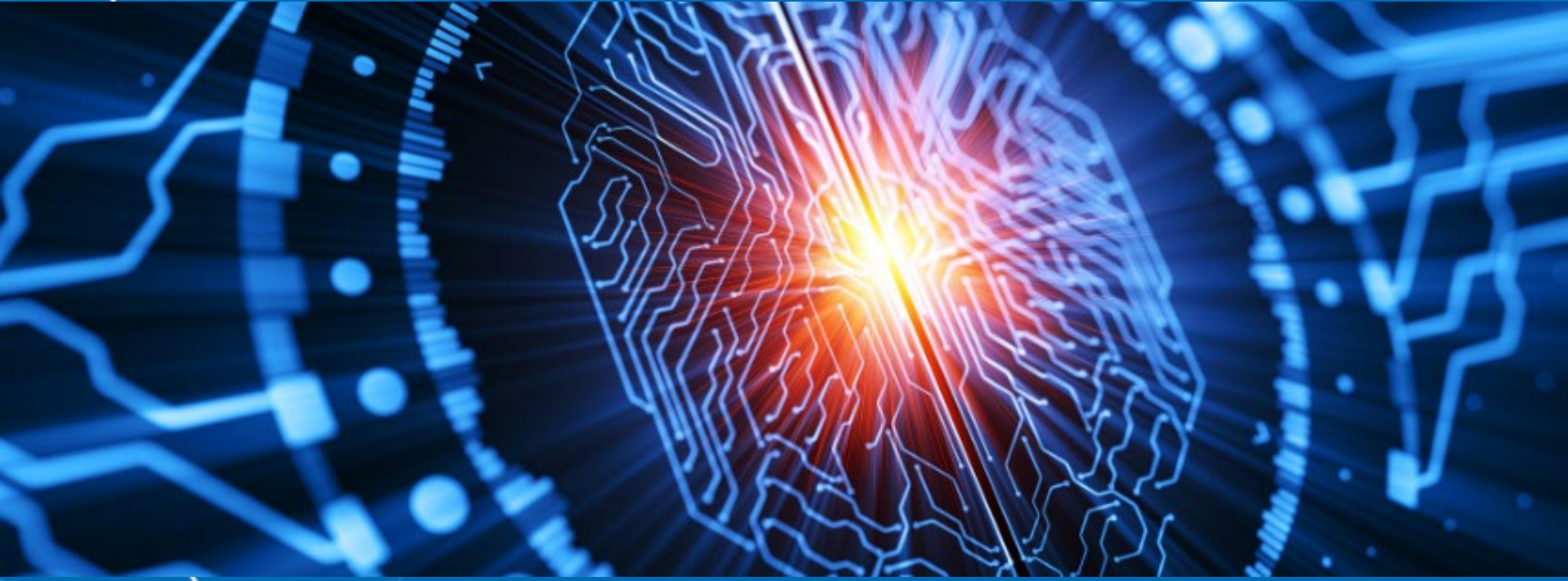
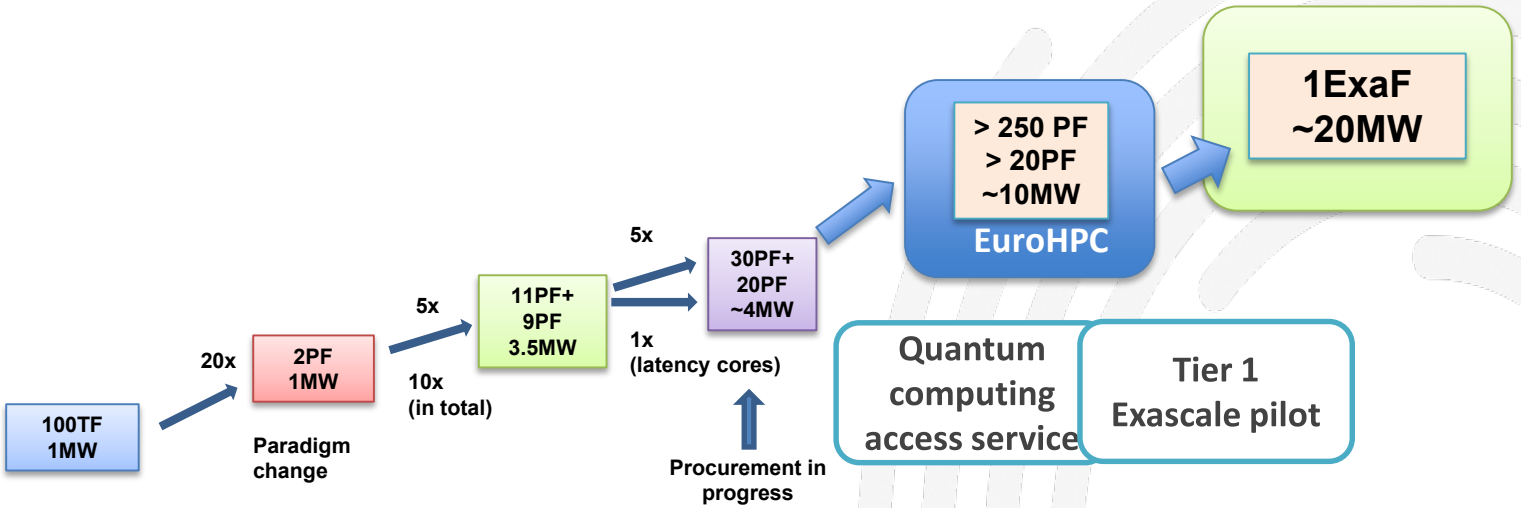


