FP7 Support Action - European Exascale Software Initiative

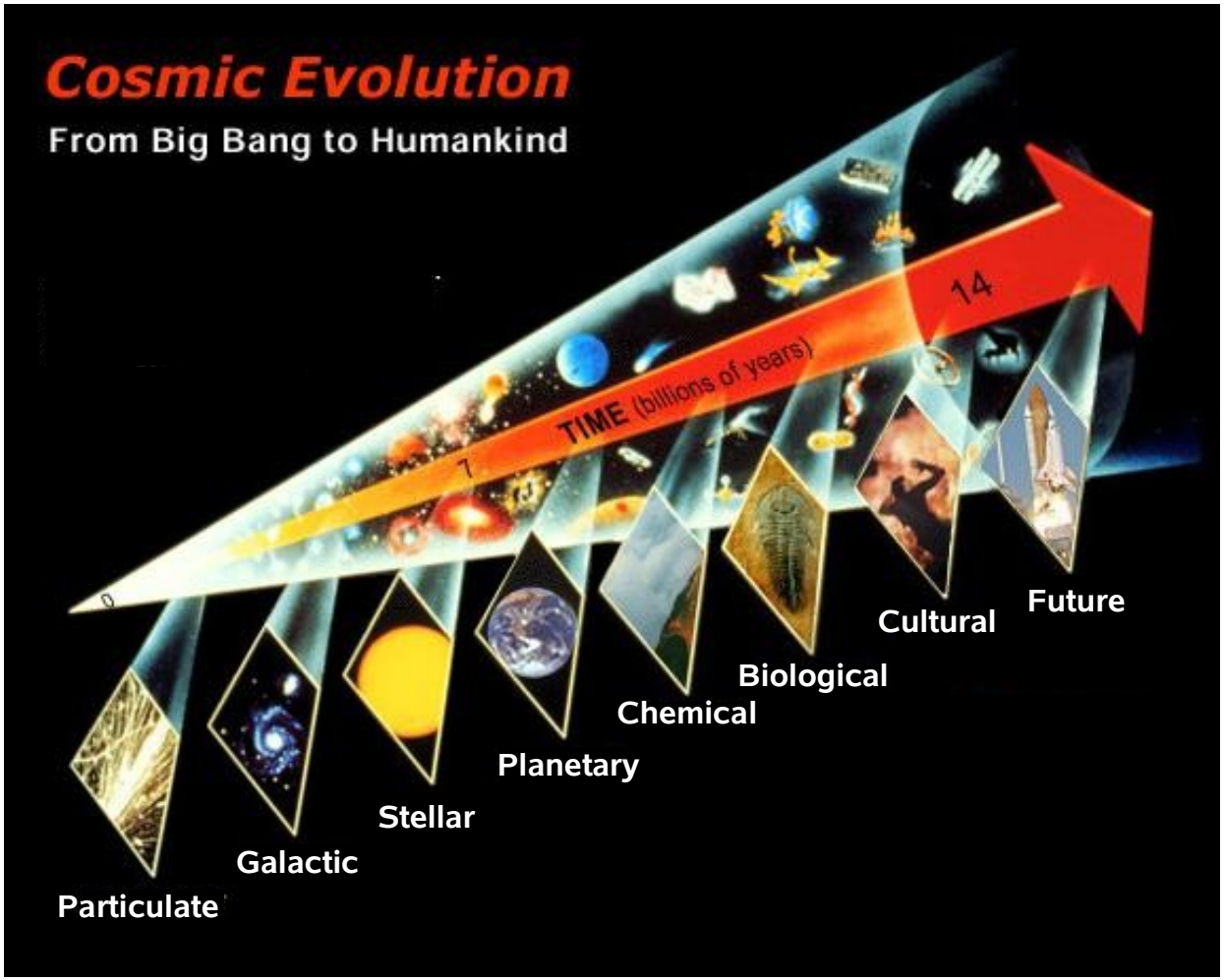
DG Information Society and the unit e-Infrastructures

