Accelerating the FlowSimulator:

Tracing and Profiling of Python Toolchains for Industry-Grade Simulations

Cristofaro Marco, Wendler Johannes, Reimer Lars, Huismann Immo

German Aerospace Center (DLR) – Dresden & Brunswick

Goal: green aviation

EU FlightPath 2050

- 75 % CO_2 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

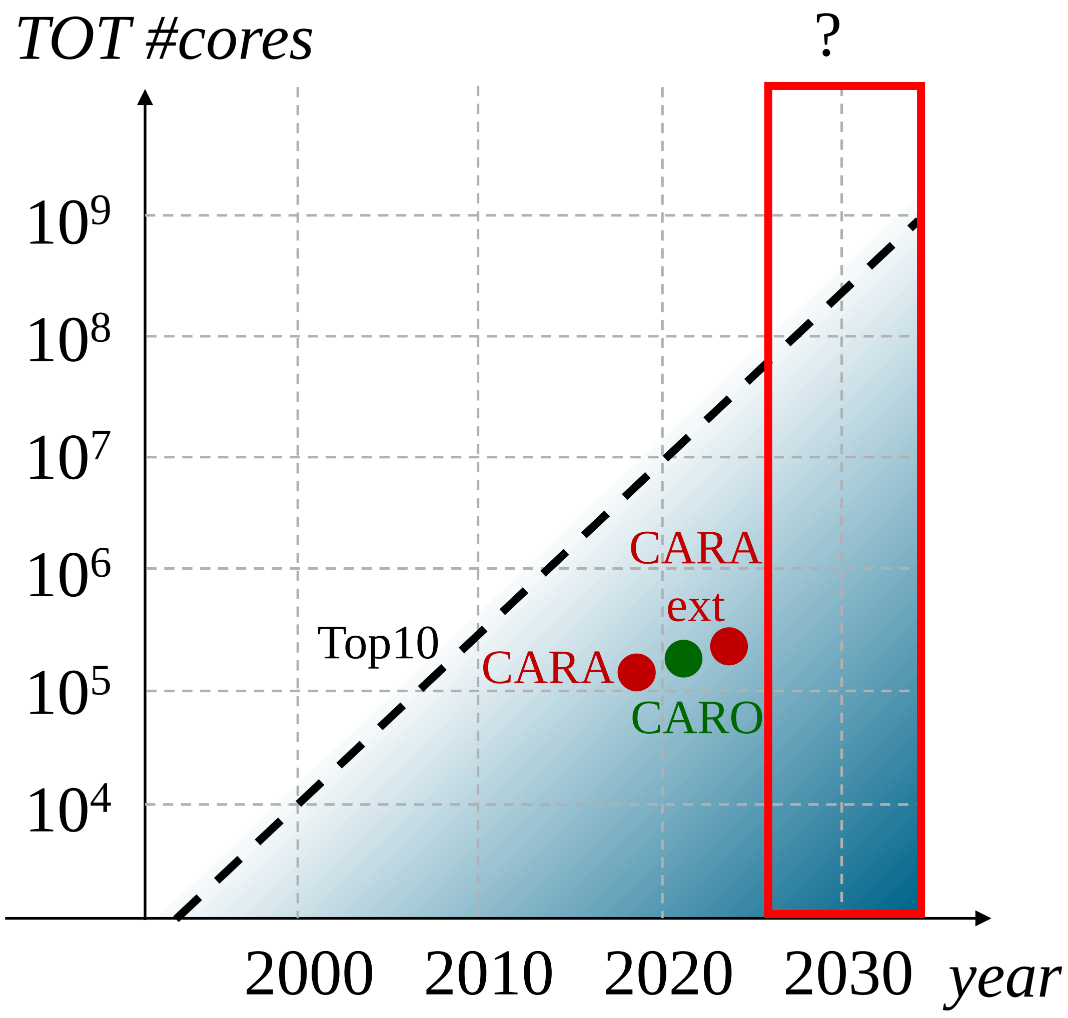
- Simulations with acceptable accuracy **may** replace costly/unfeasible testing

> 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



Increase in resources

↓

shorter time-to-solution

&

larger meshes

2006	*A380**	*~50 10^6 elements*
2024	*HLPW5***	*~1.2 10^9 elements*

BUT WE NEED

SCALABLE SOFTWARE!

* Schwammborn et al "The DLR TAU-code: recent applications in research and industry," *ECCOMAS 2006*

