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CFD Simulation of Steam Axial Turbine Stage on GPU

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Agenda

- Introduction and motivation
- **SPUMA**: a portable and non-invasive **GPU porting** of OpenFOAM
- Simulating a steam turbine stage on GPU: **missing features**
- Performance on an **industrial test case**
- Conclusions

Introduction

This presentation focuses on **compressible turbomachinery OpenFOAM** simulations, executed on both **CPUs and GPUs**, unlocking the full potential of **modern heterogeneous HPC** systems.

Turbines simulations are characterized by several complexities:

- Stator-rotor interaction
- Compressible high-speed flows
- Thermophysical modelling of steam

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Motivation

- OpenFOAM is widely regarded as the **most used open-source CFD** software.
- Specific **implementations tailored to turbomachinery** are often available only as third-party separate contributions.
- **Experienced developers are needed** to integrate these contributions and add new implementations.
- CINECA is currently putting a consistent effort in **OpenFOAM GPU porting activities**.

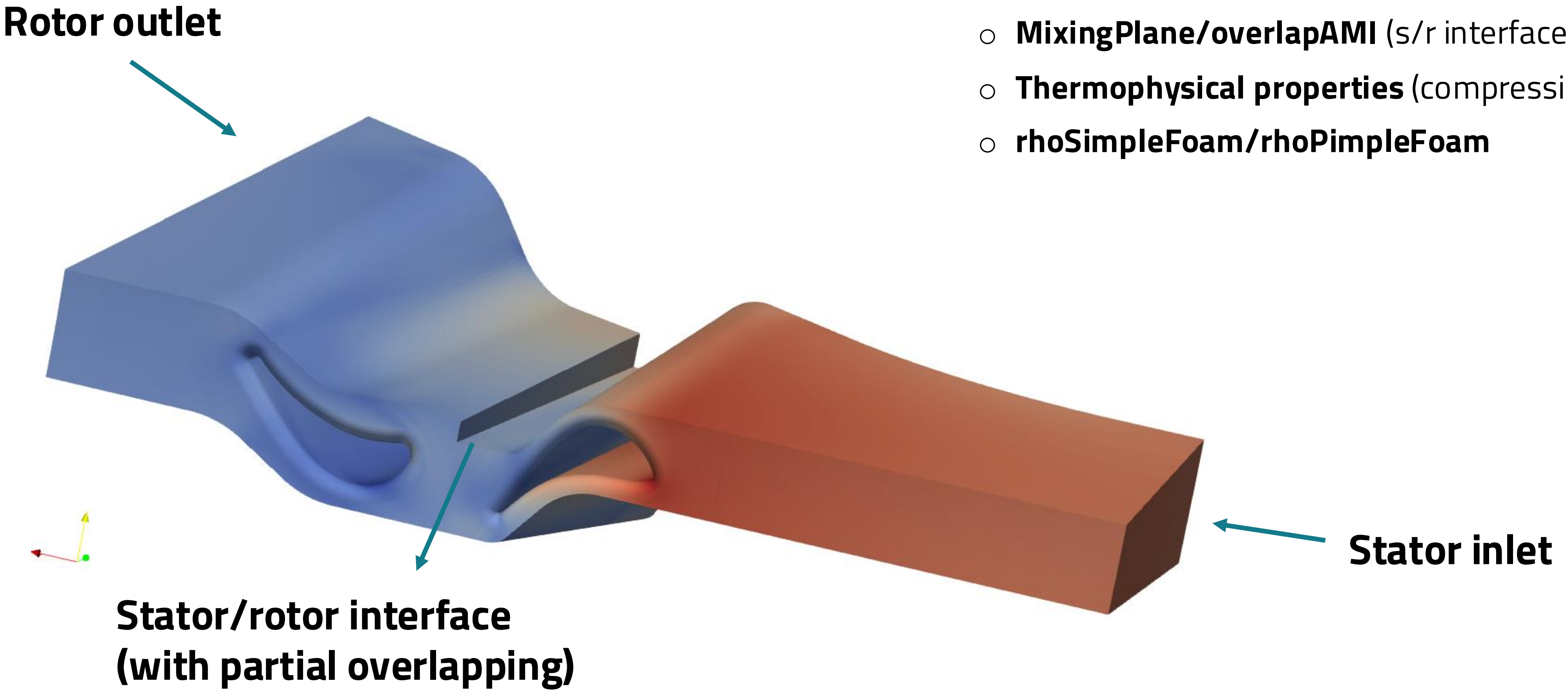
CINECA and De Pretto Industrie are collaborating to simulate turbines on CPUs

→

CINECA is porting the necessary features on GPU to execute a turbine stage pioneering analysis

Turbine stage analysis

- Simulation features:
  - **MRF** (rotor domain)
  - **MixingPlane/overlapAMI** (s/r interface)
  - **Thermophysical properties** (compressible cases)
  - **rhoSimpleFoam/rhoPimpleFoam**



CPU runs – current status

- **Final goal** -> simulating the last stages of an axial steam turbine in wet operating conditions.
- **Main third party features:**
  - **Mixing Plane** from the turboWG (credits to Hakan Nillson, Martin Beaudoin & foamExtend devs)
    https://sourceforge.net/p/turbowg/mixingPlane/ci/master/tree/
  - **OverlapAMI** from ICSFoam (credits to Stefano Oliani & foamExtend devs)
    https://github.com/stefanoOliani/ICSFoam
  - **wetSteamFoam** (credits to Jiří Fürst et al.)
    https://github.com/furstj/wetSteamFoam/tree/main
- R&D project ongoing -> **refactoring, bug-fixing and integration** of those libraries already led to satisfying results.