EESI – WP 3-4 Meeting Paris

WG 3.3: Fundamental Sciences Impacts

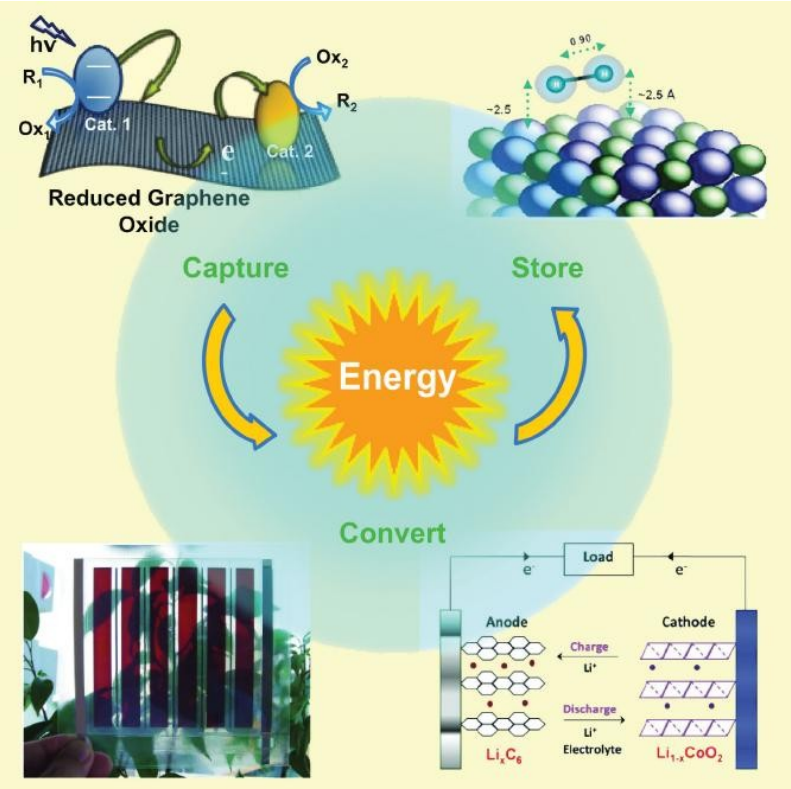
Chair: CECAM-FZJ (Godehard Sutmann)
Vice-Chair: CEA (Jean-Philippe Nominé)

Fundamental Sciences



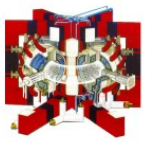
Impacts for Economy and Society

- Energy:
  - harvesting green energies
  - energy conversion
  - storage
  - supply
- Materials
  - new properties (elasticity, conductivity)
  - lower weight
  - improved lifetime
- Environment
  - reduce CO2 (efficient physical principles, reverse cycle)
  - increase efficiency



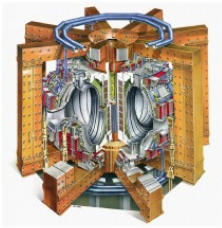
Feasibility of new energy sources

- Nuclear Fusion
  - clean energy for the future
  - design of “experiment”
  - go for future larger systems



Tore Supra

G~0



JET

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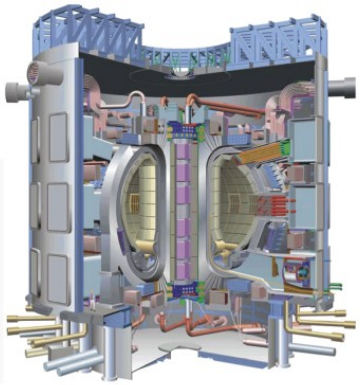