***https://commonresearchmodel.larc.nasa.gov/*

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

CARO node

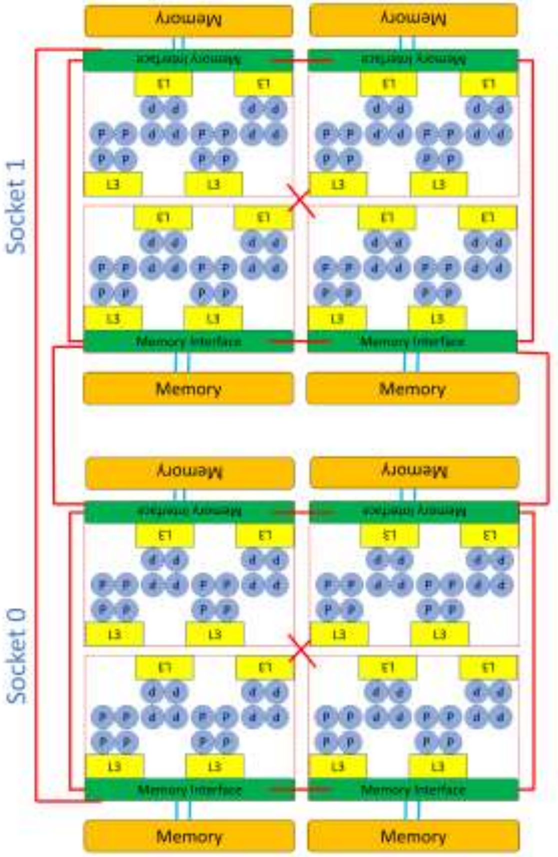


Image by Hirav Patel

FlowSimulator

Simulation frameworks for **multidisciplinary analyses** and optimizations

&

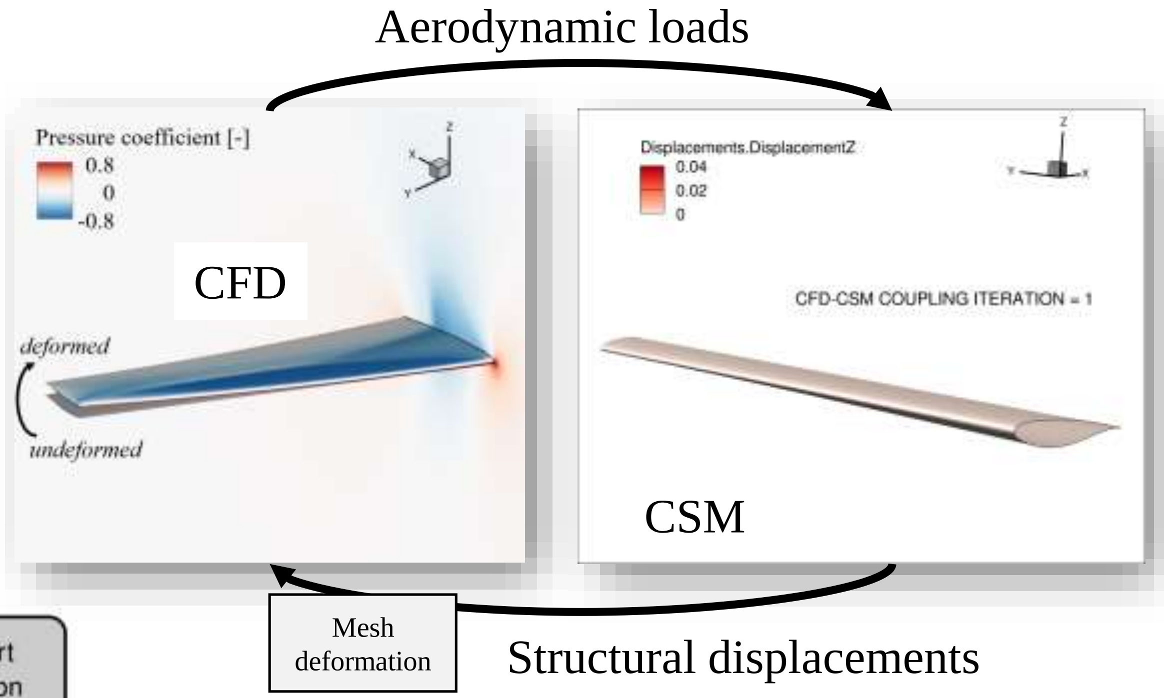
Innovative simulation softwares for high-fidelity predictions on **HPC**