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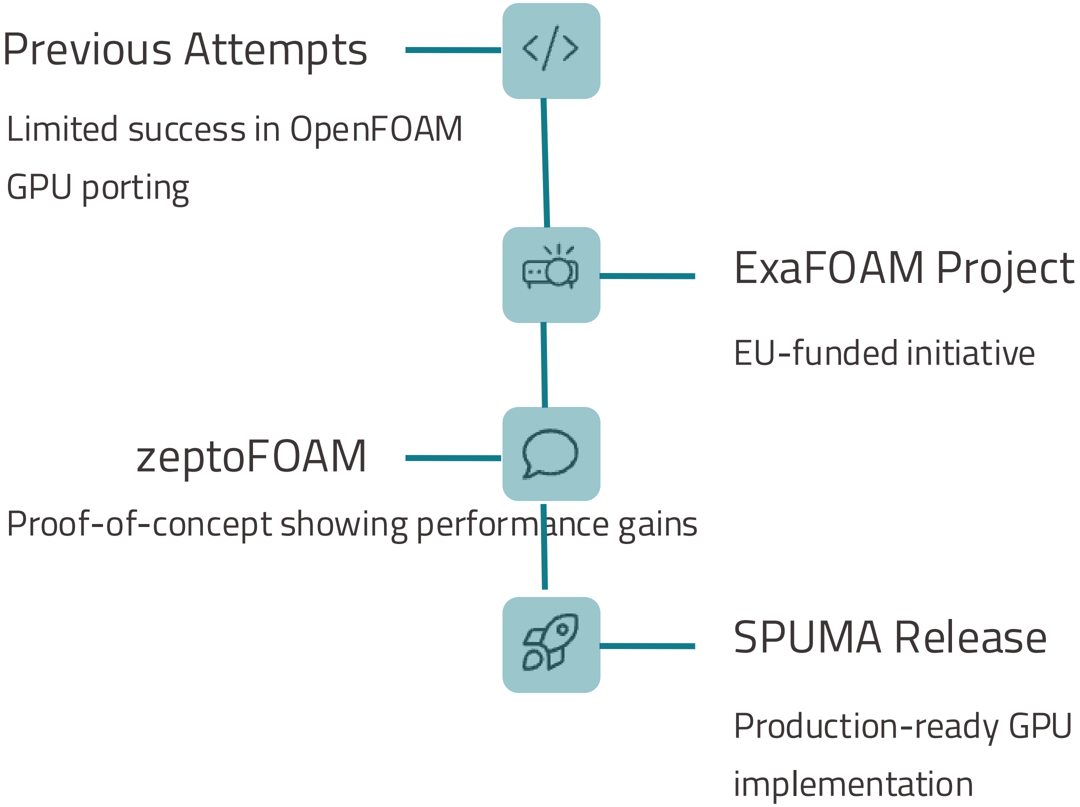
SPUMA: GPU-Ready Solution



Previous Attempts

Limited success in OpenFOAM GPU porting

ExaFOAM Project

EU-funded initiative

zeptoFOAM

Proof-of-concept showing performance gains

SPUMA Release

Production-ready GPU implementation

Minimal Code Impact

Avoid radical changes to maintain community acceptance

Efficient Memory Management

Use memory pools for GPU optimization

No External Dependencies

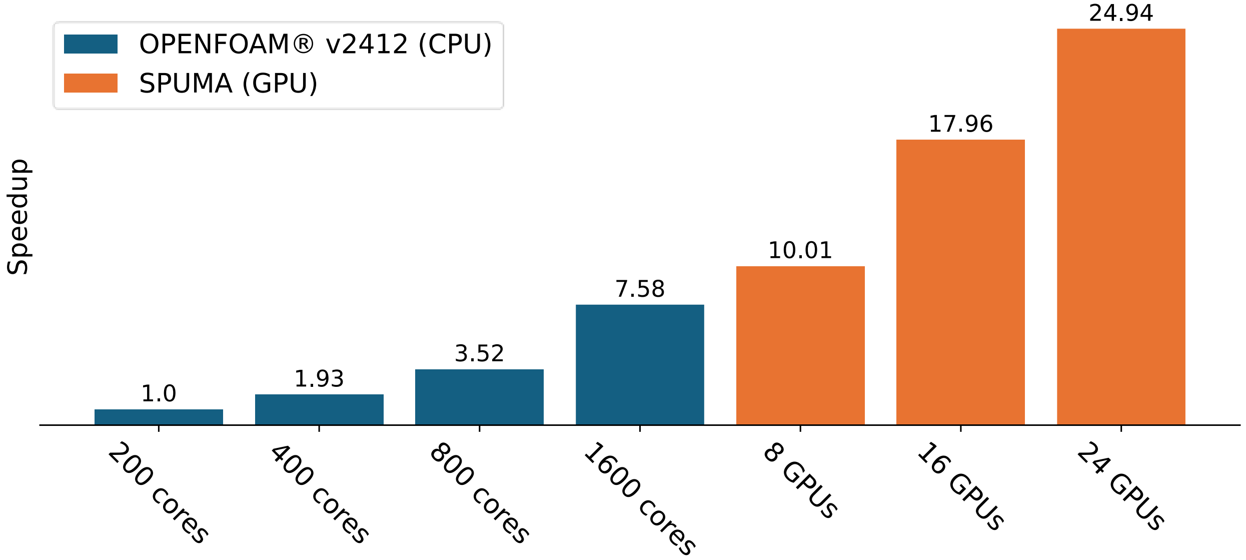
Third-party frameworks are not mandatory,

but possible (e.g., AmgX compatibility)

