Accelerating the FlowSimulator: Tracing and Profiling of Python Toolchains for Industry-Grade Simulations

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Goal: green aviation

EU FlightPath 2050

- 75 % CO₂ reduction
- 90 % NO_x reduction
- 65 % noise reduction
- => Radically different aircraft designs needed

Aircraft development & certification

Flight envelope analyses requires:

- > 10,000 data points
- > 1,000 flight hours
- > 100 steady-state, high-fidelity simulations

Motivation for simulations



• Simulations with acceptable accuracy **may** replace costly/unfeasible testing

5.5 Engineering Analysis. An engineering analysis that includes the effects of the ice accretions as defined in Part II of Appendix C and Appendix O to CS-25 may be used to substantiate the performance and handling characteristics. The

- Aeroelastic problems can be modelled with fluid-structure interaction simulations:
 - CFD solver
 - CSM solver
 - Interpolation
 - Mesh deformation
- **High-performance computing** can be exploited to reach **acceptable time-to-solution** of high-fidelity simulations

Trend in HPC computational resources







* Schwammborn et al "The DLR TAU-code: recent applications in research and industry," *ECCOMAS 2006* **https://commonresearchmodel.larc.nasa.gov/

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Measurement platform

CARO

- DLR HPC System
- 174,592 cores
- #135 Top500 (11/2021)
- Göttingen (DE)
- each node:
 - 2x AMD EPYC 7702 (64 cores)
 - RAM: 256 GB DDR4
 - 16 cores per NUMA domain
 - 16 MB L3 cache shared among 4 cores



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FlowSimulator



Simulation frameworks for multidisciplinary analyses and optimizations





&



Innovative simulation softwares for high-fidelity predictions on **HPC**



Test case



Steady aeroelastic equilibrium of LANN wing* semispan=1 m, chord=0.361÷0.144 m

non-linear

CFD solve

static

structural

deformation

interpolate

deformation

to CFD

mesh

- CFD mesh: 10⁶ elements, 1.2 10⁶ nodes
- CSM mesh: 860 elements, 1260 nodes

repartition

meshes

interpolate

loads to

CSM mesh



*Firth, George C. "LANN wing design." NASA. Langley Research Center Cryogenic Wind Tunnel Models (1983).

Yes

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load meshes

compute

CSM loads

**Cristofaro, et al. "Accelerating the FlowSimulator: Improvements in FSI simulations for the HPC exploitation at industrial level," Coupled 2023

converged?

No

FlowSimulator code structure and Score-P Python binding



core-



py-scorep-binding compiler problem



On CARO:

> spack load py-scorep-binding

> module load flowsim

> python -m scorep script.py : command ['/usr/bin/cc', '-c', '.../scorep_init.c', ...] failed

Problem:

py-scorep-binding wants to use /usr/bin/cc, but

> which cc : /usr/bin/cc > which gcc : /sw/rev/23.05/linux-rocky8-zen/gcc-8.5.0/gcc-10.4.0-xozig6/bin/gcc

Workaround:

```
In subsystem.py under py-scorep-binding installation folder add:
cc.set_executable("compiler", "gcc")
cc.set_executable("compiler_so", "gcc")
```

Only Python wrapping (no instrumentation)

Ready to use sbatch:

spack load py-scorep-binding
module load flowsim
srun python -m scorep --mpp=mpi --thread=omp script.py

Master thread:0						
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Runtime distribution (2 MPI x 4 OpenMP)



- MPI* filtered out
- Most time consuming simulation blocks:
 - *CFD*
 - MeshDeformation
- Negligible simulation blocks:
 - MeshImport
 - *CSM*
 - Interpolation
 - MeshExport



Strong scaling of steady aeroelastic simulation



"Manual" measurements need:

- Predict relevant simulation blocks
- Print runtimes
- Extract for plotting

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Strong scaling with only Python wrapping

From 2 MPIs to 512 MPIs

- main blocks runtime decrease:
 - *CFD*
 - MeshDeformation
- new blocks appears:
 - *importlib* (one time)
 - *MeshOps* for reading meshes (one time)
 - *MeshSelection* for interpolation (mostly init phase)

Not analysed with "manual" scaling measurements



Missing info in Cpp plugins

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Cpp plugins tracing requires:

- Score-P wrapper should work with all plugins build systems (implementation effort)
- Re-build everything with Score-P wrapper (a few hours)
- Define Score-P filters to limit trace size (automatic with scorep-score -g or manual)

Traces with no code instrumentation



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6 FSDL	RControl.Scenarios.CFDSolverTAU.	CFDSolverTAUSteady:Run		Fn FS	DLRContrSteady:Run F	n FSDLRContrSteady:Run	
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8 FSDL	RControl.Scenarios.CFDSolverTAU.	CFDSolverTAUSteady: RunSolve	er	Fr FS	DLRContro: RunSolver	FSDLRContro: RunSolve	
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13 FSDL	RControl.PluginControl.APIMethod:	InternalWrapper		FS	DLRContrnalWrapper	FSDLRContrnalWrapper	
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15 FSDL	LRControl.TauControl:SolverLoop	FSDLRControl.TauControl.TauCo	ontrol:SolverLoop	FS	DLRContrSolverLoop	FSDLRContrSolverLoop	
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Traces with Cpp instrumentation

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Focusing on MeshDeformation



- ConvertMatrix 73 s
 - 27% of *MeshDeformation* runtime
 - More than *FEMAssembler*
 - 16.5 s: MPI_Barrier

Matrix conversion algorithm improvement (2 MPI x 4 OpenMP)



Original algorithm



Conclusion



- Tracing of steady aeroelastic simulations
 - industrial-grade toolchain
 - aircraft design and certification with HPC
 - *FlowSimulator* (>50 plugins)
- Only Python binding
 - Readily available with pre-installed software
 - Good overview of main simulation blocks runtime
 - No info about Cpp implementations
- With instrumentation
 - Time consuming:
 - work to fit all build systems
 - re-build everything
 - define filters
 - Large traces
 - => beneficial to specific code analyses









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The authors gratefully acknowledge the scientific support and HPC resources provided by the German Aerospace Center (DLR). The HPC system CARO is partially funded by "Ministry of Science and Culture of Lower Saxony" and "Federal Ministry for Economic Affairs and Climate Action"