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

Cosmic Evolution
From Big Bang to Humankind

TIME (billions of years)

Future
Cultural
Biological
Chemical
Planetary
Stellar
Galactic
Particulate
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

- 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

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
Reduce

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

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

- Education
  - Use synergies
  - International studies (Master, PhD)
  - Co-Educational Centers

- Virtual Institutes
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