Multi-Platform Compatibility

Vendor-agnostic approach for wider accessibility

SPUMA performance (incompressible)



DrivAer Test Case

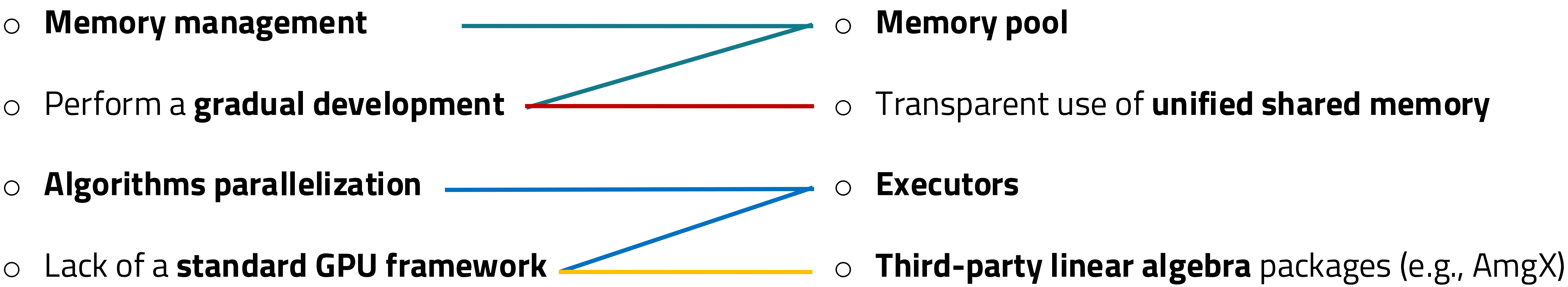
236 million cell automotive steady state simulation

1 GPU equals 220 CPU cores (1600 cores vs 24 GPUs)

This equivalence leads to **an 80% reduction of the energy** consumption

SPUMA: key features

- Major issues during a GPU porting:
- SPUMA key features



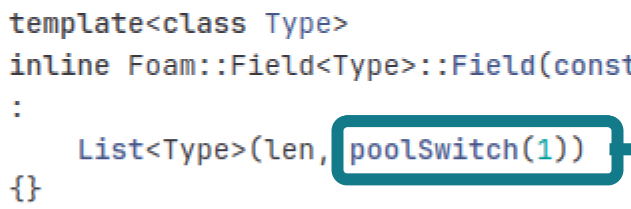
- **Memory management**
- Perform a **gradual development**
- **Algorithms parallelization**
- Lack of a **standard GPU framework**

- **Memory pool**
- Transparent use of **unified shared memory**
- **Executors**
- **Third-party linear algebra** packages (e.g., AmgX)

CINECA laid the foundations of the GPU porting by **implementing these key features**, as well as most of the **operators needed during an OpenFOAM run** (e.g., operations between Fields, GeometricFields and so on)

SPUMA: memory pool

- Foam::**Field objects** are **automatically** allocated through our memory pool APIs.



```
template<class Type>
inline Foam::Field<Type>::Field(const label len)
:
    List<Type>(len, poolSwitch(1))
{}
```

Field class constructors automatically allocate data on the pool via poolSwitch

- Unified shared memory is handling CPU->GPU and GPU->CPU copies implicitly:
  - We can **spot unported regions** of the code by profiling **CPU and GPU page faults**
  - If there are too many page faults, a **relevant slowdown** is experienced, but **the simulation is not crashing!!**

- Some OpenFOAM features use **Lists combined with Fields in computing algorithms** -> those **Lists must be allocated explicitly on the memoryPool** to avoid sudden crash of the calculation.

  - These crashes (due to invalid pointers) are <u>guiding us to spot the List</u> to be taken care of.

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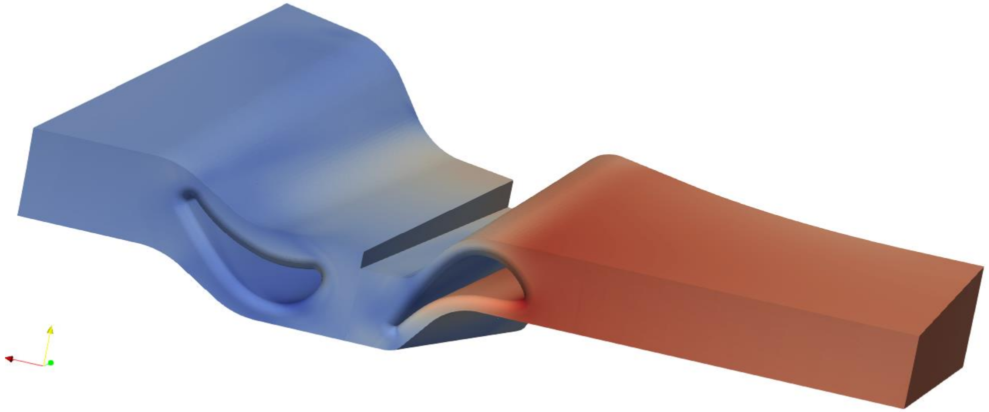
Our GPU test case

