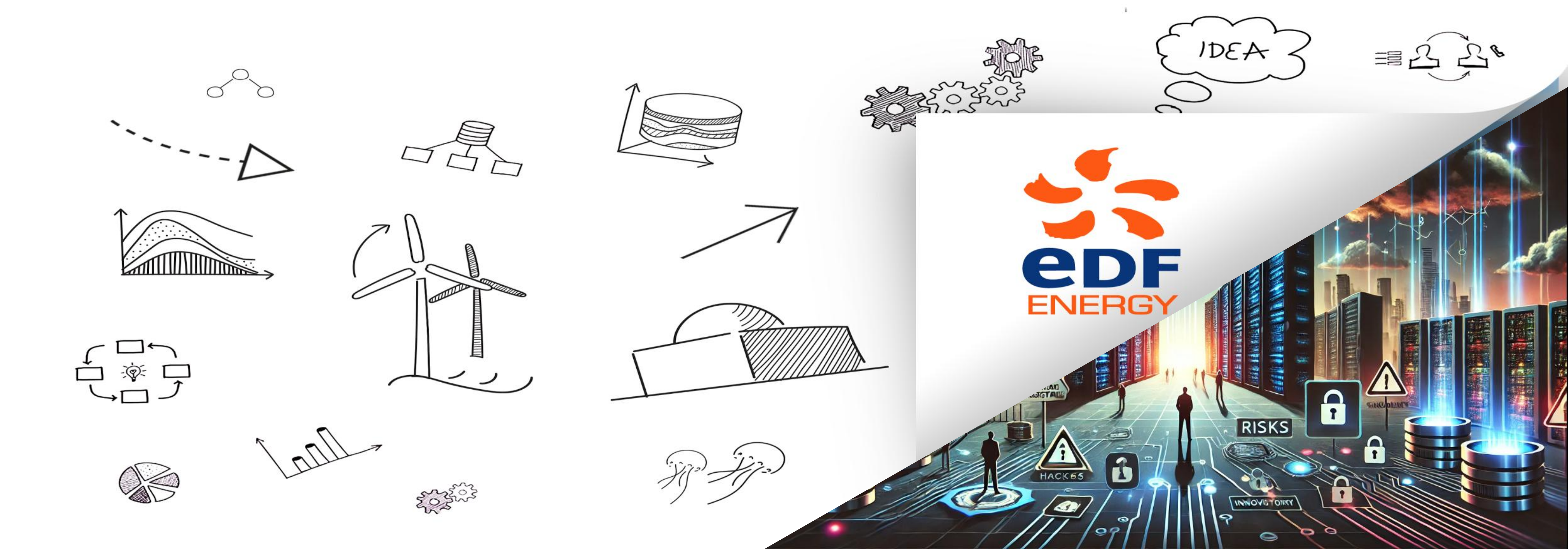

EDF R&D-ARSI HPC challenges

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24/01/25

Context-High Performance Computing needs

Challenge:

CFD and FEA simulations used for reactor plant safety (V&V), parametric studies, business tool or developing methods and code

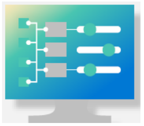
Current approach:

Tasks need computing power; provided by local clusters from University of Manchester and EDF R&D France.

Concerns- risks:

1)Data storage due to Export Control.

2) Cluster limitations i.e. peak academic periods and enterprise model used across different teams



Proposed solution:

Microsoft Azure

1) Configuration, setup and maintenance of OS, software updates, network of Azure Cycle Cloud. Policy and limits on resources on users

2) Storage needs.

3) Financial model of Azure/SKUs.

Some scenarios and job statistics to further understand and adopt on Azure Cycle Cloud

Information from Computational Fluid Dynamics (CFD) team

Hardware:

- ❑ CFD benefits from high core count; software is highly scalable and flexible to be used on serial, multicore and multinode mode (refer to hpc-code_saturne).
- ❑ Memory depends on the number of mesh elements and other operations i.e. gradient reconstruction, equations to be solved, modified source terms etc.
- ❑ Pre- and post processing of the results requires GPU acceleration and relatively high bandwidth to provide a good user experience i.e. visualisation of flow, animations.
- ❑ Storage requirements depend on flow simulation time and physics to be captured.

Software:

- ➢ "**SLURM**" configured cluster (but "SGE" also available).
- ➢ Not limited but essential software includes EDF R&D France/CEA open-source and commercial software: code_saturne , StarCCM+
- ➢ Compilers and dependencies including Intel FORTRAN, GCC, G++ Compiler, Salome, Paraview , Python, cmake, singularity, hdf5, med, medcoupling, MPI, OPENMP, PyQT5...
- ➢ Linux OS-Red Hat Enterprise Linux 9 v9.3 (and refer to last slide for more information).