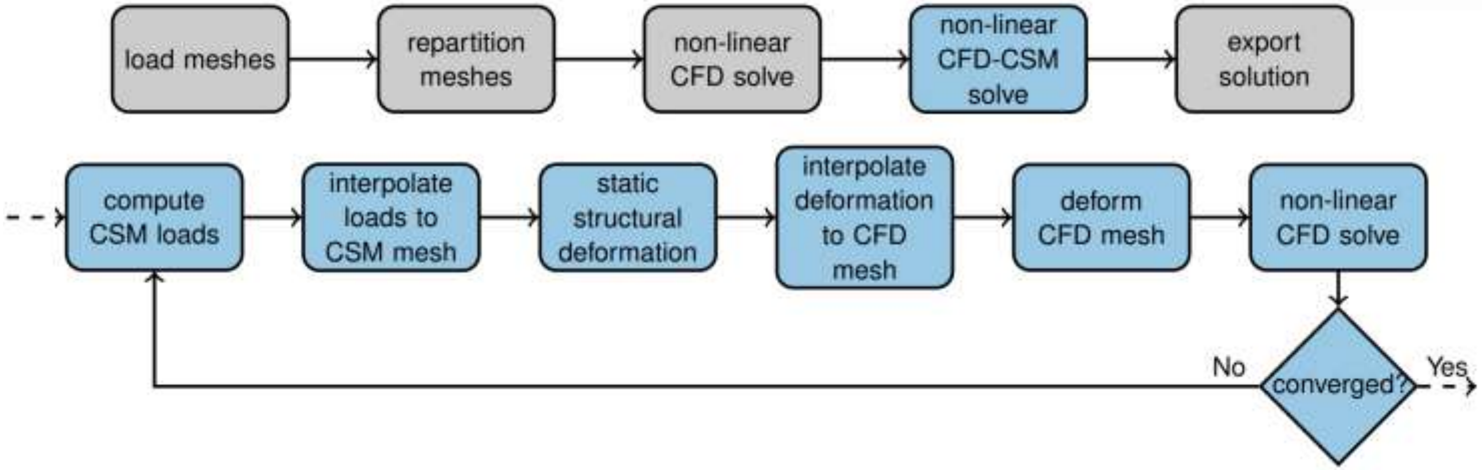
Test case

Steady aeroelastic equilibrium of LANN wing*

semispan=1 m, chord=0.361÷0.144 m

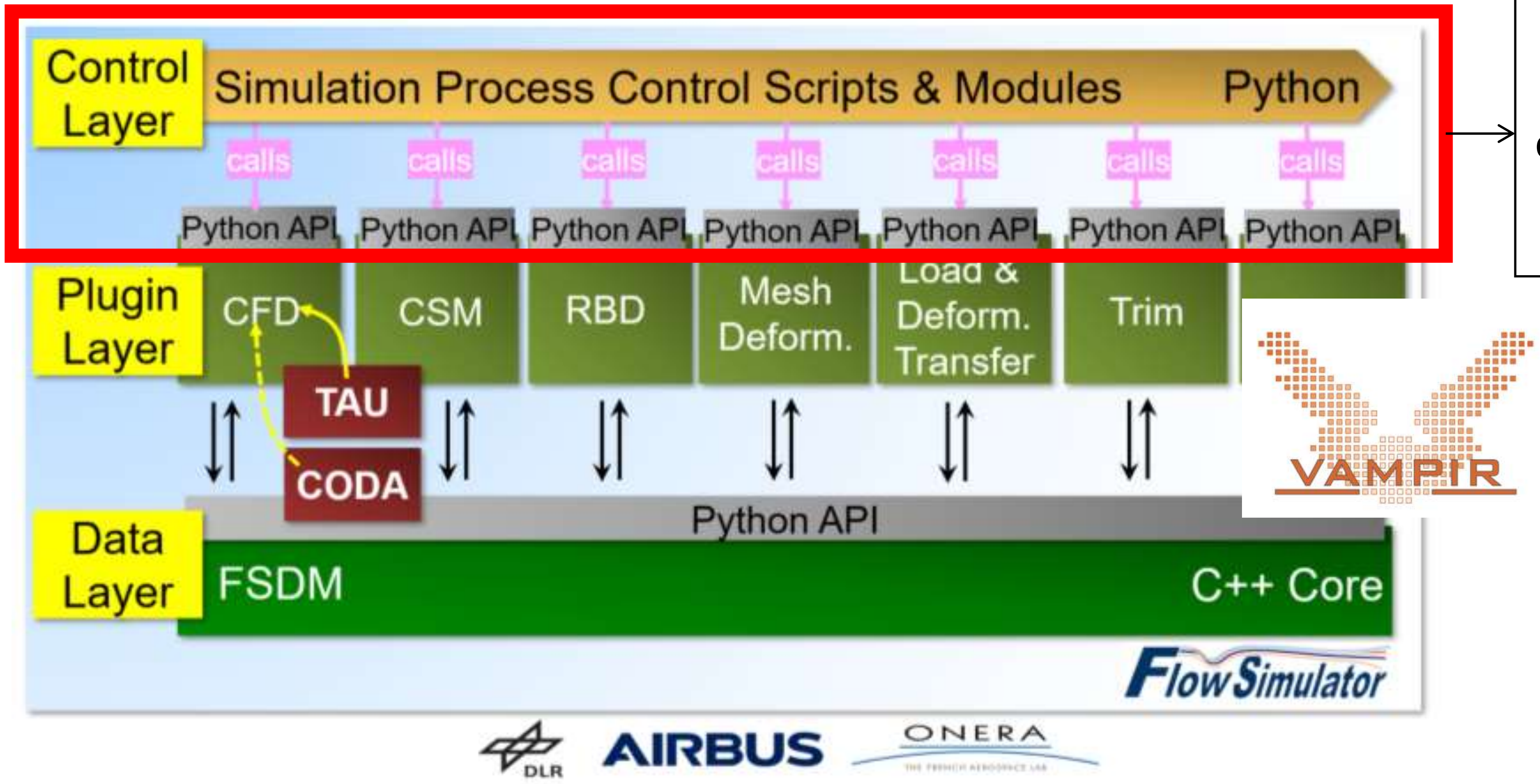
- **CFD mesh:** 10^6 elements, 1.2 10^6 nodes
- **CSM mesh:** 860 elements, 1260 nodes





*Firth, George C. "LANN wing design." *NASA. Langley Research Center Cryogenic Wind Tunnel Models* (1983).
**Cristofaro, et al. "Accelerating the FlowSimulator: Improvements in FSI simulations for the HPC exploitation at industrial level," *Coupled 2023*

FlowSimulator code structure and Score-P Python binding



py-scorep-binding
can profile and trace
complex simulation toolchains:

```
python -m scorep script.py
```

Load trace with **Vampir**

Runtime overview with almost no effort

*Reimer et al "Virtual Aircraft Technology Integration Platform: Ingredients for Multidisciplinary Simulation and Virtual Flight Testing." *AIAA 2021*

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:

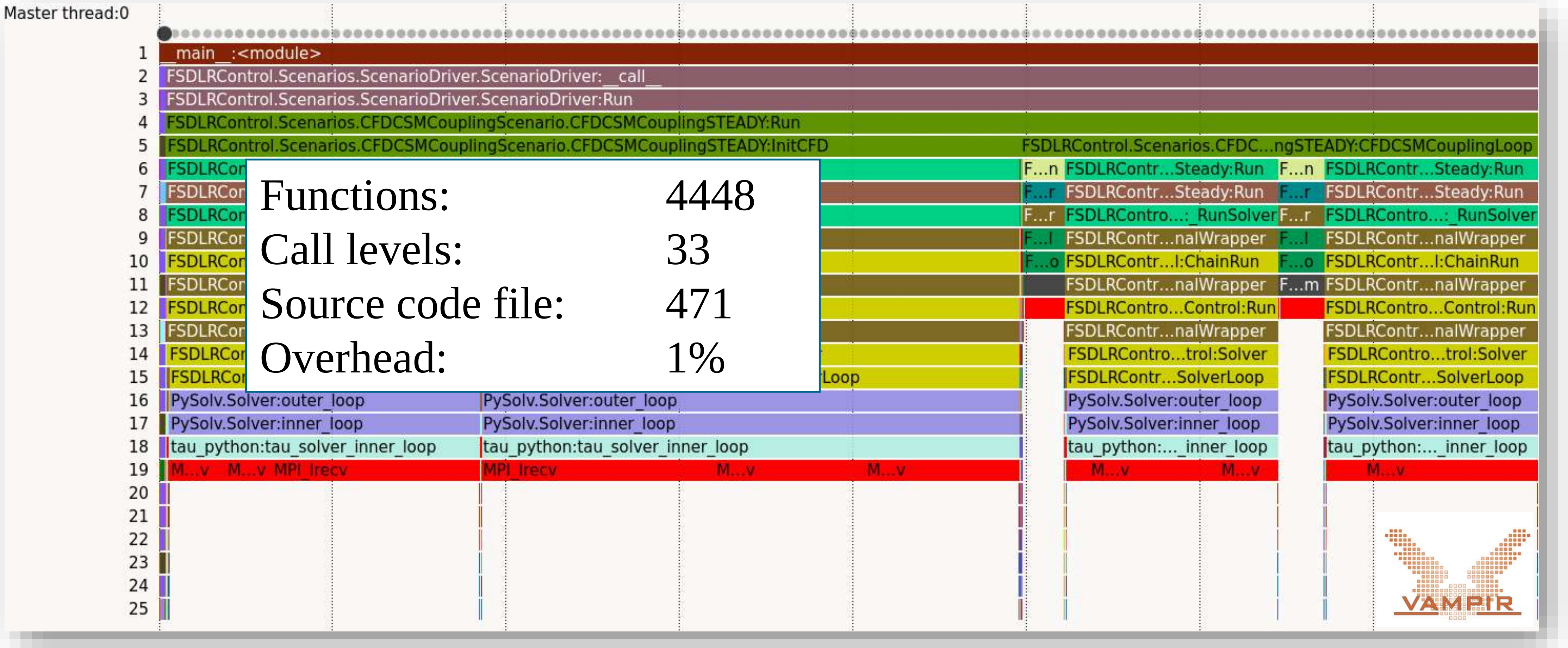
In subsystem.py under py-scorep-binding installation folder add:

```
cc.set_executable("compiler", "gcc")
cc.set_executable("compiler_so", "gcc")
```

Only Python wrapping (no instrumentation)

Ready to use sbatch:

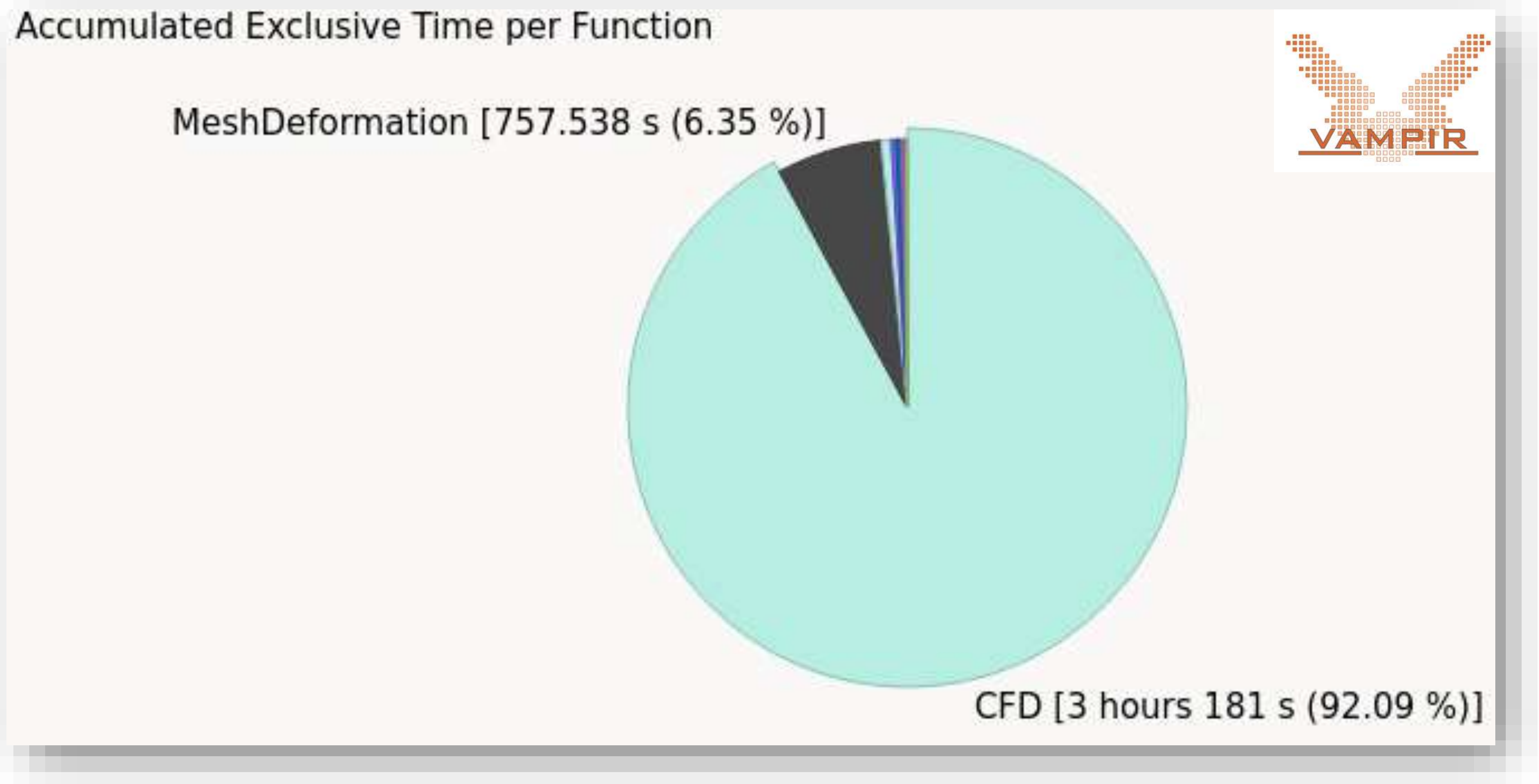
```
spack load py-scorep-binding
module load flowsim
srun python -m scorep --mpp=mpi --thread=omp script.py
```