SCAI
SuperComputing Application & Innovation
CINECA

Sanzio Bassini (CTO) – September 2019

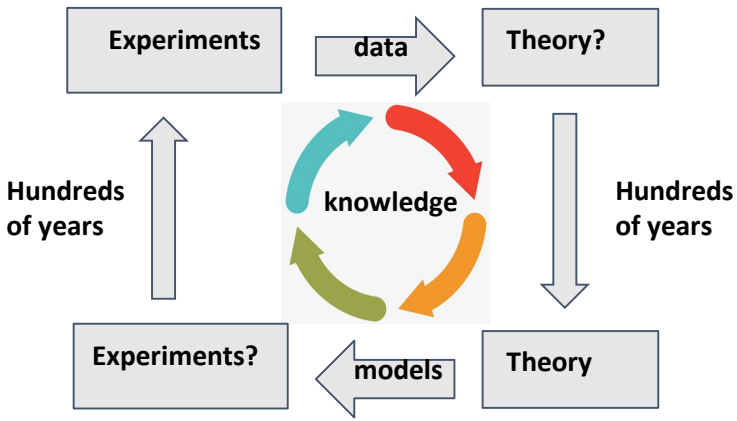
CINECA HPC Road Map



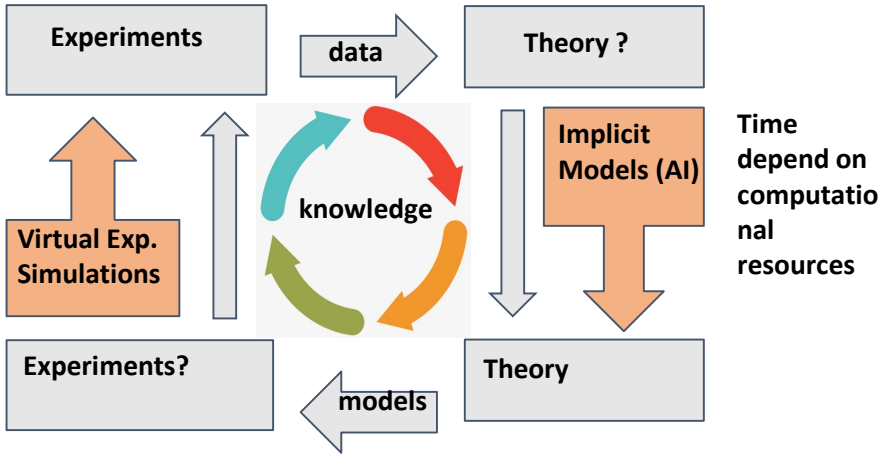
2009	2012	2016	2019/2020	2021	2025-2027
IBM SP6 Power6	Fermi IBM BGQ PowerA2	Marconi Lenovo Xeon+KNL	Marconi PPI4HPC ICEI - PPIHBP	Leonardo pre-Exascale with EuroHPC contribution	EuroHPC post Exascale/ National Full Exascale

