



Finanziato
dall'Unione europea
NextGenerationEU



Ministero
dell'Università
e della Ricerca



Italiadomani
PIANO NAZIONALE
DI RIPRESA E RESILIENZA



Centro Nazionale di Ricerca in HPC,
Big Data and Quantum Computing

Spoke 6 Multi Scale Modeling & Engineering Applications

Fabio Sciarrino
Sergio Saponara

Composizione dello Spoke

Leader



Co- Leader



Enti e Università



Spoke 6 – Multiscale Modeling & Engineering Applications

Researchers

*Involved researchers
(massa critica):*
201

Recruited researchers:
26 RTDA

Post-doctoral fellowships:
53 Assegni di Ricerca

PhD Students:
25 PhD

Funding

Overall funding:
15.900.000 €

Innovation grants:
15 Innovation Grants
> 2.000.000 €

Tender call:
3.200.000 €
50% South, 50% North
Tender Calls:
**8 project with 20 entities
involved**

Main outcomes

Publications
>300

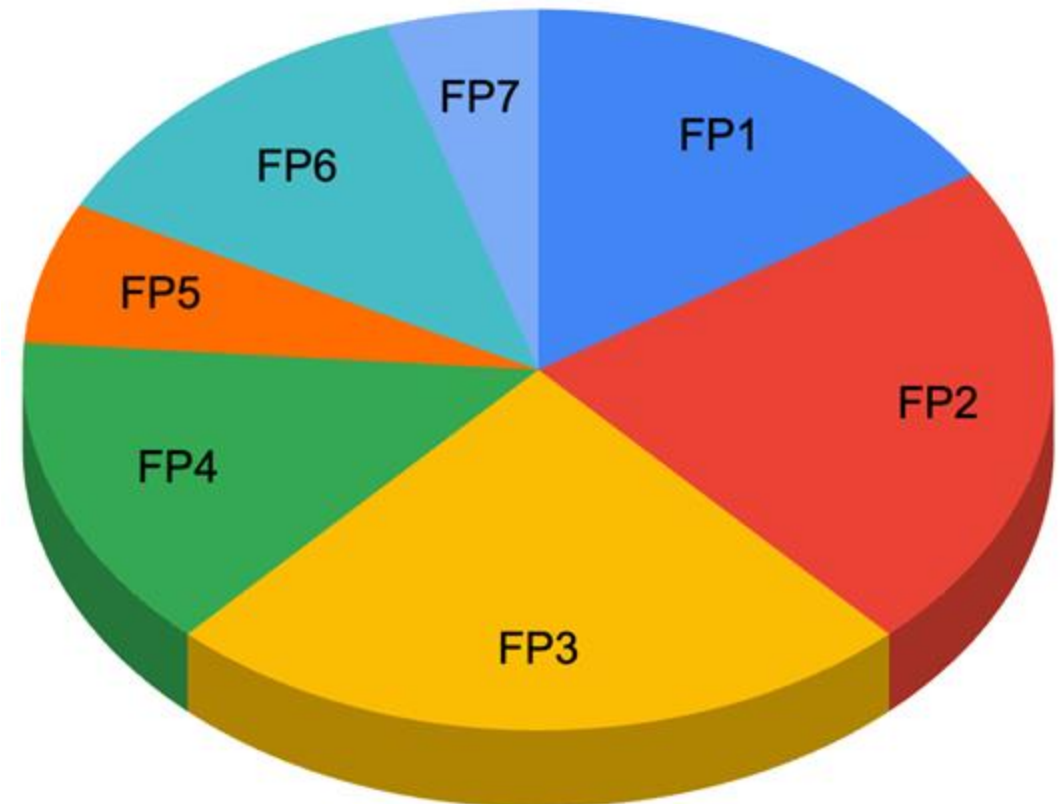
Software
>15

*Large exploitation of
CINECA resources*

Spoke 6 – Multiscale Modeling & Engineering Applications

Flagship Projects (Academia) connected with Innovation Grants (Academia & Industry)

- **FP1: Advanced materials and new devices**
- **FP2: Big data analytics & AI**
- **FP3: Computational fluid-dynamics**
- **FP4: Green energy**
- **FP5: Life science**
- **FP6: HPC for complex systems**
- **FP7: Electromagnetic systems**