ITER

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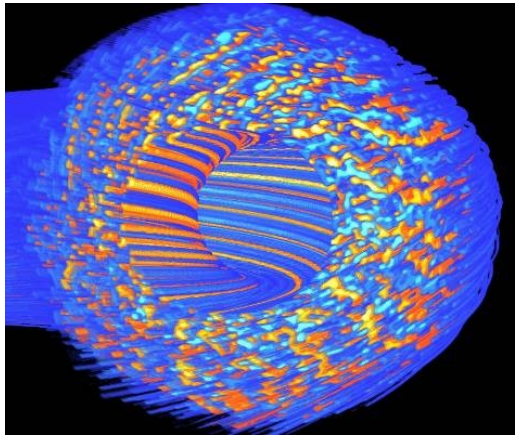
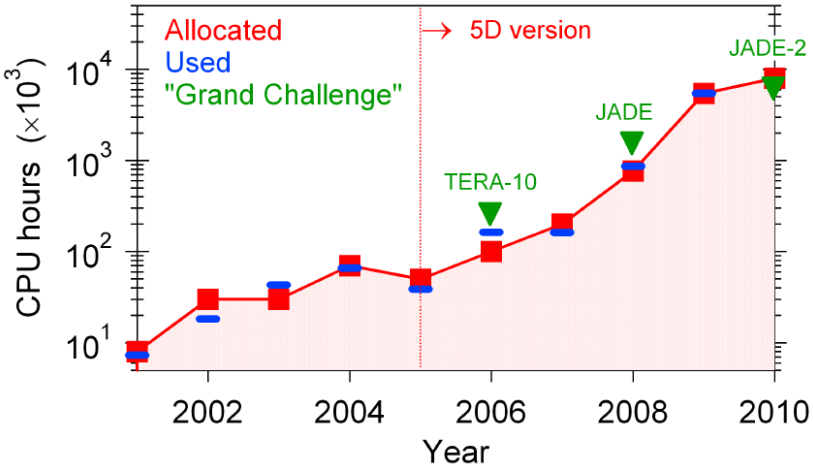


- Physical results (so far)
  - avalanche like transport
  - self-organization (turbulence – large scale flow)
  - transport barriers
  - interaction turbulence – fast particles

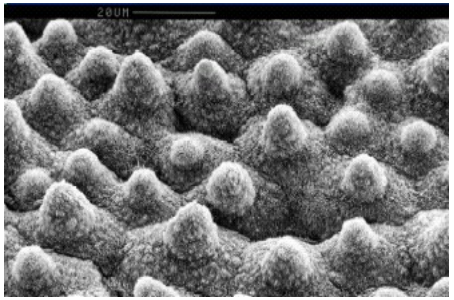


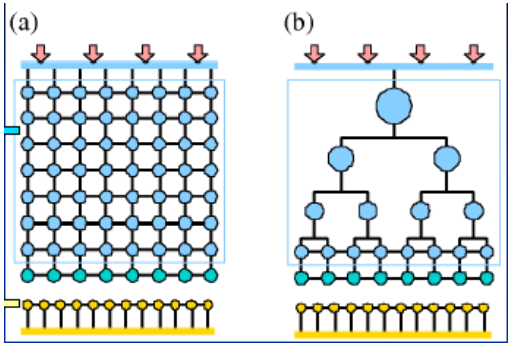
Jaguar: ~80% efficiency

272 billions grid points 10 millions CPU hours 20 TB memory

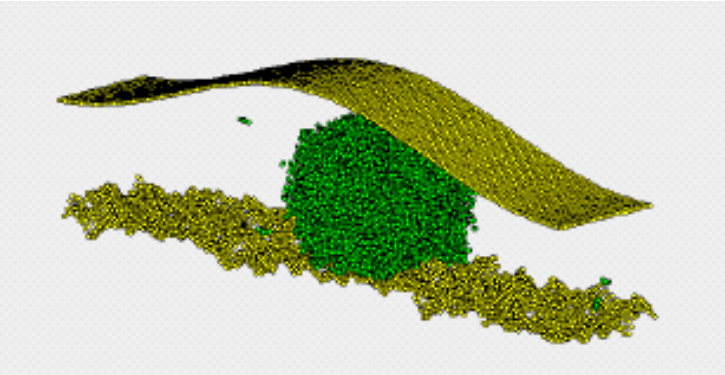
Optimization of Materials

- Understanding of (microscopic) friction
- Optimisation of materials / lubricants
- Design of new materials for specific demands
- less friction, longer lifetime, less energy-losses
- improved safety





All atom Multi-scale



Method development in combination with supercomputing enables simulation of larger and **realistic systems**

