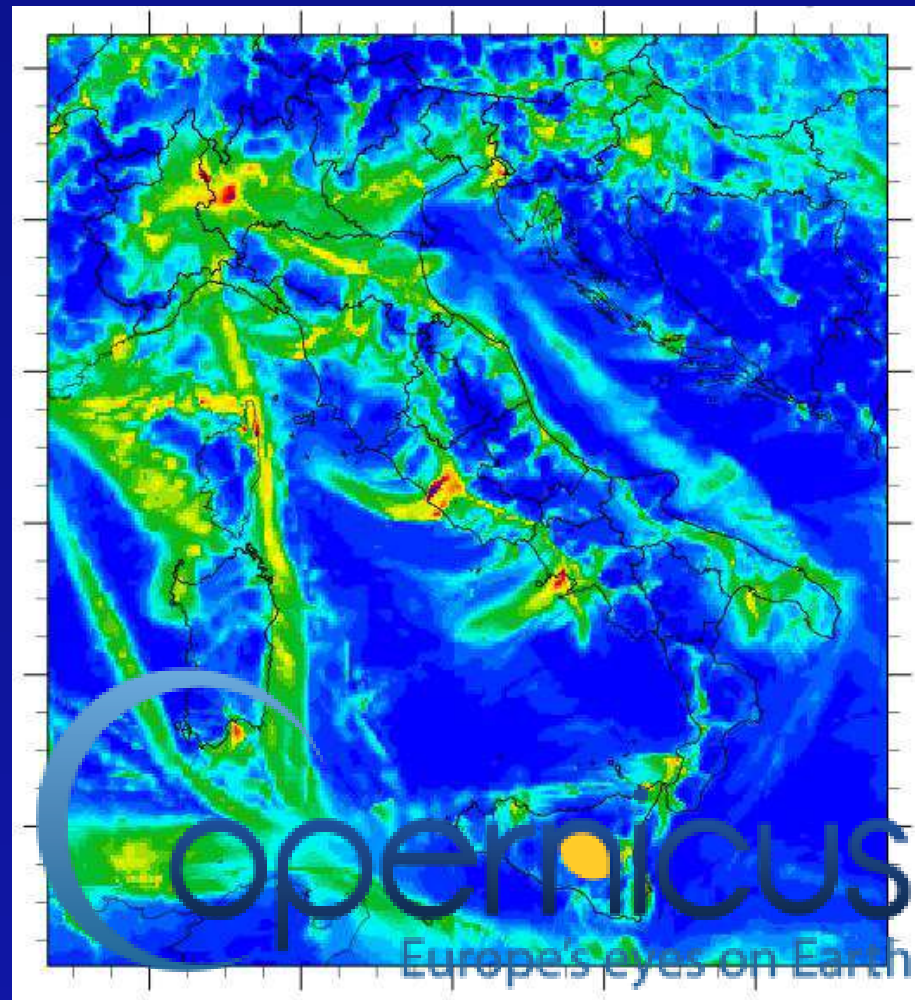
- LES (dynamic Smagorinsky for turbulence; LTSM for combustion)
- Peng-Robinson EOS in its improved Translated Volume formulation
- Accurate modelling of diffusive transport mechanisms
- Accurate calculation of diffusive transport coefficients (NIST & kinetic theory)
- Accurate numerical schemes (RK3 in time; AUSM+up/WENO3-5 & C2nd in space)
- Radiant Transfer of Energy (RTE):
 - effect of increasing pressure strongly simplified: $\kappa_{P,300bar}(T) = 103 \times \kappa_{P,1bar}(T)$
- Simplified chemical mechanism: 6 species, 4 steps [Jones & Lindstedt]
- Constitutive relations (molecular diffusion of momentum, mass and energy)



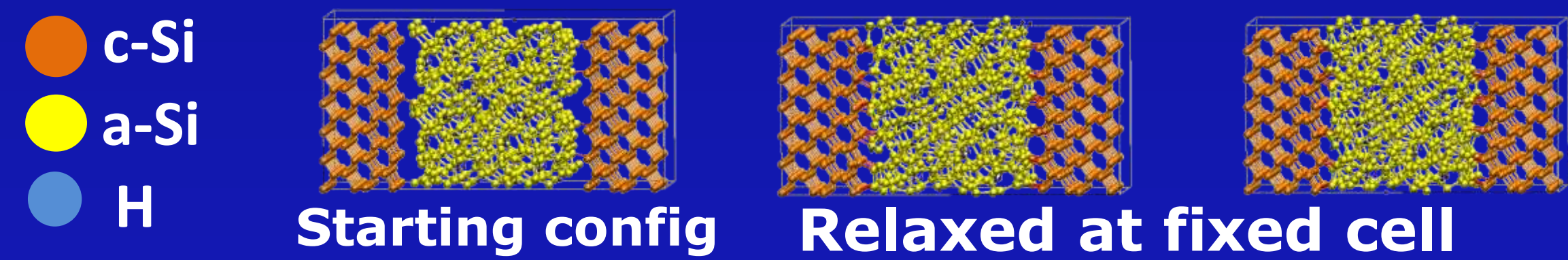
Environment: Air Quality Modeling simulations

