Symposium on HPC and Data-Intensive Applications in Earth Sciences - Day1

	Registration and Welcoming
09:00 - 10:00	Registration & Coffee break
10:00 - 10:30	Welcome, M.C. Pedicchio (OGS, Trieste, Italy)
	Keynotes Session - Convener: B. Lawrence (University of Reading, U.K.)
10:30 - 11:30	**Speaker:** V. Balaji (Princeton University & NOAA, USA) **Title:** "Climate computing: the state of play" **Short-Abstract:** Climate models represent a large variety of processes on a variety of time and space scales, a canonical example of multi-physics multi-scale modeling. In addition the system is physically characterized by sensitive dependence on initial conditions, and natural stochastic variability, and very long integrations are needed to extract signals of climate change. Algorithms generally possess weak scaling. Weak-scaling, I/O and memory-bound, multi-physics codes present particular challenges to computational performance. In this talk I will present trends in climate science driving models toward higher resolution, greater complexity, and larger ensembles, all of which present computing challenges. I will also discuss the prospects for adapting these models to novel hardware and programming models. Finally, I will introduce a set of metrics that can be used for the comparative study of computational performance of Earth System models. These measures do not require specialized software or specific hardware counters, and should be accessible to anyone. They are independent of platform, and underlying parallel programming models. We might use these measures as a basis for a CPMIP, a computational performance MIP.
11:30 - 12:30	**Speaker:** D. Komatitsch (CNRS University of Aix Marseille, France) **Title:** "Acoustic and elastic inversion and imaging on future exascale machines" **Short-Abstract:** Exascale challenges will need to be addressed in the next few years, in part based on accelerators, in the context of acoustic or seismic wave propagation for complex models as well as, even more importantly, for tomography and inversion based on these waves for unknown models, with applications in fields as diverse as geophysics, ocean acoustics, and non destructive testing. We will address some of these issues and try to illustrate possible paths to solve them in the next few years.
12:30 - 13:30	Lunch Break
	Large-Scale Computational Challenges - Convener: S. Valcke (CERFACS, Toulouse, France)
13:30 - 14:00	**Speaker:** M. Bader (Technical University Munich, Germany) **Title:** "Optimizing a dynamic rupture and earthquake simulation code for SuperMUC, Tianhe-2 and Stampede" **Short-Abstract:** SeisSol is an Arbitrary high-order DERivative Discontinuous Galerkin (ADER-DG) code to simulate earthquakes with high model complexity, featuring coupled simulation of full frictional sliding and seismic wave propagation. Complicated geometries can be tackled via unstructured adaptive tetrahedral meshes. I will present recent work on optimizing SeisSol for current supercomputers, in particular SuperMUC and the Xeon-Phi-based Tianhe-2 and Stampede. With architecture-aware optimizations we achieved up to 50% of peak performance, reaching sustained performance beyond the 1 PetaFlop/s mark. In addition to a factor-5 speedup in time-to-solution, we improved the scalability of the workflow for simulations with billions of elements and more than 10^{11} degrees of freedom.

Speaker: G. Sannino (ENEA, Rome, Italy)

Title: "Modelling the Mediterranean region under the Prace NEMERTE Project: towards enhanced resolution, accurate Strait of Gibraltar description and tidal forcing effects"

14:00 - 14:30

Short-Abstract: Over the last decades, research has demonstrated the necessity of a high resolution modelling approach to the description of the overall mechanism of the Mediterranean circulation (MTHC). Moreover, it has been observed that the counter-flowing fluxes of Atlantic and Mediterranean waters are subject to tide-induced vigorous mixing within the Strait of Gibraltar (SoG), where tidal forcing also affects the hydraulic control of volume fluxes, both processes determining larger heat, salt, and mass fluxes into the Mediterranean. A correct prescription of the lateral boundary condition at the Gibraltar inlet can therefore only be achieved by explicitly including the Gibraltar Strait in the numerical domain, at a spatial resolution sufficient to account for both the fast barotropic tidal signal propagating eastward from the Atlantic Ocean and the baroclinic mixing processes occurring within the strait. The awarded PRACE "NEMERTE" project aims to evaluate the separate and joint long-term effects of increased resolution, SoG dynamics, and tides on the simulated MTHC. During the talk the preliminary encouraging results of the "NEMERTE" project will be showed and discussed.

Speaker: P. Lazzari (OGS, Trieste, Italy)

Title: "Global Sensitivity analysis of the Mediterranean sea biogeochemical model"

14:30 - 15:00

Short-Abtract: The increasing demand of model based assessment of indicators of ecosystem state, functioning, and response climatic scenarios and/or environmental management policy has triggered the development of ecological models of increasing complexity. Here we implemented a global sensitivity analysis on a state-of-the-art 3D biogeochemical model (http://bfm-community.eu) of the Mediterranean Sea, currently applied in the framework of both climatological and operational oceanographic applications. Our results provide an estimate of the uncertainty induced on each model output assuming a 5% uncertainty in the value of each of the hundreds model parameters, together with an estimate of the cumulative effect of such uncertainty. Globally, the uncertainty is higher (up to 300%) in measures related to higher trophic level organisms, such as carnivorous mesozoopkanton, and lower for those related to planktonic primary producers. Results imply that, even assuming that the uncertainty in model parameters is higher, say around 10%, model based estimates of these indicators remain reliable, insofar other sources of errors are considered to be acceptable.