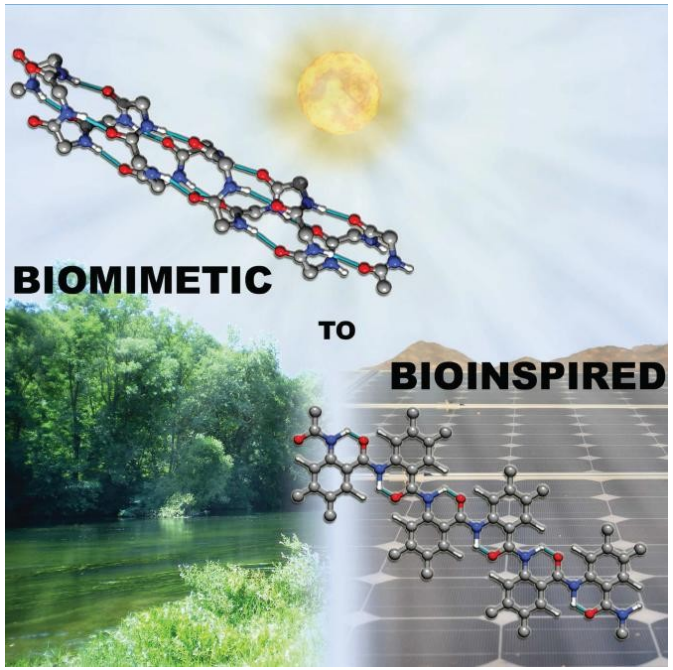
Go into new directions

- Learn from nature
  understand principles
  :: insight from simulations
  translate them to technology
  :: combine knowledge in multiscale / multiphysics simulations

  optimize and **improve** technologies by

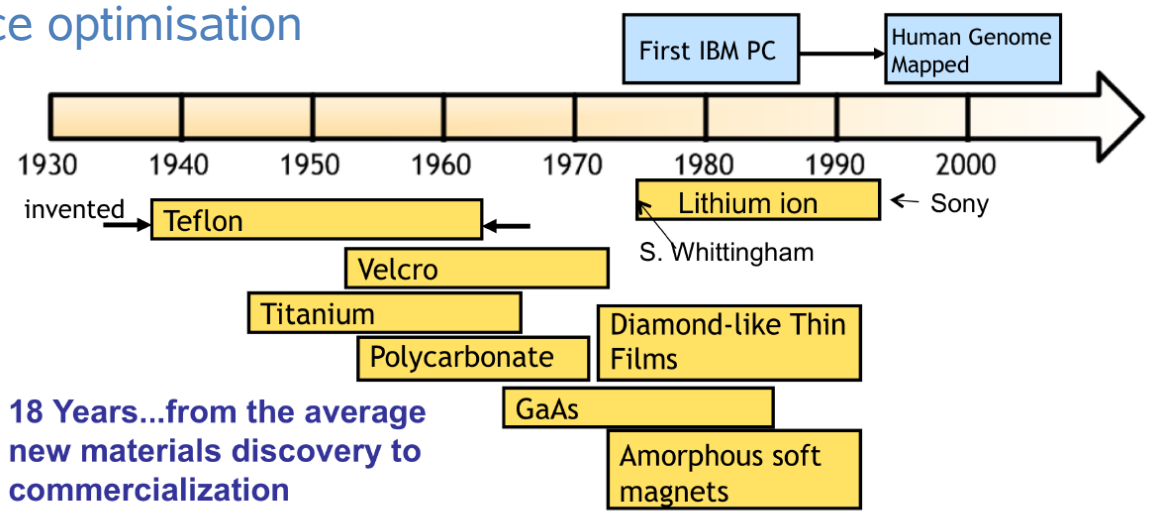
  optimal materials search
  optimal materials composition
  optimal combination of parts

- Improve principles of Nature



Impacts for Economy and Society

- Reduce
  - time-to-solution
  - interval between time-from-discovery to time-to-market
  - potential to at least halften this time by simulations:
    - materials search
    - design
    - stress testing
    - device optimisation



Materials Data from: Eagar, T.; King, M. Technology Review (00401692) ***1995****, 98, 42.*

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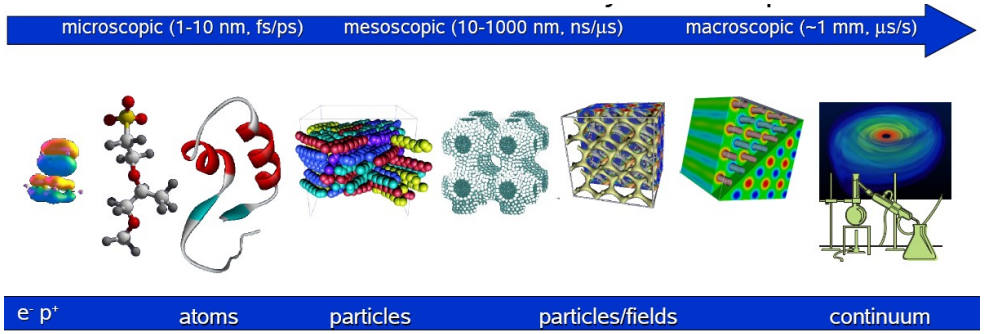
We are prepared for the next step