The persistence need for more powerful computational resources

Scientific Progress Without Computers
(two paradigms)



Scientific Progress With Computers
(four paradigms)



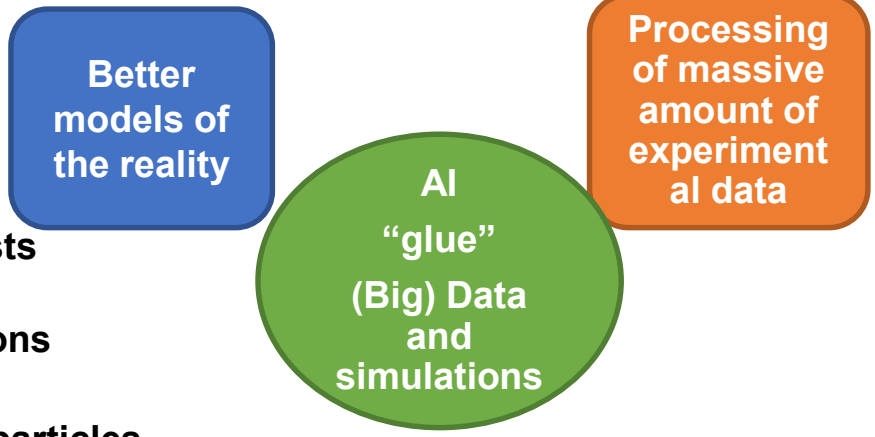
HPC & Data Processing are a knowledge accelerator: the more the better!

The progress of modern scientific research itself leads to an ever-increasing need for computational capacity as an inevitable consequence.

LEONARDO “Incomplete” list Scientific cases

	Material Science	Life Science & Bio	Meteo and Climate	Earth Science	Astrophysics & Planetary	Fundamental Physics	Engineering	Energy	Social Sci, Fintech
Batch Simulation (numerical integration)	Quantum Chemistry, atomistic simulations	**Molecular Modelling, Brain simulation**	Climate and Weather	Volcano, earthquake, sea dynamic, rivers, etc...	Cosmo, galaxy, stars, etc.. formation and dynamic	LQCD	CFD, DNS, LB, FE	Fusion (ITER)	Training DNN
Data Driven (data analysis)	Synchrotron and Neutron sources	**NGS, HBP**	Radar	Seismic	SKA, GWaves, Satellites	LHC	IoT, sensors	RTM (Oil&Gas)	Fraud detection, Sentiment. AI for complexity
Data Assimilation (simulation + data)		**Personalized medicine**	Weather	Shallow water sim. Oceanography	Space missions (e.g. GAIA)	Solar wind forecast	Autonomous Vehicles	FWFI (Oil&Gas)	Risk Management, personalized finance (pensions)
Parameter Space (ensemble simulation)	New engineered Materials, designed from scratch	**In silico Drug Design**	uncertainty quantification	Natural hazard assessment	Star Life Cycle, Black Hole, Neutron Star		Aerodynamics, wings, propellers, turbines	Batteries	
Simulation steering (interactive and visualization)	Apply forcing. Tribology Friction	**Molecular Mechanic Simulation**					Digital Twins	Reservoir Simulation	
Coupled or chained simulation (workflows)	Property Calculators, Multi-scale simulations		Include soil and ocean effects		Cosmology & Galaxies		Multi-physics simulations	wind turbines	