Speaker: D. Roten (San Diego Supercomputer Center, USA)

Title: "Implementation of nonlinear material response in scalable earthquake ground motion simulations"

15:00 - 15:30

Short-Abtract: Three-dimensional numerical simulations of dynamic rupture and wave propagation allow deterministic predictions of near-source ground motions during large, rare earthquakes, which are not well represented in observed data. Although the deployment of GPU-based supercomputers and performance optimizations have allowed researchers to push the frequency limit of such simulations from less than 1 Hz to more than 5 Hz in recent years, the ultimate goal is to extend deterministic simulations to 10 Hz to cover the entire frequency range relevant for building response. This talk introduces some technical aspects concerning the implementation of Drucker-Prager plasticity in our highly optimized, GPU-based finite difference code, which will account for nonlinear material behavior expected to occur at higher frequencies. I will also present recent simulation results which show that nonlinearity near the fault and in shallow sediments could drastically reduce the level of ground motion that must be expected during future San Andreas earthquake scenarios.

Speaker: B. Lawrence (University of Reading, U.K.)

Title: "Weather and Climate modelling at the Petascale: achievements and perspectives. The roadmap to PRIMAVERA"

15:30 - 16:00

Short-Abstract: Recent results and plans from the Joint Met Office/NERC High Resolution Climate Modelling programme are presented, along with a summary of recent and planned model developments. We show the influence of high resolution on a number of important atmospheric phenomena, highlighting both the roles of multiple groups in the work and the need for further resolution and complexity improvements in multiple models. We introduce plans for a project to do just that. A final point is that this work is highly demanding of both the supercomputing and subsequent analysis environments.

16:00 - 16:30	Coffee Break

Innovative development - Convener: D. Komatitsch (CNRS University of Aix Marseille, France)

16:30 - 17:00	**Speaker:** S. Valcke (CERFACS, Toulouse, France) **Title:** "HPC for Climate Modelling in Europe: ENES, IS-ENES and the OASIS Coupler" **Short-Abstract:** This talk will present the European Network for Earth System modelling, ENES, and its infrastructure project IS-ENES. Then details on the ENES 2012-2022 Infrastructure Strategy on computing, date and models will be given. The second part of the talk will descrive the code coupling strategies currently used in climate modelling and will present in more details the last performance results obtained with the OASIS3-MCT coupler.
17:00 - 17:30	**Speaker:** S. Denvil (IPSL-UPMC, Paris, France) **Title:** "Big Data Analysis and Metadata Standards for Earth System Models" **Short-Abstract:** Recent trends in climate modelling are to add more physical components in the modelled system, increasing the resolution of each individual component and the more systematic use of large suites of simulations to address many scientific questions. Climate simulations may therefore differ in their initial state, parameter values, representation of physical processes, spatial resolution, model complexity, and degree of realism or degree of idealisation. In addition, there is a strong need for evaluating, improving and monitoring the performance of climate models using a large ensemble of diagnostics and better integration of model outputs and observational data. High performance computing is currently reaching the exascale and has the potential to produce an exponential increase of size and numbers of simulations. However, post-processing, analysis, and exploration of the generated data have stalled and there is a strong need for new tools to cope with the growing size and complexity of the underlying simulations and datasets. This talk will expose the strategy of the French community to face those challenges.
17:30 - 18:00	**Speaker:** M. Lieber (Technical University Dresden, Germany) **Title:** "FD4: Four-Dimensional Distributed Dynamic Data structures" **Short-Abstract:** Load balancing and efficient model coupling in large scale scientific simulations are challenging tasks that should be implemented preferably in an independent and reusable software framework. In this talk, the open source framework FD4 (Four-Dimensional Distributed Dynamic Data structures) is introduced. It helps to parallelize a simulation model by managing the 3D domain decomposition and dynamically balancing the workload among the MPI ranks. Additionally, FD4 offers scalable model coupling (e.g. for coupled atmospheric simulations) and dynamic allocation of grid blocks (e.g. for multiphase problems). FD4 has been used in COSMO-SPECS+FD4, a coupled model for detailed cloud simulations, and enables a scalability to 256k ranks.
18:00 - 18:30	**Speaker:** Tomaso E. Ongaro (Istituto Nazionale di Geofisica e Vulcanologia Pisa, Italy) **Title:** "Challenges in multiphase flow modeling and numerical simulation of explosive volcanic eruptions" **Short-Abstract:** The main objectives of numerical simulations of explosive volcanic eruptions are the prediction of the impact of future eruptive scenarios on the natural and anthropic environment and the interpretation of the available geological and geophysical information by means of reliable physical models. However, our simulation capability is currently limited by: 1) incomplete knowledge of the physical processes taking place during eruptions; 2) insufficient numerical model resolution and difficulty of estimating the related numerical error; 3) large epistemic uncertainty associated to initial and boundary conditions. The problem of modeling and numerical simulation of eruptive phenomena is here presented by discussing recent computational applications to volcanic eruption plumes and pyroclastic flows and the problems related to the comparison with natural events. From these examples, the main challenges for future improvement in numerical simulations can be identified, namely: 1) high-performance code design, 2) multiscale modeling, adaptive meshing and numerical accuracy, 3) subgrid scale modeling (including topography), 4) multidomain coupling. At the same time, numerical model validation should be addressed by constraining as much as possible models to observational/experimental data and by estimating uncertainty and errors in large numerical codes. To address this challenges, a synergetic multidisciplinary effort will be required in the future among geophysical, mathematical and computer science researchers.