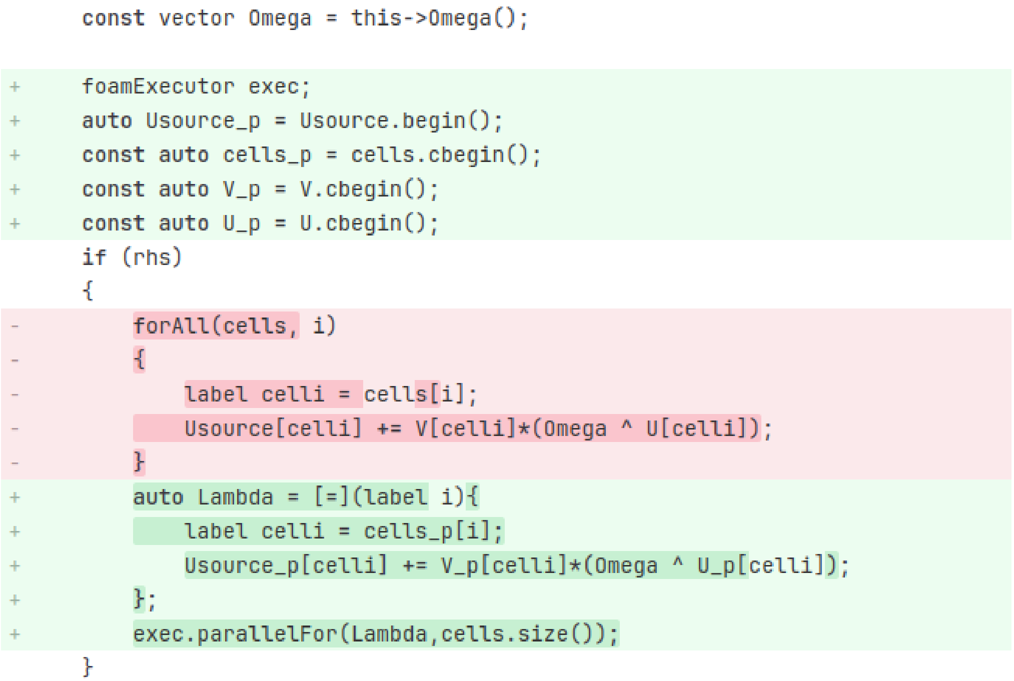
- Axial turbine – low pressure stage exploiting rotational periodicity. **Real operating conditions** (high Re, transonic, fully turbulent)
- Finite volume, second order, mesh size -> **more than 20 million cells (for a single blade periodic segment).**
- Superheated steam operating conditions (approximation)
- Needs the following features to be ported on GPU:
  - **MRF**
  - **Thermophysical models**
  - **cyclicAMI**
  - **Mixing plane/ partially overlapping interfaces.**



MRF: porting GPU

The MRF classes contain a typical example of **how we can remove page faults and speed up** the calculation.

MRFZone::addCoriolis (example)

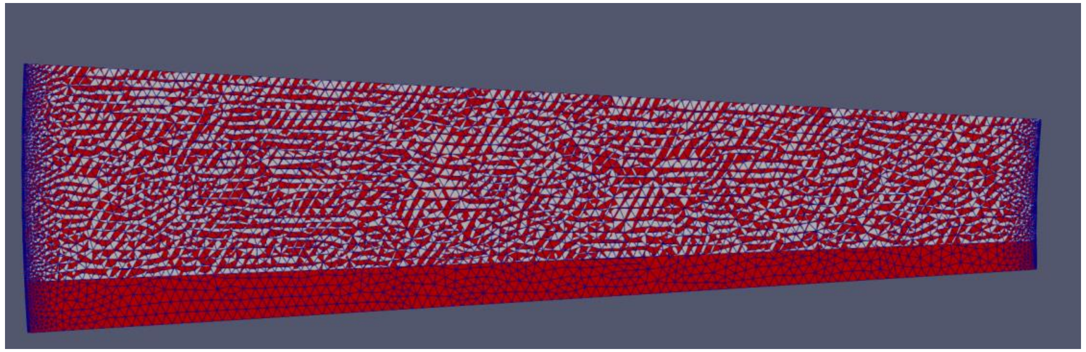


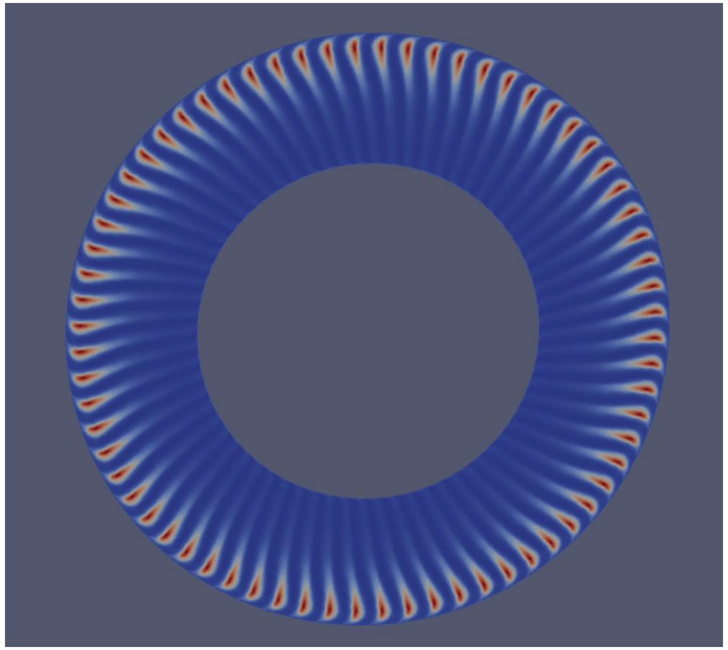
```
    const vector Omega = this->Omega();

+   foamExecutor exec;
+   auto Usource_p = Usource.begin();
+   const auto cells_p = cells.cbegin();
+   const auto V_p = V.cbegin();
+   const auto U_p = U.cbegin();
    if (rhs)
    {
-       forAll(cells, i)
-       {
-           label celli = cells[i];
-           Usource[celli] += V[celli]*(Omega ^ U[celli]);
-       }
+       auto Lambda = [=](label i){
+           label celli = cells_p[i];
+           Usource_p[celli] += V_p[celli]*(Omega ^ U_p[celli]);
+       };
+       exec.parallelFor(Lambda,cells.size());
    }
```

