Materials design At the eXascale

European Center of Excellence for HPC applications
an H2020 e-infrastructure

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Information & Communication Technology Section (ICTS)
International Centre for Theoretical Physics (ICTP)
... a Centre of Excellence in materials modelling, simulations, and design able to unleash the EU leadership in this field and in high-performance computing

and to empower our core communities with powerful new instruments to address the key scientific, industrial and societal challenges that require novel materials.
BUSINESS

TECHNOLOGY

SCIENCE

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action lines

1. creating an ecosystem of capabilities, applications, data workflows and analysis: needed now, and ready for the exascale

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- community codes for quantum simulations: their capabilities and reliability
- transition to exascale architectures, energy awareness, codesign, ...
- workflows; data provenance, preservation, sharing and analytics
- an ecosystem that integrates capabilities, available to researchers in academia and industry
- a set of pilot cases: excellent science of direct industrial relevance
action lines

2. training, dissemination, industry

- **key services to the core communities:**
  codes, data, expertise, training
- **training:** coordination, integration, access
- **turn-key solutions for end users in research and industry**, incl. SMEs:
  build a ‘market place’ starting from our pilots, outreach
Pilot case 1: M.C. Righi (Cnr Modena)
Computational protocol for friction and tribochemistry

**Goal:** controlling friction through materials design → coatings, lubricants (in collab with Toyota and Total)

**Problem:** enhanced reactivity, classical MD not enough → computational tribochemistry incl. quantum effects

**Strategy:** Ab initio mol. dynamics based on modified versions of Born Oppenheimer MD + Car Parrinello cp.x computer code

**Deliver:**
- workflow: MD tribochemistry simulations
- automated procedures & database
- training through research in MaX labs
Pilot case 2: P. Ordejón (ICN2)  
Computational protocol for understanding thermal storage in molten salts and nanofluids

Molten salts:
- Heat storage and transport medium
- Allow electric energy generation in the absence of sunlight (with heat stored during daylight)
- Melting: ~200°C
- Operation: ~500°C
- High heat capacity
Pilot case 3: S. Baroni (SISSA)
Computational protocol for simulating the color optical properties of natural dyes for food industry applications

- study and understand the properties of the colors
- replace synthetic colorants with natural colorants
Pilot case 4: N. Marzari (EPFL)
Design and discovery of optimal solid-state electrolytes

The search for novel Lithium-ion conductors

Motivation:
- Safety of current systems
- Increase performance
- Enable high-voltage

Key objectives:
- Find candidates for electrolyte in solid-state lithium-ion batteries
- Find descriptors of ionic conductivity

Approach:
- 1207 structures (containing O, Li, insulating) from database
- 2264 deriving structures
- BOMD simulation from first-principles at 3 temperatures
- Analysis

BOSCH
Invented for life
GLOBAL CONTEXT: Increasing Recognition of Impact of HPC Enabled Applications

U.S. President Barack Obama issued an executive order establishing the National Strategic Computing Initiative with initial allocation of $450 M from the U.S. Department of Energy. (29/07/2015)

French President François Hollande announced the launch of French National “Plan Supercalculateur” with €50M of national funding. (07/05/2014)

Former Vice President of the European Commission Neelie Kroes announced the launch of a contractual Public-Private Partnership (cPPP) on Big Data (€500M EC funding) and for the development of a European HPC Eco-system (€700 M EC funding). (17/12/2013)

Chinese President Xi applauds success of world’s fastest supercomputer Tianhe-2 built by China’s National University of Defense Technology with the fundamental purpose of “providing a driving force for the construction of an innovation-oriented country”. (18/06/2013)

Social and scientific priority issues to be tackled by using Post ‘K’ Computer

Priority issues (9 issues)

1. We selected nine social and scientific priority issues from the following point of view:
   (1) High priority issues from a social and national viewpoint
   (2) Promising Creation of World-Leading achievement
   (3) Promising Strategic Use of Post ‘K’ computer
Executive Order
Creating a National Strategic Computing Initiative

[...] This coordinated research, development, and deployment strategy will draw on the strengths of departments and agencies to move the Federal government into a position that sharpens, develops, and streamlines a wide range of new 21st century applications. It is designed to advance core technologies to solve difficult computational problems and foster increased use of the new capabilities in the public and private sectors.

[...] It is also important to note that HPC in this context is not just about the speed of the computing device itself. [...] HPC “must now assume a broader meaning, encompassing not only flops, but also the ability, for example, to efficiently manipulate vast and rapidly increasing quantities of both numerical and non-numerical data.”

over the next decade HPC systems are expected to be capable of one exaflop \(10^{18}\) operations per second) and to manage and analyse data sets up to one exabyte \(10^{18}\) bytes)
Conclusion and Acknowledgements

- In 2014-2015 EU founded the EINFRA5 for ~ 37.5M euros
- About 4M were awarded to intalian Institutions (0.8M to the Trieste area)
- About 1.8M were awarded to the MaX project

*data provided by APRE (TS)
MATERIALS DESIGN AT THE EXASCALE

European center of excellence - a H2020 e-infrastructure

THE CENTER
a centre of excellence aimed to disenthrall the EU leadership in materials modelling, simulations, discovery and design

THE CHALLENGE
what if material simulations were 1000x faster and more workable? driving the exascale transition

THE CREW
5 research teams, 5 supercomputing centres, 1 educational institute, 2 business partners

www.max-center.eu