Spoke 6 – Multiscale Modeling & Engineering Applications

FP6: HPC for Complex Systems

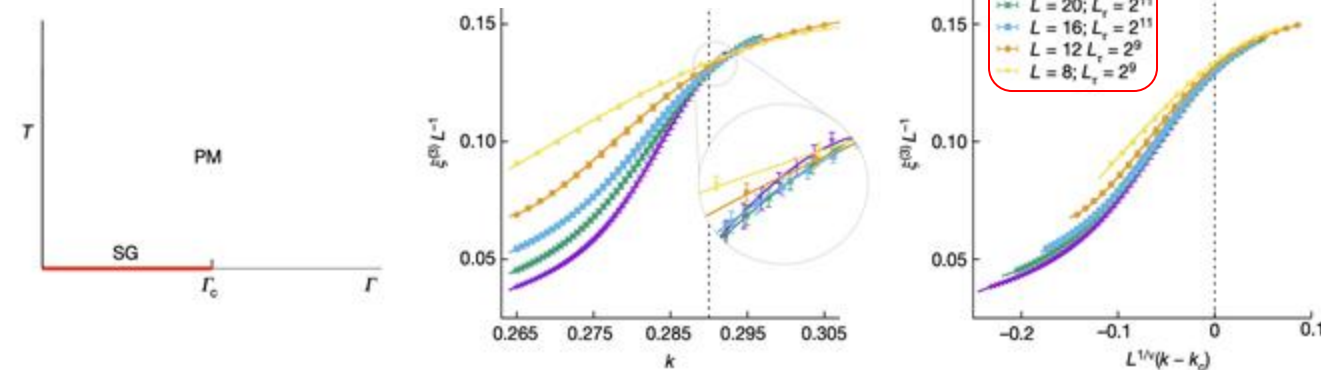
First clear evidence for a quantum transition in 2D Ising spin glasses.

Not only intensive use of GPUs (Leonardo) but smart analysis exploiting symmetries.

Same exponents found later by D-wave!

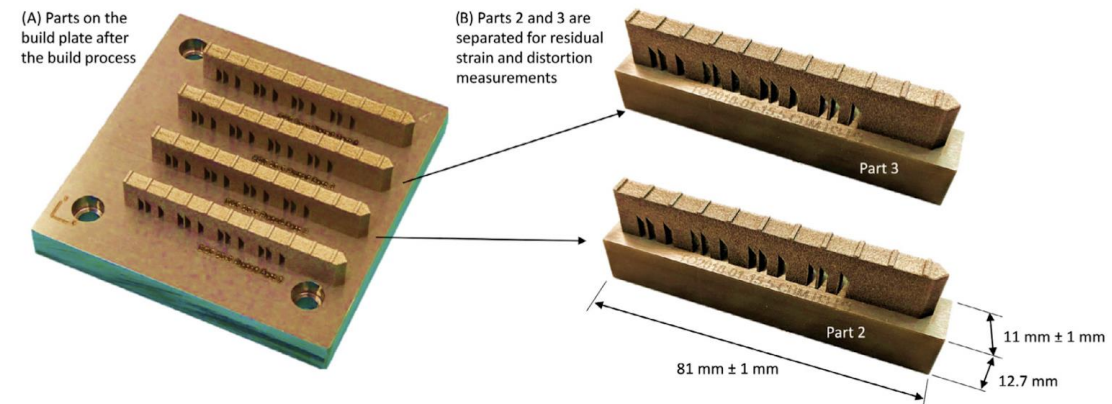
very large sizes!
intense use of Leonardo

nature 631, 749–754 (2024)



FP3: Computational Fluid Dynamics

Uncertainty Quantification in Laser-Based Powder Bed Fusion Simulations

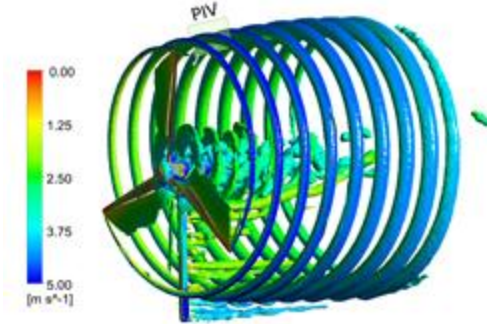


33% reduction in uncertainty of residual strain predictions using **Bayesian inversion**.

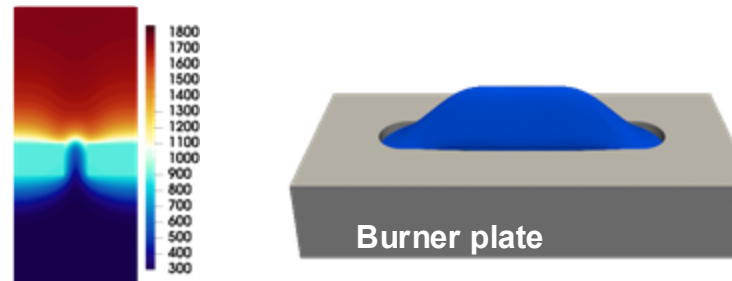
Spoke 6 – Multiscale Modeling & Engineering Applications

FP4: HPC to unleash decarbonization technologies

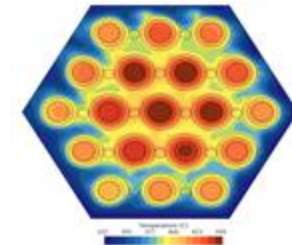
HPC tools for simulation of floating
wind farm in deep water environments