- Explicit **forAlls are originally executed** on the CPU, producing unwanted copies.
- We construct a **lambda expression**, copy pass all the pointers and ship the content to the SPUMA executor.
- In this case, the forAll corresponds to a **parallelFor** method of the executor.

overlapAMI: optimize the code while porting it

- OverlapAMI can be exploited to run **frozen rotor** simulations when **domains are partially overlapped.**
- Example:
  - Rotor -> 66 blades
  - Stator -> 51 blades

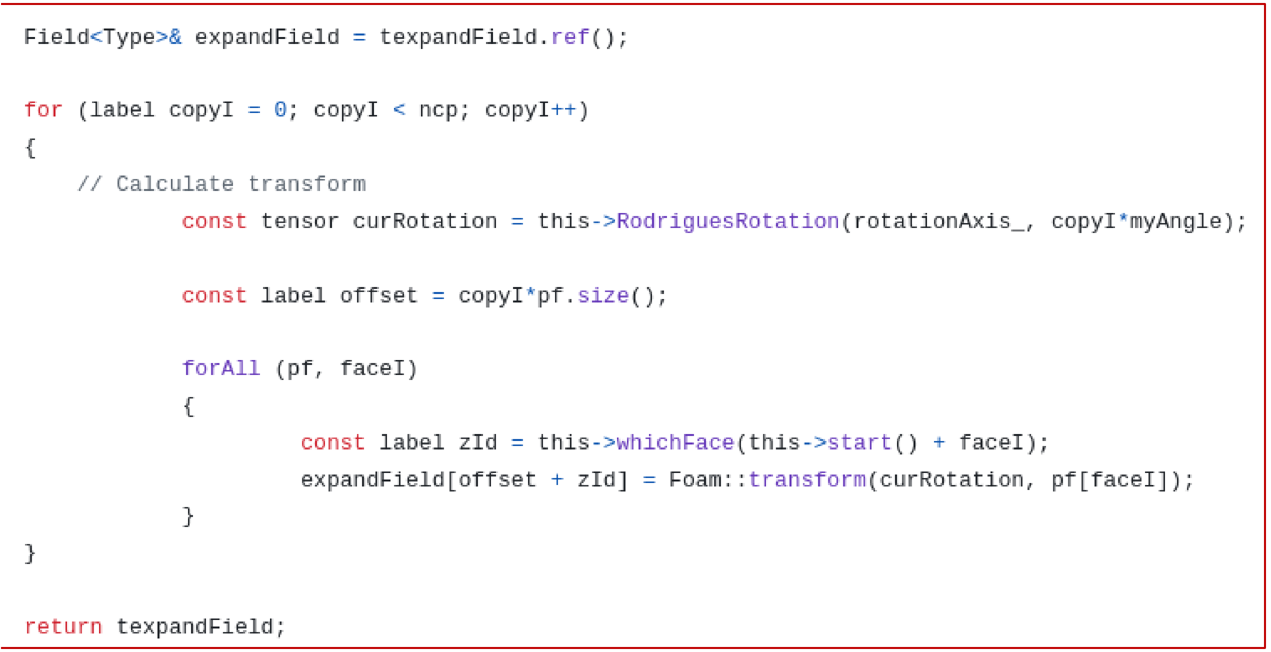




Both patches are expanded periodically to obtain a 360° patch, then the AMI interpolation is performed.

