EESI Presentation at IESP

San Francisco, April 6, 2011

WG 3.1 : Applications in Energy & Transportation

Chair: Philippe RICOUX (TOTAL)
Vice-Chair: Jean-Claude ANDRE (CERFACS)

WG3.1 Scientific and Technical Vision

Best coupling between **Architecture / Algorithm / Application**, in order to address and solve on Exaflop systems crucial issues in Energy & Transportation industries, and more generally Engineering industries.

Multi-domain applications

Geophysics, Oil & Gas, Multiphase flows, Flight physics, Aeronautics, Chemical engineering , Mechanical engineering, Structure deformation, Propulsion and engine flows, Combustion, Hydraulics, Neutronics, Nuclear industry, Surface transportation, Trains, …

Applied mathematics, Numerical analysis, Particle dynamics, CFD, Computing

Team of experts : Largely distributed , methodological and applied

Experts from Large Companies in Industry : Oil, Aeronautics, Electricity, Nuclear, Hydro, Train

Experts from Academy : LES, CFD, Particle, Computer sciences, Algebra, …

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WG3.1 List of Experts

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Henri CALENDRA	(TOTAL, F)	Geophysics, Oil and gas
Keld NIELSEN	(ENI, I)	Multiphase flows, Oil and gas
Thierry POINSOT	(CERFACS, F)	Combustion, CFD
Eric CHAPUT	(EADS/Airbus, F)	Flight physics, Aeronautics
Demetrios PAPAGEORGIOU	(Imp. College, GB)	Applied math., Physics
Ulrich RUDE	(U. Erlangen, D)	HPC, Particle dynamics
Jean-Daniel MATTEI	(EDF, F)	CFD, Hydraulics
Christian HASSE	(BMW, D)	Propulsion and engine flows, Automotive
Heinz PITSCH	(Univ. Aachen, D)	Propulsion, Engine flows
Norbert KROLL	(DLR, D)	CFD, Aeronautics
Tanguy COURAU	(EDF, F)	Neutronics, Nuclear industry
Ali TABBAL	(ALSTOM, F)	Surface transportation, Trains
Chuan-yu WU	(U. Birmingham, GB)	Chemical Engineering
Mark SAWYER	(Univ. Edimburgh)	Computing
Jacek MARCZYK	Ontonix	Computer Aid Engineering

WG 3.1 First Experts Meeting Résumé

Questions and issues to address:

- for efficiently reaching goals: which effort ? where to spend the money?

- the roadmap must be implemented in several industries

Roadmaps are different depending upon particular industries :

Aeronautics :

Exaflop not ultimate goal, need at least Zetaflop for LES aircraft
Mostly “farming” applications (almost independent simulations)
Data mining and data assimilation
Steady cases (RANS, URANS) with improved physical modeling

Seismics, O&G :

Largely embarrassingly parallel
Major problems are programming model, memory access and data management
Need Zetaflop for full inverse problem

WG 3.1 First Experts Meeting Résumé

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Combustion: Turbulent combustion modeling, LES in large scale reactors
Coupling multi-physics
Exaflop for Combustion at the right scale,
Multi-cycle engine (Weak scalability)

Engineering : Optimization, Monte Carlo type simulations, “farming applications”, …
Main problem : equations themselves, physics, coupling, …

Multi-Fluids Flows , Fluid Structure Interactions, Fluidized beds:
Particle simulations , stochastic PDE, …
Multi-scale approach
Main problem : physics, fluid in particles?

…

WG 3.1 First Experts Meeting Résumé

Experts consider that

Only few “hero” applications to push the limit, real goal is Zetaflop and not Exaflop

Major applications corresponding to production problems, will be “farming” applications

Some flexibility in architecture : several applications on the same large computer (computer center) and the same application on different architectures (true for farming only)

4 important areas defined :

- Co-existence of (new) common software platforms and legacy codes
- Multi-physics simulation: establishment of standard coupling interfaces and software tools
- Open-source jointly developed grid-generation tool
- Standardized efficient data management

WG 3.1 First Experts Meeting Résumé

Common main issues to be addressed (where to spend the money)

- Scalable program ,
  - Strong and weak scalability, load balancing, flexibility
  - Numerical analysis, algebra, time scales,
- Legacy code, open source,
  - Standards (MPI, OpenMP, C++, Fortran, …)
- Mesh generation
- Coupling multi physics codes with efficiency

  Data management (sorting memory for fast access, allocating new memory as needed in smaller chunks, treat parts of memory that are rarely/never needed based on heuristic algorithms, …)
- Particle simulation
- Human resources, training (what level?)
- Toward “defensive programming” …

WG 3.1 First Experts Meeting Résumé

For each of important issue , a roadmap could be proposed :

