Some HPC challenges for multi-physics extended CFD computations

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retour sur innovation

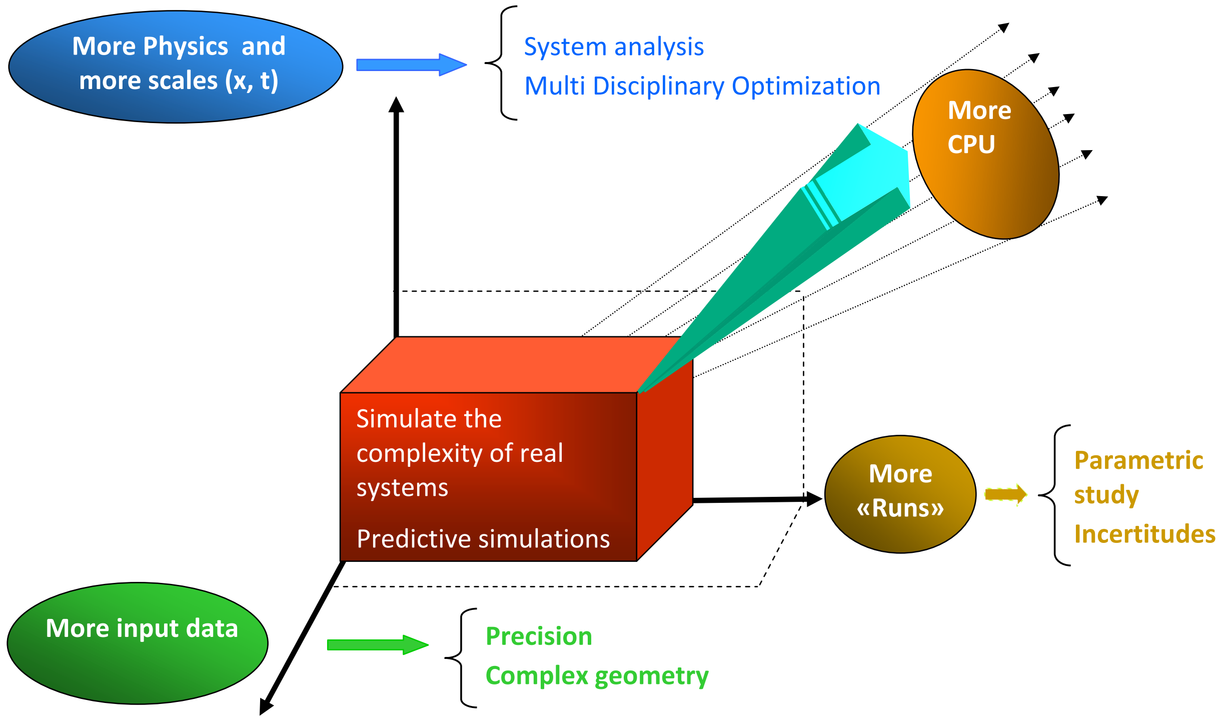
Outline of presentation

- Context (multi-physics extended CFD for research and industry)
- ONERA's CEDRE code

1) Some HPC challenges
   - Memory
   - I/O library
   - Lagrangian vs Eulerian
   - Coupling and CWIPI library
   - Scalability
2) Large scale LES examples
   - Aeroacoustics
   - Reactive flows
   - Two-phase flows

- Conclusions

HPC challenges: 1 target – 3 axes



Context

- Hardware evolution
  - From vector mainframes (Cray, NEC, Fujitsu), large memory per core
  - To scalar parallel clusters, reduced memory per core
  - Towards HPC clusters and exascale machines, limited memory per core
- Multi-physics extended CFD
  - From pure aerodynamic conditions (1 species, perfect/ideal gas)
  - To reactive conditions (multi-species, chemical kinetics, real gases)
  - To multi-phases conditions (dispersed, separated, mixed)
  - To multi-physics conditions (aeroacoustics, fluid-solid interactions (heat transfers, mechanics), electro-magnetism, moving meshes, ...)
- Code challenges
  - Memory and I/O managements
  - Automatic partitioning and balancing
  - Coupling procedures
  - HPC requirements at every level

ONERA's CEDRE code

- ONERA's reference code for energetics and propulsion
- Unstructured meshes
  - Cell centered (finite volume), expl/implicit, MUSCL up to high order
  - Generalized, full polyhedral, meshes (face based)
- Parallel
  - MPI based
  - Automatic partitionning and balancing
- Multi-physics
  - Internal (different CEDRE solvers for different physical systems)
    - Charme: Navier-Stokes, turbulent, reactive, real gases, multi-phases
    - Sparte: dispersed phases (Lagrangian)
    - Spirée: dispersed phases (Eulerian)
    - Astre: radiation (Monte-Carlo)
    - Réa: radiation (discrete ordinate)
    - Acacia: thermal solutions in solids
    - Film: liquid films
  - External (coupling libraries: MpCCI, CWIPI, OpenPalm)
  - Moving/deformable mesh (conservative ALE approach)
- Zonal approach (models per user's domain)