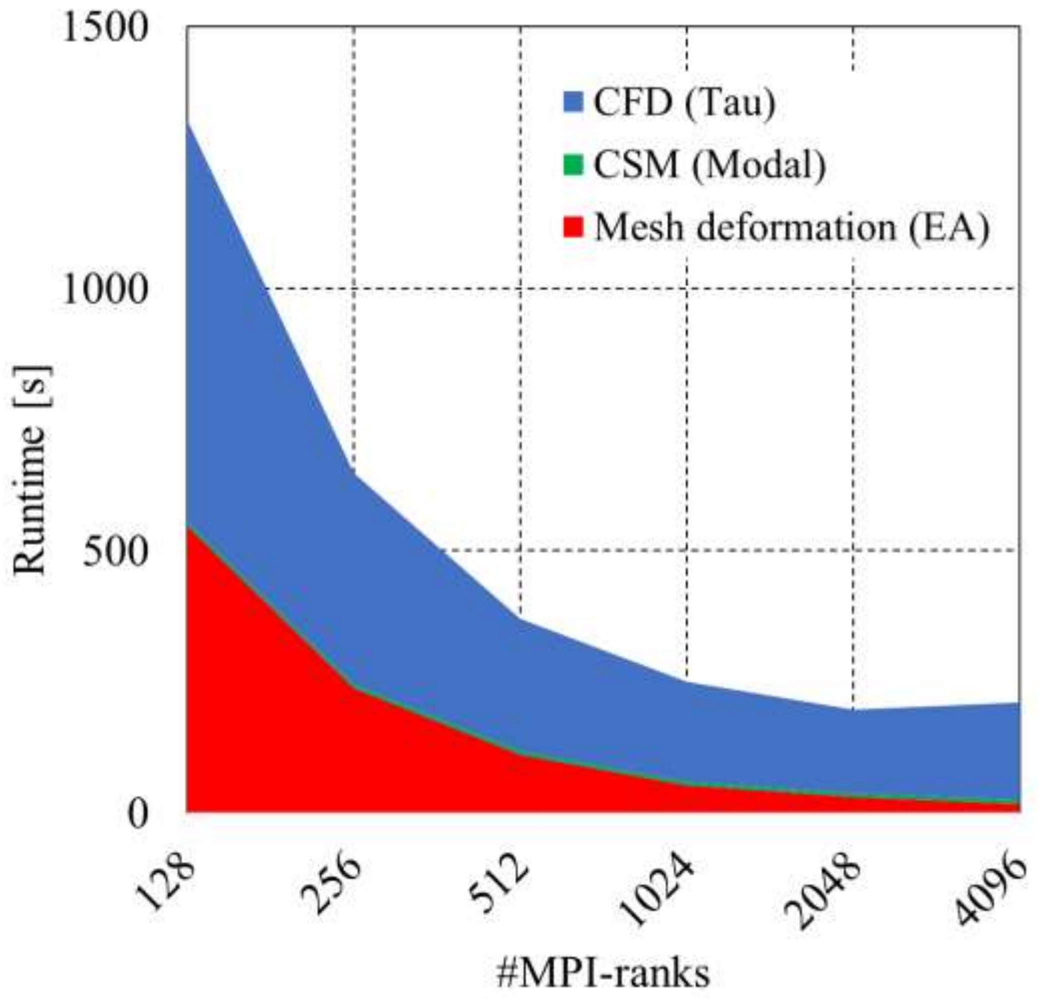
Functions:	4448
Call levels:	33
Source code file:	471
Overhead:	1%