Leonardo will enable



New algorithms

new material from scratch

use information from sensors deployed in an internet-of-things

Simulate formation of galaxies

batteries

source of gamma-ray bursts

predict how solar eruptions

properties of elementary particles

treatments tailored both to the patient

understanding of general relativity

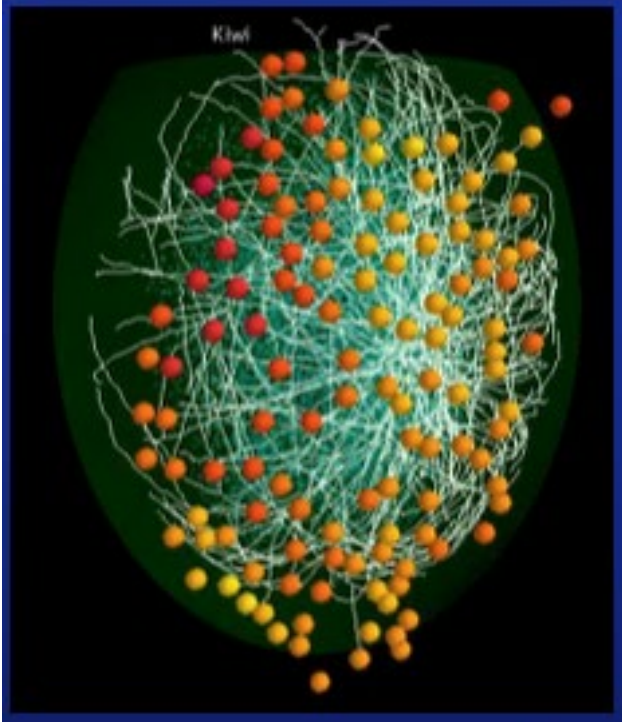
uncertainty quantification in predictions

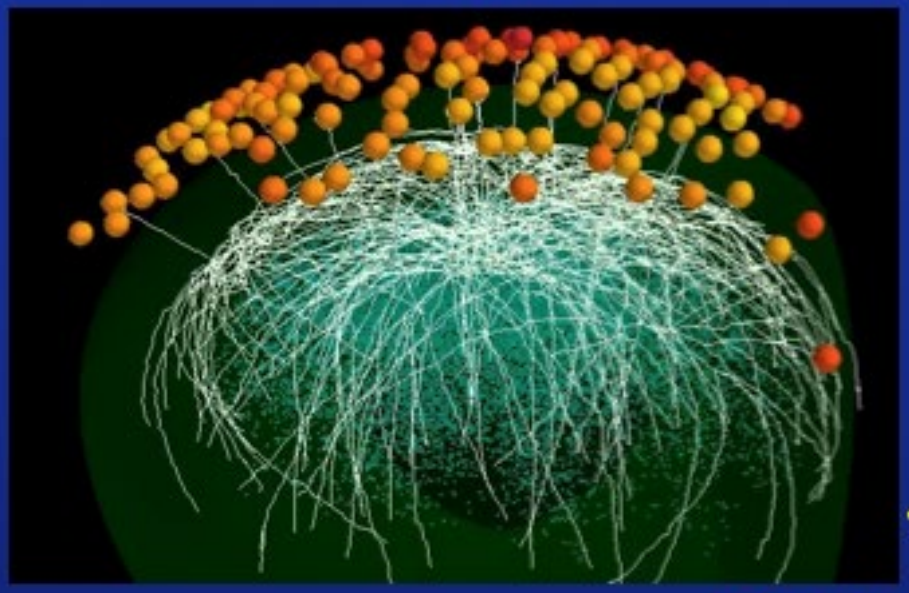
Next-generation weather forecasting

Improve the efficiency of nuclear power, hydropower, wind turbines

direct numerical simulations of the Navier-Stokes equations

advance quantum chromodynamics





Human Brain Project

635 mitral cells
100K granule cells
$7 \cdot 10^5$ synapses
(1/20 of the real system area
32,000,000 nonlinear ODEs)

Table 2 | Model parameters and execution times for a typical simulation.