2012 – 2015:

- decision process concerning the software
- establishment of a core development group
- funding of a small number (at least one) of pilot projects and establishment of the tool framework described above , grid generation tool, common solver software

2015 – 2020:

- establish first projects with both the software platform and at least one legacy code for the specific application. Choose a HPC application with scientific and social impact
- establishment of a growing number of research projects based on the common platform especially for multi-physics applications requiring very high memory
- Review of the approach until 2020

WG 3.1 First Experts Meeting Résumé

Europe Strengths

- Scalable program ,
  - Strong and weak scalability, load balancing, flexibility
  - **Numerical analysis, algebra, time scales,**
- Coupling multi physics codes with efficiency
  - **O- PALM,**

Europe strengths but to be reinforced

- Mesh generation
- Particle simulation

Europe weaknesses

- Standards (MPI, OpenMP, C++, Fortran, …)
- Data management
- Training ?

WG 3.1 Cross Cutting Issues

Common issues with others applications and WG :

Develop new software approaches in **industrial geometries**

- multi-level parallelism , parallel I/O, data management
- load-balancing
- fault-tolerance techniques
- dynamic reconfiguration
- automatic and adaptive meshing
- Increase efficiency in
  - numerical methods, algorithms, libraries,
  - standard programming tools,
  - compilers (including for hybrid architectures)

Crucial for achieving simulation which can effectively scale up to a few hundred of thousand cores, if not a million cores.

WG3.1 Next steps

1. Experts Meetings

- 18th January 2011 (Paris, TOTAL)

Brainstorming, discussion about main issues (these slides)

- 12th April 2011 (Frankfurt Airport)

Synthesis of previous meeting, draft of deliverable 3.1

Focus on : how much effort , communication, social , Europe strengths

2. Deliverable 3.1

Working Group Report on Energy and Transportation (engineering) applications: **Month 12 (June 2011)**

BACKUP / RESERVE

Partner
Logo

WG 3.1 First Experts Meeting Résumé

Data management , database access while:

- sorting memory for fast access
- allocating new memory as needed in smaller chunks
- splitting needed from unneeded memory
- treat parts of memory that are rarely/never needed based on heuristic algorithms
    - o with compression
    - o with writeout to disk
    - o deletion of memory, giving reference to recalculation if ever needed
- optimize memory access for points not discretized in database supplying
    - o built-in interpolation schemes
    - o local database refinement (change in discretization/resolution)

Efficient data management libraries supported in a similar fashion as the software platform.

Increase efficiency in

numerical methods, algorithms , libraries,

standard programming tools, compilers (including compilers for hybrid architectures)

Crucial for achieving simulation which can effectively scale up to a few hundred of thousand cores, if not a million cores.

Develop new software approaches in **industrial geometries**

multi-level parallelism , parallel I/O,

automatic and adaptive meshing,

load-balancing , fault-tolerance techniques , dynamic reconfiguration,

…

Partner Logo

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WG3.1 OBJECTIVES and STARTING POINT (2/2)

Main challenges (F/0)

- ***Aeronautics*: full MDO, CFD-based noise simulation real-time CFD-based in-flight simulation: the digital aircraft**
- ***Structure calculation***: design new composite compounds, …
- ***Special Chemistry*** : atom to continuum simulation for macro parameters estimation in catalyst, surfactants, tribology, interfaces, nano-systems, …
- ***Energy*: computations with smaller and smaller scales in larger and larger geometries : Turbulent combustion in closed engines and opened furnaces, explosion prediction, nuclear and fusion plants, …**
- ***Oil and gas industries***: full 3D inverse waveform problem, multi-scale reservoir simulation models, …
- ***Engineering (in general)*: multi-scale CFD, multi-fluids flows, multi-physics modelling,, complex systems modelling, …**

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Memory bandwidth. No tricks, no apologies.
– Uniform, low-latency petascale memory matched to floating-point speed
– Full speed no matter where operands and processes reside
– 100x historical I/O speeds relative to flops allow realtime embedded uses
– Checkpoint/restart can be done in under 5 seconds
– Removes pressure on programmers to be “clever,” improving productivity

Portable Object Code and Run-Time Environment
– New, industry-standard (open) high-level HPC model
– Zero porting cost; tuning burden entirely on system instead of programmer
– Legacy languages, codes, and parallel models fully supported
– A collection of innovations assure *correctness and clarity.*

Hardware protection helps security, debugging, admin, OS scaling

v Interval Arithmetic assures validity and provides parallelism
– Makes uncertainty in floating-point math visible and controllable
– Enables new, massively parallel approaches for nonlinear optimization

v Purpose-Based Benchmarks measure productivity explicitly