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

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

Strong scaling with only Python wrapping

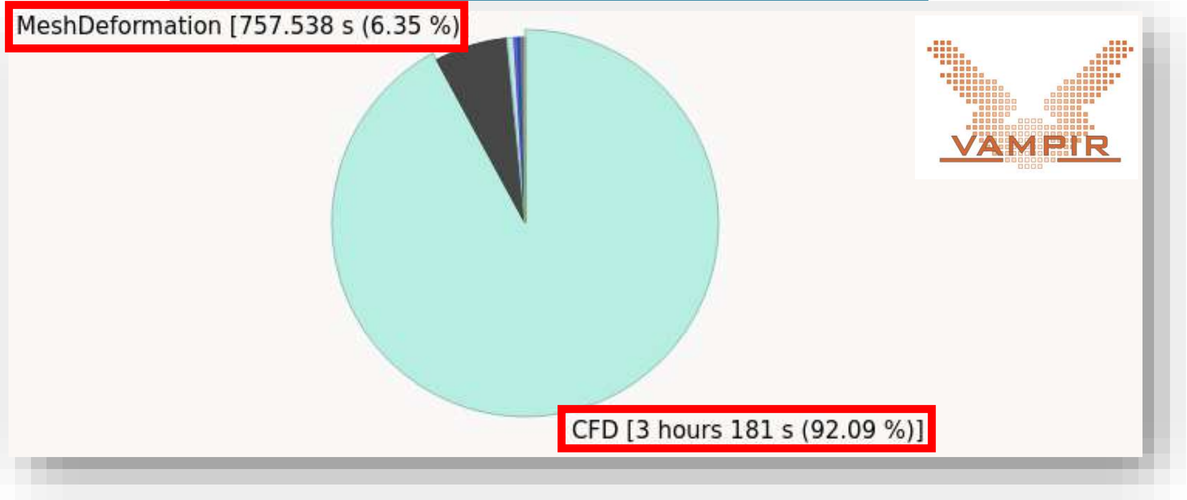
From 2 MPIs to 512 MPIs

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

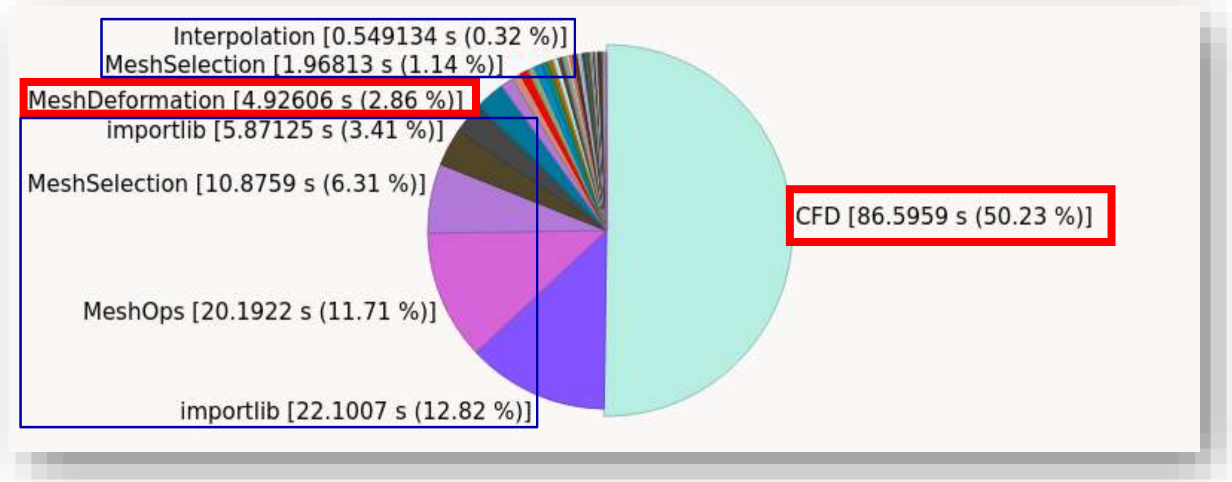