	Seg (min-max)	States (min-max) (v, channels, and syn. gates)	Syn (min-max)
MC (n = 635)	380,348 (169–1433)	5,259,735 (2536–20,029)	707218 (309–2796)
GC (n = 68013)	4,344,724 (33–257)	26,892,317 (261–668)	707216 (1–62)
Total	4,725,472	32,152,052	

	Computation time	Comm. time (spike exchange)	Comm. time (multisplit)	Total run time (2048 procs)
Average (sec)	27149.35	68.53	555.94	32,552.86
Max (sec)	27756.25	813.44	1453.96	

Currently installed on

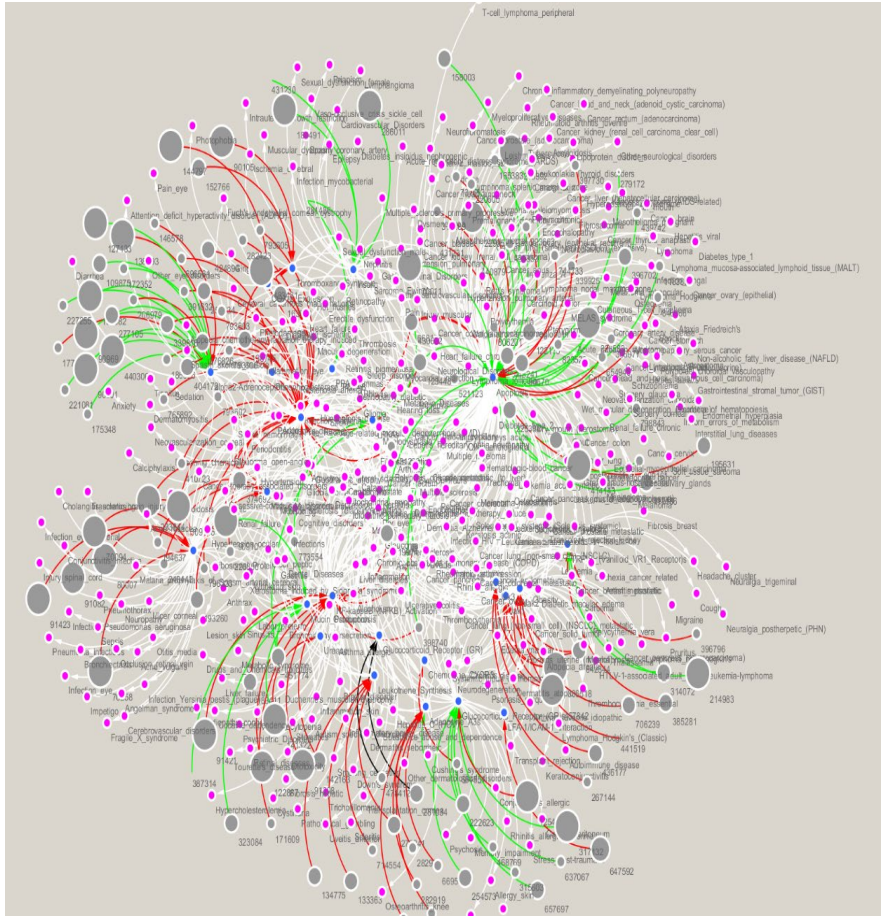
CINECA Marconi

JSC JURECA, JUQUEEN

Typical 40 sec of sim. on 2048 processors, fully integrated NEURON+python implementation, $750 \cdot 10^6$ spikes: 9 hours, 10 Gb output, 99% eff.

Genome-wide molecular docking

Approaching disease-specific poly-pharmacology by connecting drugs with biological targets and diseases



Genome-wide molecular docking simulations will predict

- Drug Efficacy
- Drug Safety
- Averse Effects
- Novel Use of Known Drugs

- In the Zika case study, the ANTAREX (AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems) team identified 26 binding sites from the crystal structures of five Zika proteins: NS5, NS1, NS2B/NS3, NS3 and the envelope protein.

- A total of 1.2 billion molecules were tested via computer simulation on 1 million computational threads available through the Marconi supercomputer.