ENEA is in Copernicus, the European Union's Earth Observation Programme, looking at our planet and its environment for the ultimate benefit of all European citizens

IT modeling system provides on daily basis forecast up to 3 days. The system runs on European domain at 20 km resolution and on Italian domain at 4 km resolution using two-way nesting approach. The modeling chain downloads GFS meteorological forecast from NCEP (U.S. meteorological system); NCEP fields are used to feed RAMS (Cotton et al., 2003) prognostic meteorological model. SURFPRO (Finardi et al., 2005) computes the turbulent parameters from RAMS model output. Chemical boundary conditions are retrieved by Copernicus Atmospheric Service (CAMS, <http://atmosphere.copernicus.eu>).



Materials Science: Interface modeling for heterojunctions solar cells



- The PBC model of large c-Si/a-Si:H/c-Si interface has been built with the aid of the classical MD simulations.
- The thermalization, quenching and equilibration processes during hundreds of pico-seconds were simulated by the ReaxFF approach (CIEMAT)

- The simulation cell of 1152 atoms (1088 Si + 64 H), with dimensions $L_x = L_y = 23.22 \text{ \AA}$; $L_z = 46.44 \text{ \AA} \Rightarrow 43.45 \text{ \AA}$ has been relaxed by ab initio approaches (ENEA)
- Band structure, density of states, charge density, and total potential is produced as input for the calculation of non-equilibrium Green's functions transport properties (ENEA/FZJ)

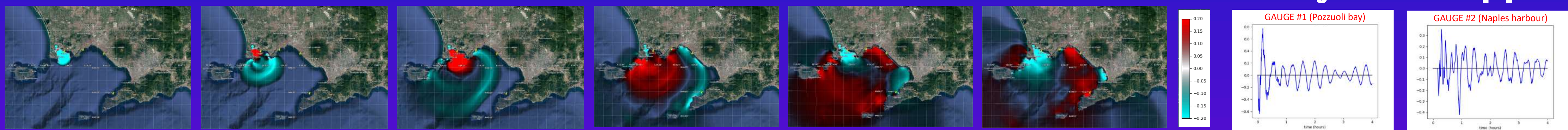


Critical Infrastructure Protection: Tsunami simulations in Southern Italy

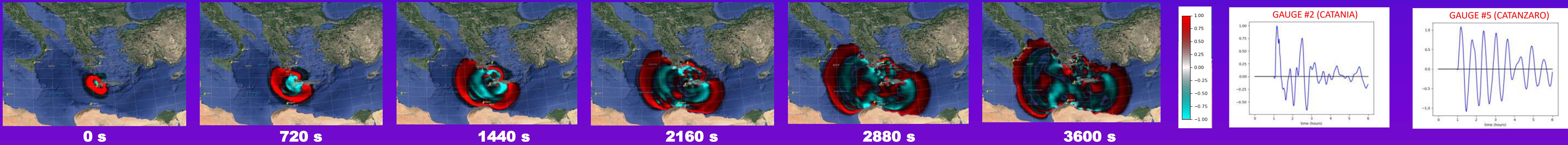
ENEA jointly INGV (National Institute Geophysical and Volcanology) is the Italian node of European Infrastructure Simulation and Analysis Centre aiming at establishing a collaborative, european-wide platform in the domain of Critical Infrastructure Protection (CIP), for supporting Operators and Public Authorities in better protecting assets and in enhancing their resilience with respect to all hazards.

ENEA HPC CRESCO6 provides Tsunami simulations running GeoClaw , open source software, in three Southern Italy scenarios

Gulf of Naples: Phlegraean Fields Eruption



Mediterranean Sea: Hellenic Arc 356 AD earthquake (M_w = 8.5)



Messina Straits: 1908 earthquake (M_w > 7)