HPC challenges for specific industrial needs

- Unstructured mesh – no aligned data
- Memory
- I/O
- Multi-physics - coupling approaches
- Scalability
- Moving mesh (not presented)

MEMORY

- Importance of memory – measure inside code (house keeping)
- Current trend of decreasing available memory per core

HOWEVER:

- Resilience problem: MTTI checkpoint-restart
- Impact of Big Data (also needs of big memory)
- Advances in technolgy
  - PRAM (parameter random access memory) in place of RAM
  - ReRam (HP – "The Machine" project)
- More memory can also have an influence on multi-physics coupling

Memory reduction trend may be counter balanced (fortunately)

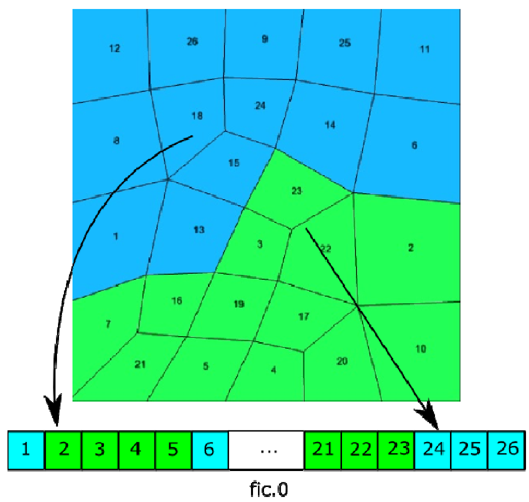
I/O issue (1/2)

Unstructured data
=> non continuous / inteleaved data

Large number of small files (per core):
Problem for backup and for parallel file system (Lustre, GPFS)

Single file:
in-house library,
binary,
compatibility little-endian/big-endian

Restart of computations on different number of cores (strong users demands)

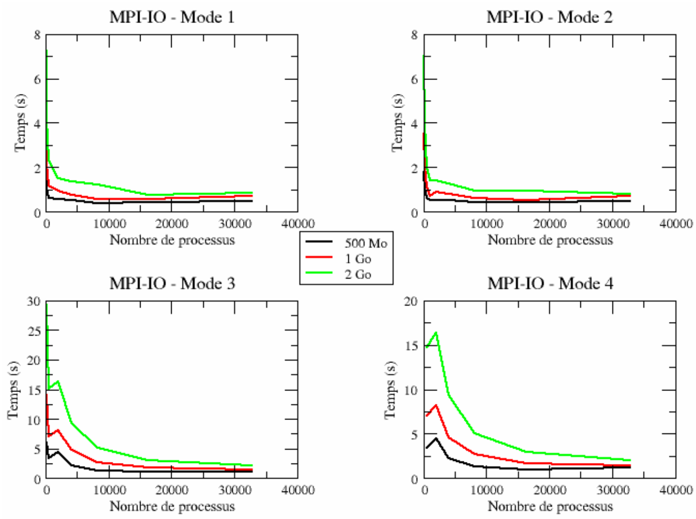


I/O issue (2/2)

Actual bottleneck: ways to escape

- Test through Projet PRACE: Cedre Preparatory project n° PRA017, 2010, computer Jugene from Juelich, 1Mh
- I/O library tests on 32 000 cores, GPFS is better than Lustre
- "Interleaved" cost is limited for restart files

- Collective writing per bloc :
  - Mode 1 (reference)
  - Mode 2 (use of MPI_TYPE_HINDEXED)
- Interleaved writing
  - Mode 3 (use of MPI_TYPE_SUBARRAY)
  - Mode 4 (use of MPI_TYPE_HINDEXED)