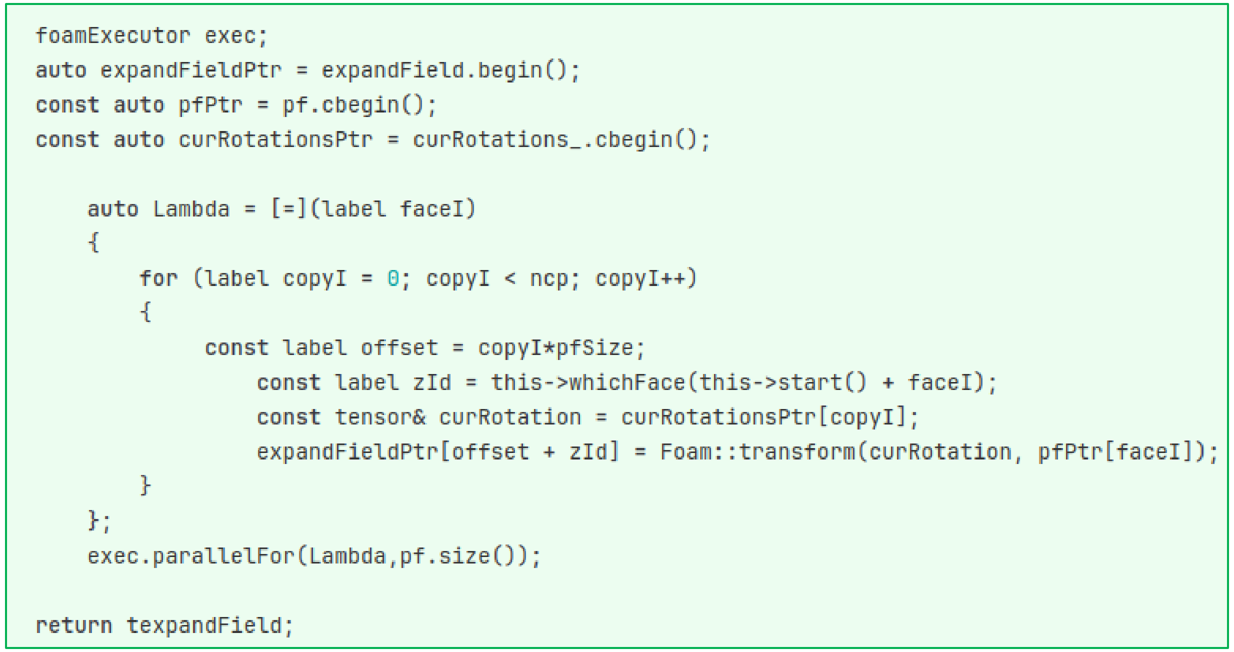
overlapAMI: optimize the code while porting it

overlapAMIPolyPatch::expandData



```
Field<Type>& expandField = texpandField.ref();

for (label copyI = 0; copyI < ncp; copyI++)
{
    // Calculate transform
            const tensor curRotation = this->RodriguesRotation(rotationAxis_, copyI*myAngle);

            const label offset = copyI*pf.size();

            forAll (pf, faceI)
            {
                    const label zId = this->whichFace(this->start() + faceI);
                    expandField[offset + zId] = Foam::transform(curRotation, pf[faceI]);
            }
}

return texpandField;
```

Original

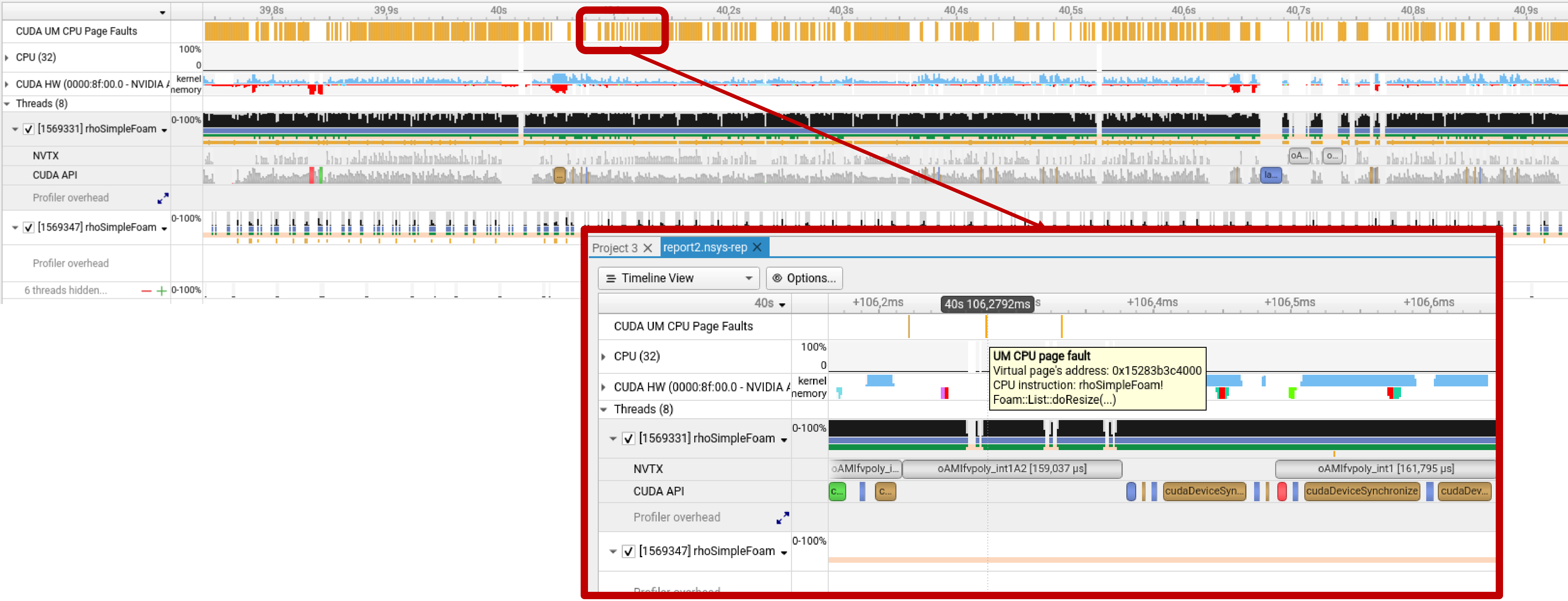


```
foamExecutor exec;
auto expandFieldPtr = expandField.begin();
const auto pfPtr = pf.cbegin();
const auto curRotationsPtr = curRotations_.cbegin();

    auto Lambda = [=](label faceI)
    {
        for (label copyI = 0; copyI < ncp; copyI++)
        {
             const label offset = copyI*pfSize;
                 const label zId = this->whichFace(this->start() + faceI);
                 const tensor& curRotation = curRotationsPtr[copyI];
                 expandFieldPtr[offset + zId] = Foam::transform(curRotation, pfPtr[faceI]);
        }
    };
    exec.parallelFor(Lambda,pf.size());

return texpandField;
```