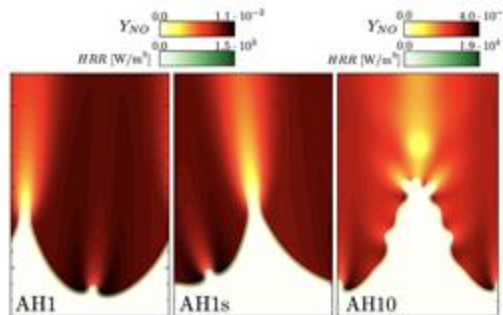
Flashback of H₂-enriched flames in
household burner



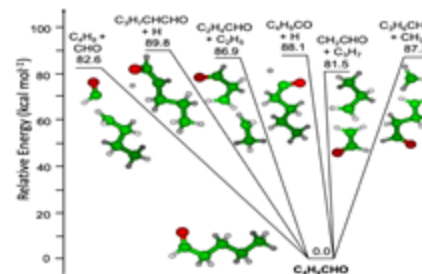
HPC tools for the simulation of
nuclear systems



Fundamental physics of hydrogen
and ammonia



Estimation of rate constants for the
decomposition paths of high
molecular weight aldehydes during
the combustion of biofuels

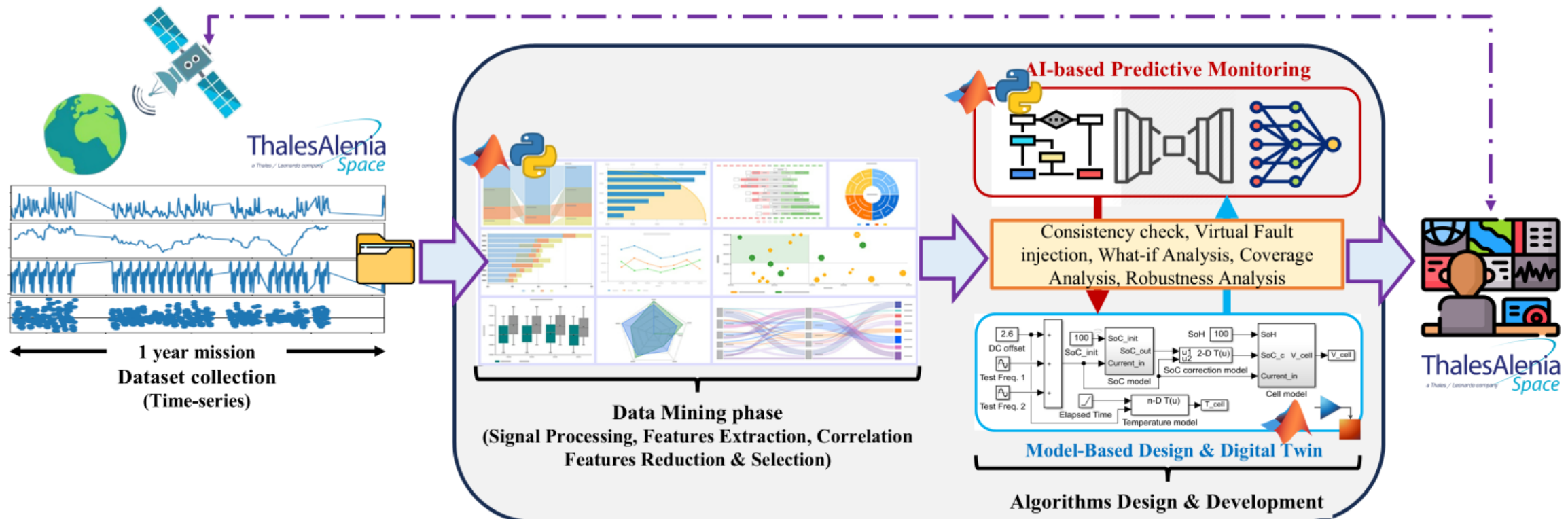


Advanced Computational Digital Twins
for the development of sustainable
transport solutions with Highly Efficient
Fuel Cell Hybrid Electric Vehicles



Spoke 6 – Multiscale Modeling & Engineering Applications

FP2: Use of digital twins for consistency checks, evaluation of operation limits and effect of anomalies and failures in simulation without direct stress on physical systems



Spoke 6 – Multiscale Modeling & Engineering Applications

- **Further strengthen collaborations** with industries to **transfer** ideas and knowledge from fundamental research
 - *Action: Large Innovation Grants over longer period with high-impact goal*
- Enhance **accuracy and computational efficiency** of computational models, crucial in engineering, applied sciences and innovation
 - *Action: integrate advanced physics-based and data-drive (AI, reduced and surrogate models) paradigms to improve simulation accuracy while reducing computational costs.*
- Foster **cross-sector contaminations** and **innovation** in the design and optimization of solutions
 - *Action: span the TRL scale by knowledge exchange between researchers, engineers, and industrial stakeholders from different sectors*