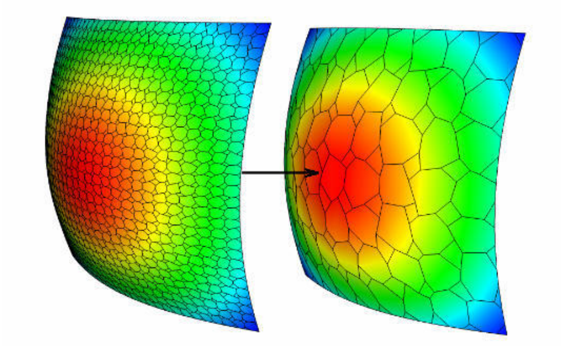


Multiphysics: Eulerian vs Lagrangian

- Multi-physics: more challenges to be faced
- Eulerian approach: parallel by domain
- Lagrangian approach: parallel by trajectory (e.g. photons)
- Both approaches in CEDRE
- Problem of load balancing for the complete simulation
- Some Lagrangian approach needs all the mesh on each core (e.g. solver Astre)
  - Limit of memory: hybrid solution through OpenMP
  - Today this solution permits to push the limit from 3M elements to 20 M elements (48Go/node)
- Works are still needed on that subject

CWIPI: Coupling With Parallel Interface

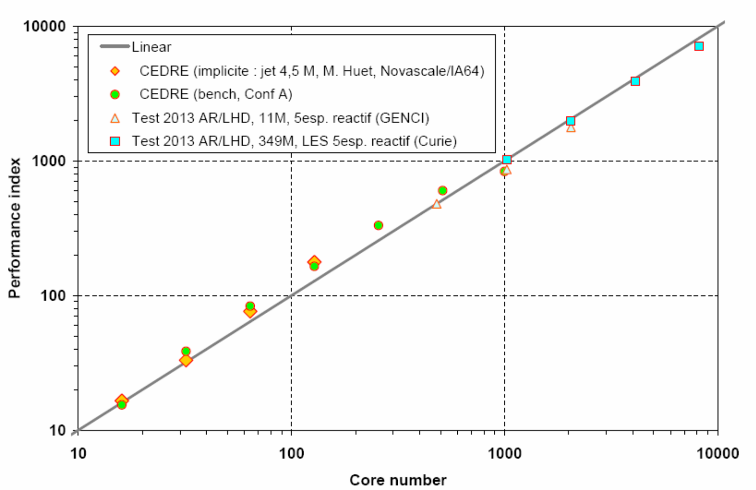
- Developed at ONERA
- Open source (cedre.onera.fr)
- Test on Curie 32k cores – 1 Billion nodes
  - Simulates the coupling between two softwares through an exchange across an interface consisting of a partitioned surface. The discretization of the surface is unique to each code.
  - Synchronous vs asynchronous: speed ratio 10-15



CEDRE: Scalability tests

We acknowledge PRACE for awarding us access to resource CURIE based in FRANCE at TGCC, Project PA1389, 2013, 200 kh

- Study of combustion instabilities in a variable-length combustor by Large Eddy Simulation on 350 Mcells



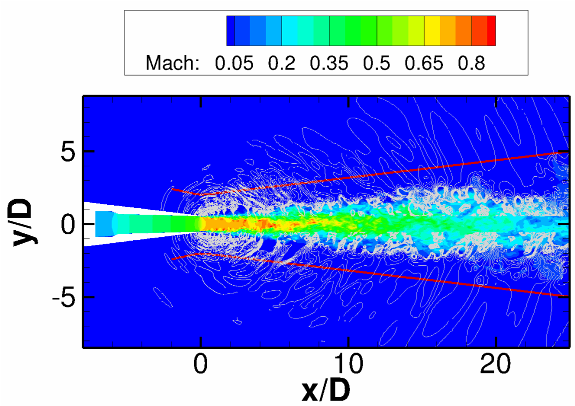
Aggregated results from several projects

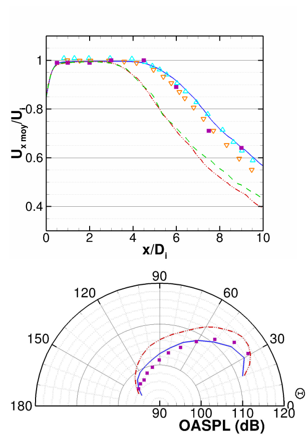
Examples of large scale LES "real life" applications

- Aeroacoustics
- Reactive flows
- Two-phase reactive flows

Large scale LES: Aeroacoustics (1/2)

- Jet noise
  - Aircraft noise reduction studies
  - Hybrid approach: CEDRE LES-CFD + KIM acoustic code
  - 250 Mcells + resolved nozzle boundary layer tripping, 960 cores