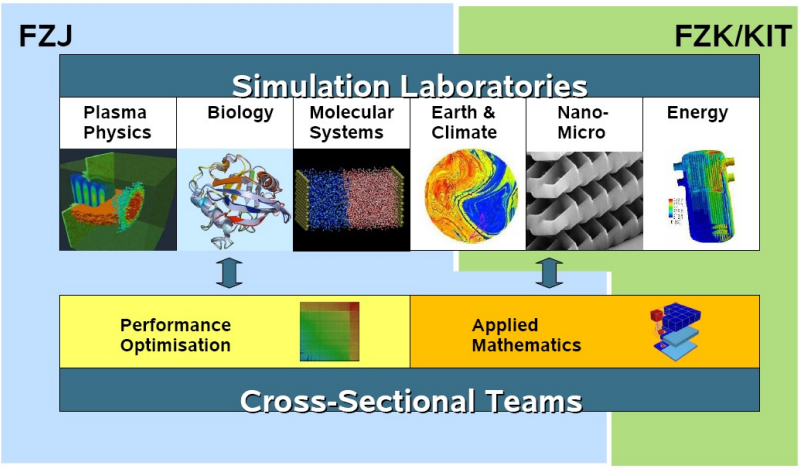
- European strengths include
  - best simulation codes / software development centered in Europe
    - Ab initio: BigDFT, ADF, GPAW, VASP, CPMD, CP2K, AbInit, Castep, Onetep, Fleur, Columbus, Turbomole, QuantumEspresso,...
    - Classical MD: Gromacs, DL_Poly, IMD, ESPRESSO,...
    - Astrophysics: GADGET, Arepo, Pluto, RAMSES, PKDGrav, Nbody,...
    - Plasma Physics: PEPC, GYSELA, Orb5, Elmfire, Euterpe, ...
  - highly developed methods and algorithms
    - FFT, fast multipole, multigrid, wavelets, ...
  - well organized communities
    - material sciences, astro, quantum chemistry



- weaknesses include
  - multiscale modeling

Needs for Training and Education

- International Networking
  - Scientific organizations (CECAM, Psi-k, Virgo,...)
  - Tutorials, workshops
- Support for scientific community
  - Simulation laboratories
  - Bilateral Support actions
  - Co-design centers
- Eductation
  - Use synergies
  - International studies (Master, PhD)
  - Co-Educational Centers
- Virtual Institutes



Swiss Platform for High-Performance and High-Productivity Computing (HP2C, see www.hp2c.ch)

Scientific problem — Simulations + Theory + Experiment

Swiss Universities / Federal Institutes of Technology
(presently **12 domain science projects** in HP2C Platform)

Interdisciplinary teams consisting of:
> model & method development
> application software design / engineering
> system software (everything between apps & hardware)
> numerical libraries / programming environments
> mapping methods onto computer hardware/ systems
> hardware design / engineering

Swiss National Supercomputing Center (CSCS) & U. of Lugano (USI)
(collaboration with industry: Cray, IBM, Mellanox, SCS)

Supercomputer — IT manufacturers – system integrators

Costs and Efforts

- Cost estimate according to current initiatives
  5 FTEs from each side (i.e. 10 FTEs/year)

- Taking into account ~ 7-10 domains and need for co-design and support unit (for whole EU) with e.g. 8 scientists and 2 technical staff members
  - 70-100 FTEs (co-design) **+** 70-100 FTEs (SimLabs, support units)

- Enable small number of codes to **ExaFlop – Computing** and move large number of codes (and broad scientific community) to **Peta-Scale**

  - large impact for user community to make the transition to PetaFlop-Computing
  - parallel programming will be “standard”

Conclusions

- Exaflop computing in fundamental sciences will have huge impacts for
  - education (e.g. master programs, international exchange)
  - scientific community (e.g. distributed groups)
  - scientific discoveries (e.g. large scale dynamical simulations)
  - technological improvements (e.g. multiscale device simulation)
  - new materials (e.g. memory, energy storage)

Thank you for your attention