GPU ported

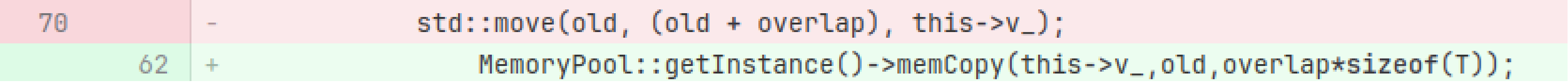
- The baseline kernel is again a **parallelFor.**
- We precalculate a rotation tensorField (curRotations_) and move the copyI loop inside the kernel, strongly **reducing the number of GPU kernels launched during the calculation**.

overlapAMI: optimize the code while porting it



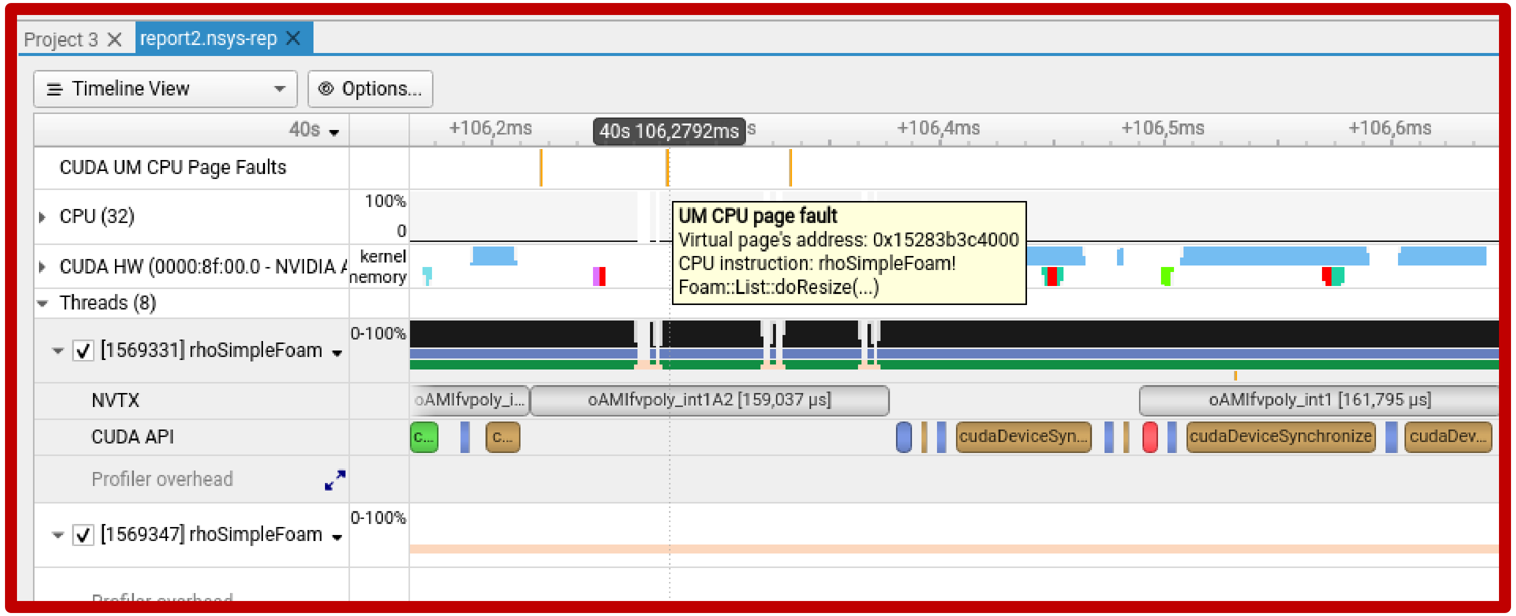
UM CPU page fault
Virtual page's address: 0x15283b3c4000
CPU instruction: rhoSimpleFoam!
Foam::List::doResize(...)

overlapAMI: optimize the code while porting it



```
-            std::move(old, (old + overlap), this->v_);
+                MemoryPool::getInstance()->memCopy(this->v_,old,overlap*sizeof(T));
```