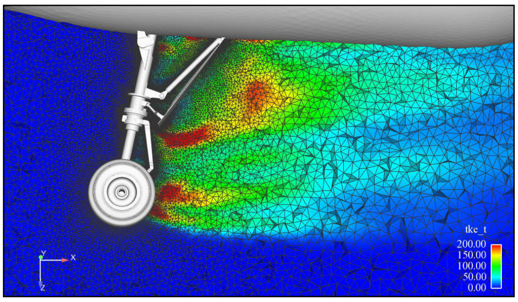




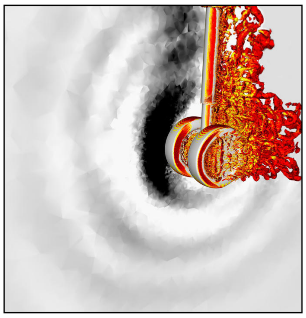
M. Lorteau, F. Cléro, F. Vuillot, "Recent progress in LES computation for aeroacoustics of turbulent hot jet. Comparison to experiments and near field analysis", AIAA 2014-3057, 20th AIAA/CEAS Aeroacoustics Conference, 16-20 June 2014, Atlanta, Ga, USA

Large scale LES: Aeroacoustics (2/2)

- Landing gear noise
  - Aircraft noise reduction studies
  - Complex geometries: unstructured meshes are required
  - Hybrid approach: CEDRE LES-CFD + KIM acoustic code
  - 70 Mcells + ZDES turbulence modeling



Gulfstream/Nasa PDCC nose landing gear (BANC workshop)



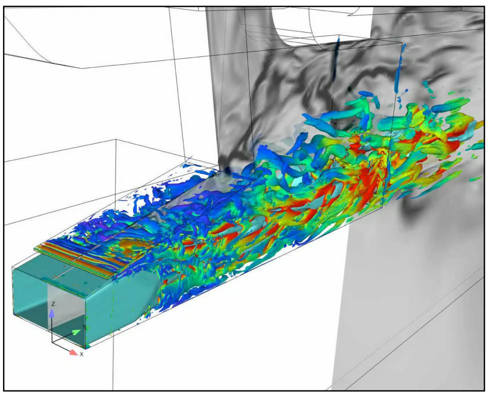
Airbus Lagoon NLG (BANC workshop)

L. Sanders, N. Lupoglazoff, F. Vuillot, E. Manoha, D. Luquet, F. de la Puente, "Further flow and noise predictions of the Gulfstream PDCC nose landing gear based on the CEDRE unstructured solver", 19th AIAA/CEAS Aeroacoustics Conference, 27-29 May 2013, Berlin, Germany

F. de la Puente, L. Sanders, F. Vuillot, "On LAGOON nose landing gear CFD/CAA computation over unstructured mesh using a ZDES approach", AIAA 2014-, 20th AIAA/CEAS Aeroacoustics Conference, 16-20 June 2014, Atlanta, Ga, USA

Large scale LES: Reactive flows

- Supersonic reactive flow in over-expanded nozzle + film cooling
  - Launcher studies (CNES, ATAC project)
  - 6 species + seven steps reactive scheme
  - 7.5 Mcells + ZDES turbulence modeling

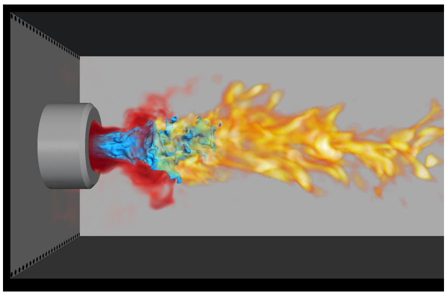


Iso-Q surface coloured by mod(Ux)

B. Sainte-Rose, N. Bertier, S. Deck, F. Dupoirieux, "Numerical simulations and physical analysis of an over-expanded reactive gas flow in a planar nozzle", Combustion and Flame 159 (2012), 2856-2871

Large scale LES: Two-phase reactive flows

- Liquid propellant rocket motor combustion chamber
  - MASCOTTE cryogenic test bench (LOX-GH2 type)
  - Coupling of two CEDRE Eulerian solvers
    - CHARME for separated phase flow (gas and liquid jet)
    - SPIREE for the dispersed droplet spray flow
  - 10 Mcells grid, 2x480 cores



A. Murrone, N. Fdida, C. Le Touze, L. Vingert (2014), "Atomization of cryogenic rocket engines coaxial injectors. Modeling aspects and experimental investigations", Space Propulsion, 2014, Cologne, Germany, 19- 22 mai, 2014

Wrap-up

- HPC challenges for research and industrial flows
  - Unstructured data structures
  - I/O and memory management
  - Exchange and coupling procedures
- ONERA's CEDRE code for energetics and propulsion
- Large scale LES: recent examples
- Clear HPC needs
  - Unsteady flow solutions
  - Multi-physics
  - Data management
- Works are in progress in these areas

Thank you for your attention

- QUESTIONS ?