Predicting novel materials with specific desirable properties is a major aim of ab initio computational materials science (aiCMS) and an urgent requirement of basic and applied materials science, engineering and industry. Such materials can have immense impact on the environment and on society, e.g. on energy, transport, IT, medical-device sectors and much more. Currently,...

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EXSCALATE4CoV: EXaSCale smArt pLatform Against paThogEns for Corona Virus
ALFONSO VALENCIA

The EXSCALATE4CoV (E4C) project aims to exploit the most powerful computing resources currently based in Europe to empowersmart in-silico drug design. Advanced Computer-Aided Drug Design (CADD)
in combination with the high throughput biochemical and phenotypic screening will allow the rapid evaluation of the simulations results and the reduction of time for the discovery of new...

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**HBP-SGA3: HUMN BRAIN PROJECT - FLAGSHIP**

**JAVIER BARTOLOME RODRIGUEZ**

The HBP is now poised to start the last of four multi-year work plans, which will take it to the end of its original incarnation as an EU Future and Emerging Technology Flagship. Our plan is that the end of the Flagship will see the start of a new life for the HBP, as an enduring European scientific research infrastructure, EBRAINS, that is on the European Strategy Forum on...

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**Edge Twins HPC: Bringing Digital Twins to the Edge for mass Industry 4.0 applications**

**ROSA M BADIA**

Digital twins, along with the Internet of Things and Edge computing, are expected to play a decisive role in the next decade's industrial markets (Industry 4.0) enabling dramatic improvements in complex systems...
design and operation. However, this technology has not been yet widely implemented, since it requires the collaboration of experts in multiple fields and costly...


**EDUARDO QUINONES MORENO**

The main goal of Rising STARS is to enable a parallel programming framework for the development and execution of advanced large-scale Cyber Physical Systems (CPS) with High Performance Computing (HPC) and real-time requirements. Overall, there is an urgent necessity to develop run-time parallel frameworks, compatible with HPC, capable of guaranteeing that decisions made at...

**CAMS_61: Development of regional air quality modelling and data assimilation aspects**

**ORIOL JORBA CASELLAS**

The proposed project will deliver development plans, guidelines, working examples and tools for the continuous upgrade of the CAMS regional service. This will encompass (i) a in depth assessment of the CAMS regional forecasts and a prioritized list of proposed model developments, (ii) best practices for coupling forecasts to analyses, and (iii) model-agnostic tools for the...

**MEEP: MareNostrum Experimental Exascale Platform**

**JOHN DAVID DAVIS**
The MareNostrum Experimental Exascale Platform (MEEP) is a flexible FPGA-based emulation platform that will explore hardware/software co-designs for Exascale Supercomputers and other hardware targets, based on European-developed IP. MEEP provides two very important functions:

- An evaluation platform of pre-silicon IP and ideas, at speed and scale and
- A...

LiverScreen: Screening for liver fibrosis - population-based study across European countries

Liver cirrhosis is a very common and severe chronic disease, responsible for high morbidity, impaired quality of life, major healthcare costs, and poor survival, causing an estimated 170,000 deaths per year in Europe. Liver cirrhosis is preceded by a long period of slowly developing, asymptomatic, liver fibrosis; most commonly caused by non-alcoholic fatty liver disease...

UP2DATE: Intelligent software UPDATE technoloties for safe and secure mixed-critically and high performance cyber physical systems

FRANCISCO JAVIER CAZORLA ALMEIDA
Mixed-Criticality Cyber-Physical Systems (MCCPS) deployed in critical domains like automotive and railway are starting to use Over The Air Software Updates (OTASU) for functionality improvement, bug fixing, and solving security vulnerabilities (among others). But, OTASU entails several difficulties:

1) Safety including non-functional properties like...

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AMPERE: A Model-driven development framework for highly Parallel and EneRgy-Efficient computation
EDUARDO QUINONES MORENO

A Model-driven development framework for highly Parallel and EneRgy-Efficient computation supporting multi-criteria optimi...

Complex, dependable and physically-entangled systems of systems must be supported by innovations to allow a significant reduction of the cost and complexity of system design targeting computing platforms composed of parallel heterogeneous architectures. Software development is one key challenge, as current programming tools do not fully support emerging processor...

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