SALOME + code_aster = salome_meca

code_saturne

ParaView

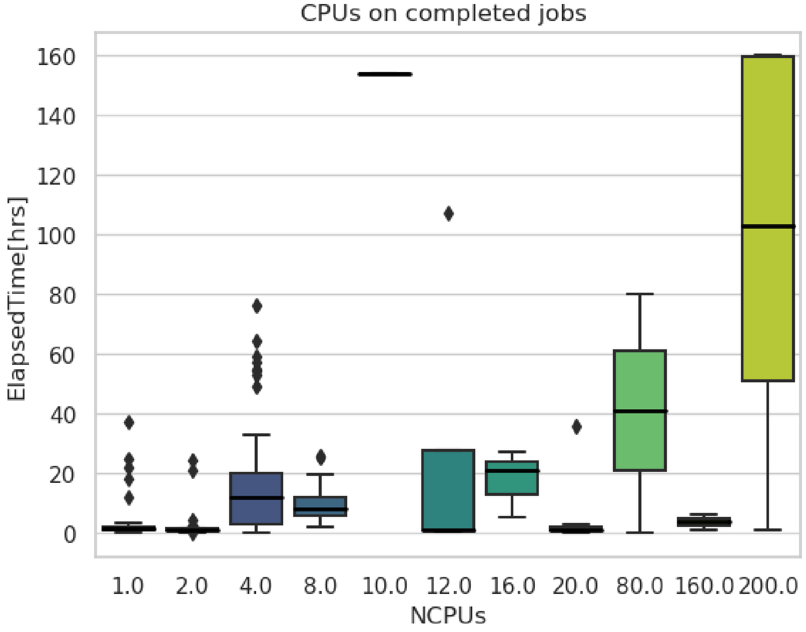
Some data overview from last year CFD simulations

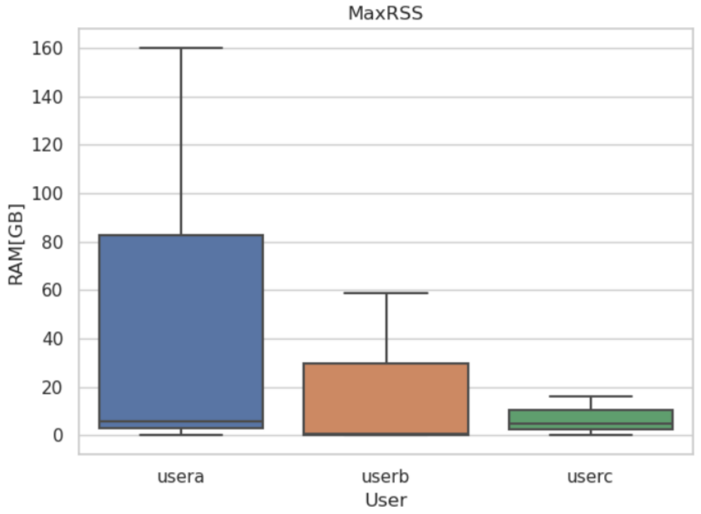
Based on jobs completed/failed from last 365 days

- Variability of resources for CFD and associated on project demands.
- Core ranges from 1 to a few 100s and maximum time for job last on average 4.1 days.
- RAM allocated on basis of 4-6GB/CPU but most jobs did not require more than 200GB in total (based on maximum max RAM used on task node.)

	JobID	Time Elapsed[hrs]	Alloc. CPUs	Alloc. RAM
count	525.00	525.00	525.00	525.00
mean		15.42	70.34	282.90
std		34.26	88.51	353.45
min		0.00	0.00	2.00
max		161.21	200.00	800.00

Data analysed from CPUs, MaxRSS and time elapsed:





Based on Finite Element Analysis (FEA) needs

Hardware:

- ❑ FEA tends to be CPU limited, i.e. the width of the matrices being solved are large and not benefits much when increasing core count.
- ❑ FEA tends to benefit (based on cost perspective) from high amounts of RAM/CPU. i.e. 40 CPUs are generally enough for any given FEA model but need up to 1TB of RAM for the largest models.
- ❑ Post processing would need GPU acceleration and relatively high bandwidth to provide a good user experience.
- ❑ Storage requirements per model can be quite low. Probably less than 1TB for most of what team does.

Software

- ➢ Abaqus, Intel FORTRAN Compiler and C++ compilers.
- ➢ Abaqus 2023 and older versions don't align well with AMD EPYC chips and thus FEA would prefer Intel chips.
- ➢ Code_Aster, Salome MECA, Paraview-Intel FORTRAN Compiler + Required GCC- C++ Python compilers.

Overview of average job stats based on FEA users:

Users	Job count	Time Elapsed [hrs]	Alloc. CPUs	Alloc. RAM (GB)
A	160	70	20-40	150
B	160	84	20-30	100

Workflow for a simulation of FEA/CFD and Azure Cycle Cloud

Problem Identification
1. Objectives
2. Domain identification

Pre-Processing
3.Geometry
4.Meshing
5.Physics
6. Solver Settings/code development

Solve
7. Simulation solution

Post processing
8. Analysis of results

Meet the objectives

No

Yes

End (Reporting, updating repository and backing up)

Time and compute resource demanding tasks.

- ➢ Utilisation of Azure Cycle Cloud effectively and efficiently to best accomodate ARSI compute needs.
- ➢ Further support on configuration and SKU financial model.

Thank You

Example of cluster configuration

▪Example of cluster (SLURM v22.05.10) which is managed by HPC IT specialists:

- **11,960** cores/ A-100/ V100 GPUs: 299 nodes of 40-core Intel “Cascade Lake” Xeon Gold 6230 CPU @ 2.10GHz.
- All of the instruction sets available in Skylake CPUs (SSE, SSE2, SSE3, SSE4.1, SSE4.2, AVX, AVX2, AVX-512, and AVX512BW,CD,DQ,F,VL, the new AVX-512 Vector Neural Network Instructions (VNNI) for more efficient deep-learning inference calculations).
- Software is configured centralised loaded via *modules environment* on login node, then copied to compute node for job.
- 954TB scratch running (GPFS 5.0.4-2).
- InfiniBand throughout (Mellanox 100 Gb/sec (4X EDR)).#
- About 200GB home storage for user and scratch of 250GB