List::doResize



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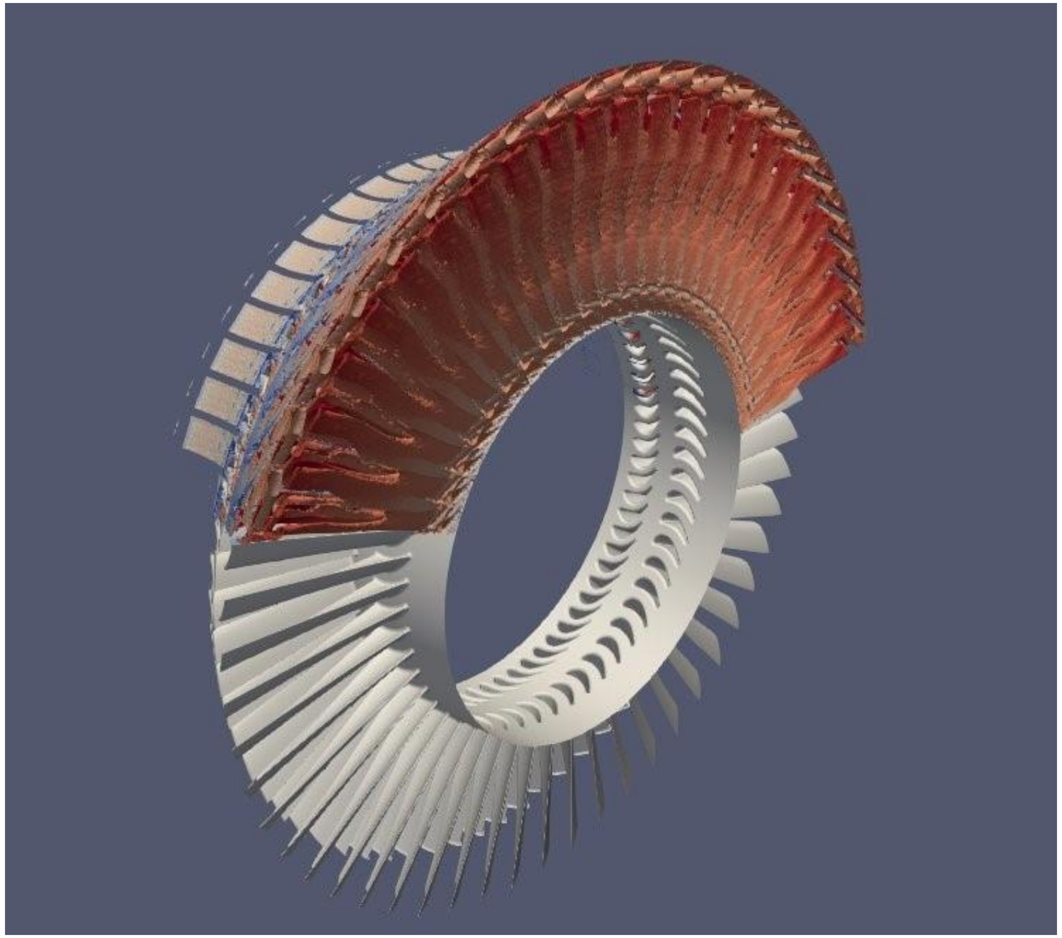
CPU runs

- Test case executed on both Galileo100 and Leonardo DCGP HPC systems.
- The simulations converge smoothly at the testing conditions provided by the industrial end-user.
- Steady RANS (Reynolds Averaged Navier Stokes) simulation wall time ranges from 5 to 8 hours on 2 nodes of G100
- 1 G100 node = 2 x CPU Intel CascadeLake 8260, with 24 cores each)



Performance comparison

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GPU run

- Time per iter = 2.07 s
- N GPUS = 1 NVIDIA A100

CPU run #0

- Time per iter = 8.625 s
- N cores = 48 (Leonardo DCGP)

CPU run #1

- Time per iter = 6.755 s
- N cores = 96 (Leonardo DCGP)

CPU run #2

- Time per iter = 6.135 s
- N cores = 192 (Leonardo DCGP)

Cores per GPU ratio

*timeCPU*coresCPU / timeGPU* nGPU*

Cores per GPU ratio (run #0) = 200

Cores per GPU ratio (run #1) = **313**

Cores per GPU ratio (run #2) = 569

Warning: the coresPerGPU indicator can be easily altered by variating the CPU conditions

Performance breakdown

GPU run

Step	**% of Total Time**
Simple loop	**100.00%**
Uassembly	**23.17%**
Upredictor	**1.23%**
Usolve	**7.75%**
Eassembly	**20.60%**
Esolve	**1.80%**
ThermoCorrect	**0.05%**
Passembly	**2.82%**
Psolve	**7.52%**
Turbo correct	**26.74%**

CPU run #1

Step	**% of Total Time**
Simple loop	**100.00%**
Uassembly	**25.00%**
Upredictor	**1.29%**
Usolve	**5.33%**
Eassembly	**20.48%**
Esolve	**1.49%**
ThermoCorrect	**0.09%**
Passembly	**2.34%**
Psolve	**3.78%**
Turbo correct	**31.37%**

Performance vs mixingPlane

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GPU run - overlapAMI

Step	% of Total Time
Simple loop	**100.00%**
Uassembly	**23.17%**
Upredictor	**1.23%**
Usolve	**7.75%**
Eassembly	**20.60%**
Esolve	**1.80%**
ThermoCorrect	**0.05%**
Passembly	**2.82%**
Psolve	**7.52%**
Turbo correct	**26.74%**

CPU run - mixingPlane

Step	% of Total Time
Simple loop	**100.00%**
Uassembly	**22.25%**
Upredictor	**1.23%**
Usolve	**6.09%**
Eassembly	**20.28%**
Esolve	**1.84%**
ThermoCorrect	**0.15%**
Passembly	**2.89%**
Psolve	**4.67%**
Turbo correct	**32.45%**

Cores per GPU ratio = **180**

Conclusions

- The compressible axial turbine test case **run successfully on CPU** after the required **software integration/development activities**.

- **SPUMA**, a recent development by CINECA, already supported most of the OpenFOAM features needed to simulate the test case.

- **GPU porting of missing features has been performed** working on:
  1. MRF
  2. Thermophysical models
  3. cyclicAMI and overlapAMI
  4. Velocity and temperature limiters

- The resulting **cores to GPU ratio (approx. 2-300)** is in line with results obtained in incompressible cases.

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Thank you for your attention!