Engineering and Industrial Applications

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Engineering and Industrial Applications

Transport	Aerospace
	Propulsion
	Automotive
	Marine

Energy (renew)	Wind
	Batteries
	Fuel cells
	Solar
	Electrolysis

Mftg	Chemicals
	Metals and materials processing

Environ-ment	Water management
	Air quality
	Built environment

Energy (conv)	Heating
	Gas turbines
	IC engines
	Oil/gas
	Electrical generation /motors
	Electrical transmission/ networks
	Nuclear

Structures	Mechanics of materials and structures
	Construction

IT	Signal processing
	Control engineering
	Optics and lasers
	Information
	ML and AI

Panel members

Keywords/Short description	First Name	Last name	Organisation	Country	Org type
Combustion; Heat transfer; Turbulence; Simulation; Large Eddy Simulation; nuclear; rockets	Guilhem	**Lacaze**	Transmutex	FR	industry
Fluid mechanics, Heat transfer; Turbulence; Simulation; Large Eddy Simulation; rockets, nuclear energy	Benedicte	**Cuenot**	Safran/ CERFACS	FR	industry
Climate, machine learning, image processing, power networks.	Thomas	**Brunschwiler**	IBM Zurich	CH	industry
Structural engineering; Structural Health Monitoring, Hybrid Modeling, Nonlinear Dynamics, Data-driven Diagnosis & Prognosis	Eleni	**Chatzi**	ETH Zürich	CH	acad
Physics of Fluids; Turbulence; Drops & Bubbles; Multiphase Flow	Detlef	**Lohse**	U Twente	NL	acad
Applied mechanics, continuum methods and algorithms, FEM	Garth	**Wells**	U Cambridge	UK	acad
HPC algorithms, applied simulations to energy networks	Olaf	**Schenk**	U Swizz Ital	CH	acad

Questions for panel

- What are currently the **most important topics** in the field from the point of view of science, society or industry ?
- What are the **main challenges** for simulations? Can you identify **key bottlenecks** whose resolution would open up new frontiers ?
- What **recent high-performance simulations**/models have offered the **most exciting breakthroughs** or examples of what is possible?
- How is the computational resource landscape changing regarding **code development and portability** to different machines? What are the **needs and how are they being served**?
- How are **machine learning and other forms of AI being applied to your field**, and how are they evolving? Are **custom tools** required and being developed?
- **Other thoughts** in general, whether specific to an area or across all areas on the needs and potential evolution of HPC usage and potential?

Expected headlines

Energy

- Energy & propulsion:
  - Aero/vehicle/marine: drag reduction, DNS + ML models for turbulence, model coupling with acoustics
- Renewable Energy:
  - Wind: blade and windfarm large scale modeling (LES, fluid-structure interaction, atmospheric turbulent flow)
  - Solar/batteries/electrochemical: materials search using DFT+MD+ML+AI
  - Fuel cells/electrolysis: microscale + macroscale two phase simulations including catalysis (hybrid material + DNS)
  - Catalysis and reforming: development of new catalytic surfaces and materials for e-fuel reforming, advanced DFT+MD models for catalysis, coupling with fluid mechanics

Expected headlines

Energy

- Conventional
  - Combustion (heating, gas turbines, engines, propulsion) + oil/gas : fluids+reaction DNS, turbulence modeling, two-phase flow (liquids). ML for turbulence+chemistry model reduction. New fuels: H_2, NH_3, SAFs change chemistry and models.
  - Nuclear: Coupled MC modeling of core, and CFD of cooling circuit. Significant increase in interest in Small Modular Reactors (SMR)

Expected headlines

- Structures:
  - Multiscale models for predictions of properties of complex structures with vastly different spatial scales and materials (aerospace, automotive, buildings)
  - Structure-flow interactions: wind turbines, bridges, but also flows through porous materials (catalysis, PEM)
  - Multiphase calculations for 3D printing: LMD/SLM processes and structure design and property predictions

Expected headlines

- Manufacturing:
  - New process development: net zero e-fuels, ammonia, SAFs
  - Chemicals discovery: materials, processes using DFT/MD combined with ML for model order reduction
  - Process intensification: AI/block-chain tracking/data flows for higher manufacturing throughput
  - …

Expected headlines

- Hardware & software engineering:
  - Sensor and imaging integration: generation of lower order models for imaging/recognition and multisensor integration with multiple applications: navigation, robotics, autonomous operation
  - Telecommunications, networks, optical computing: simulation and design of new protocols and processes
  - Design and simulation of highly integrated circuits
  - …too many others

Cross-cutting scientific themes

- Advanced meshing techniques for multiscale models: adaptive meshing for continuum modeling (flow DNS, mechanics/acoustics FEM). Algorithms to automate vastly different scales
- Machine learning everywhere: specialized algorithms for submodel encoding using hierarchical level simulations
- Flexible code development: code development for portable use GPU/CPU/hybrid
- Increasing use of low-cost cloud computing: HPC in parallel/complement: HPC centers to think about seamless access/how it fits in landscape