↓

Not analysed with "manual" scaling measurements

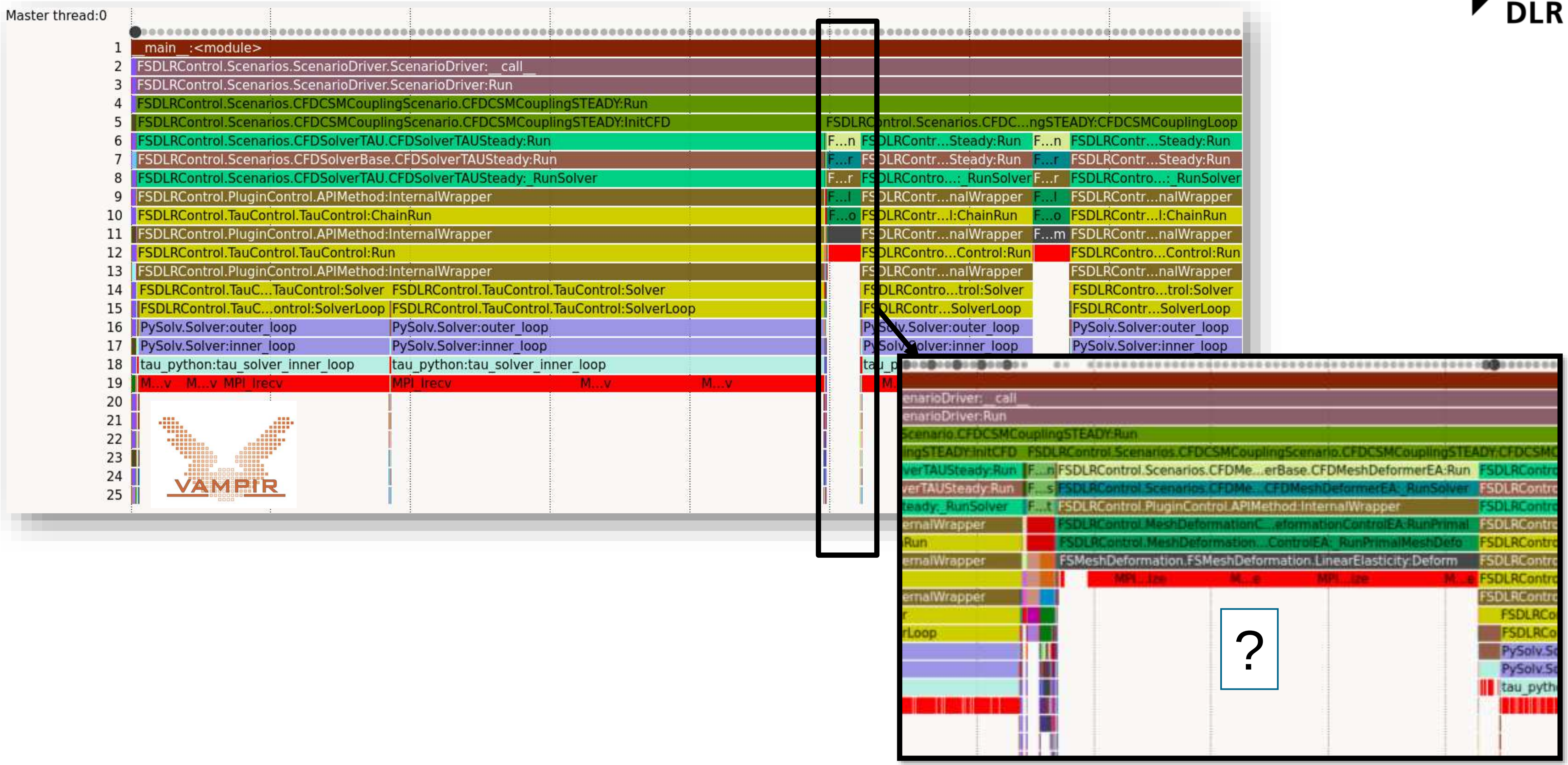
1 node x 2 MPI x 4 OpenMP



16 node x 32 MPI x 4 OpenMP



Missing info in Cpp plugins



Cpp instrumentation for Score-P

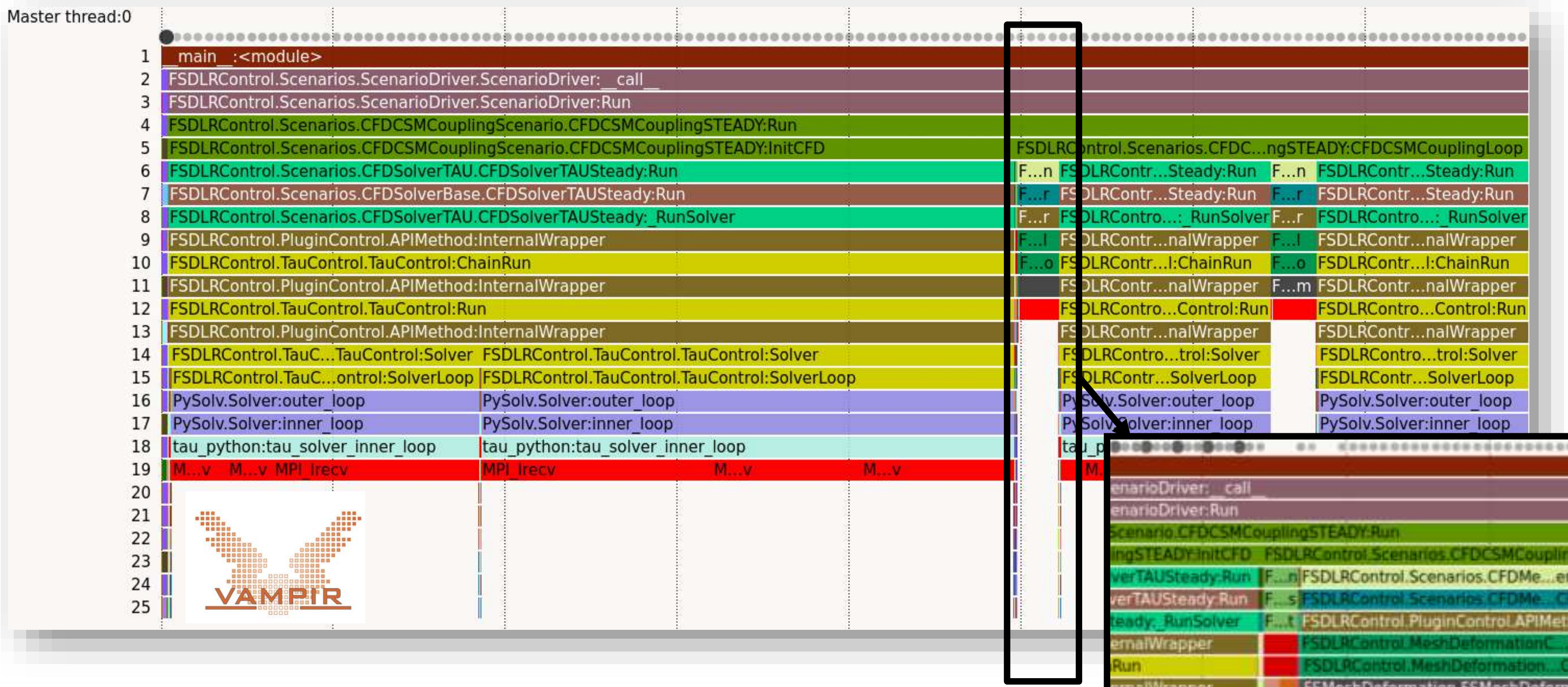
Cpp plugins tracing requires:

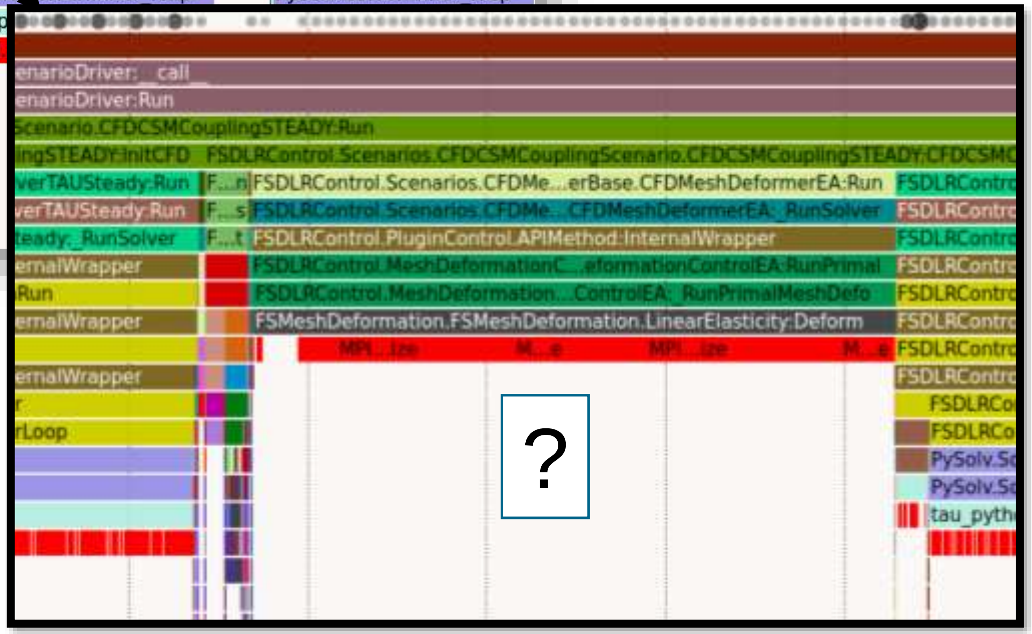
- Score-P wrapper should work with all plugins build systems
  (implementation effort)

- 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

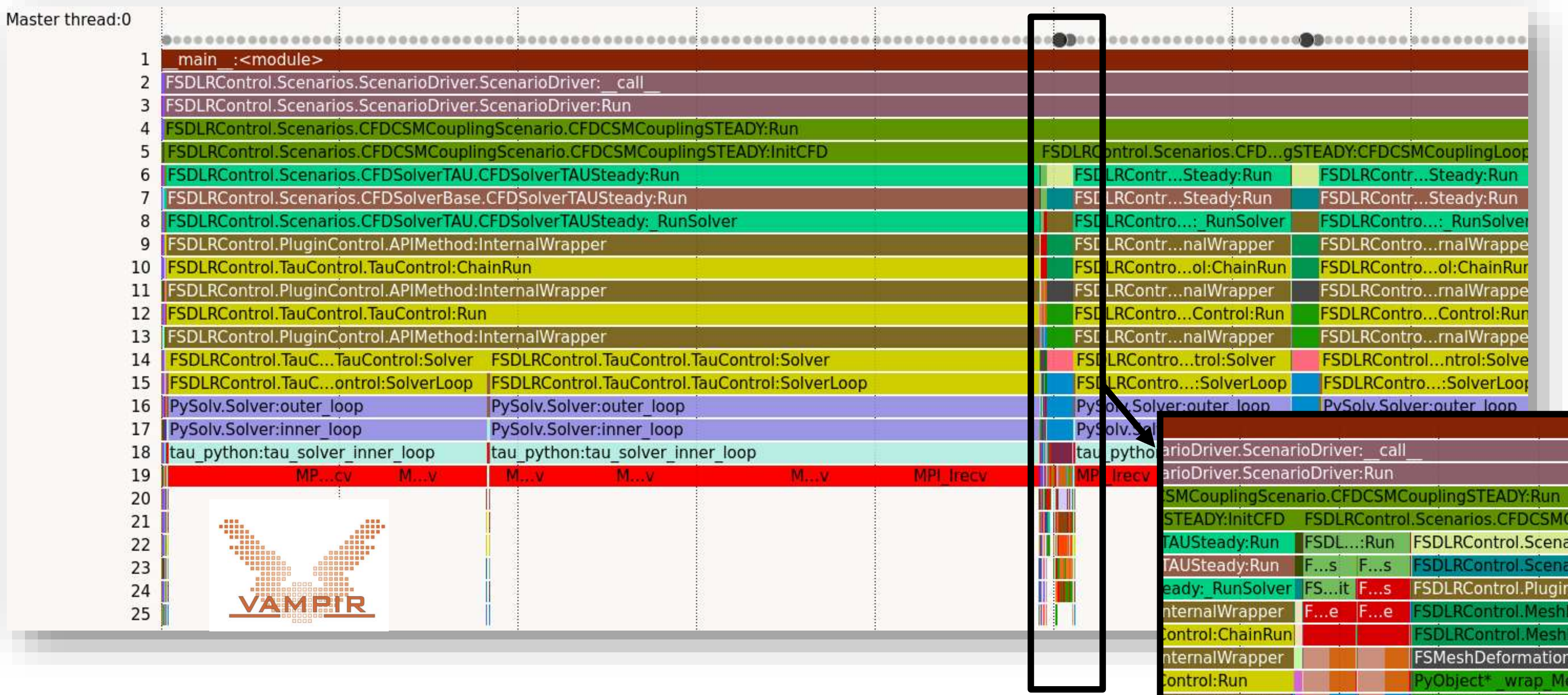


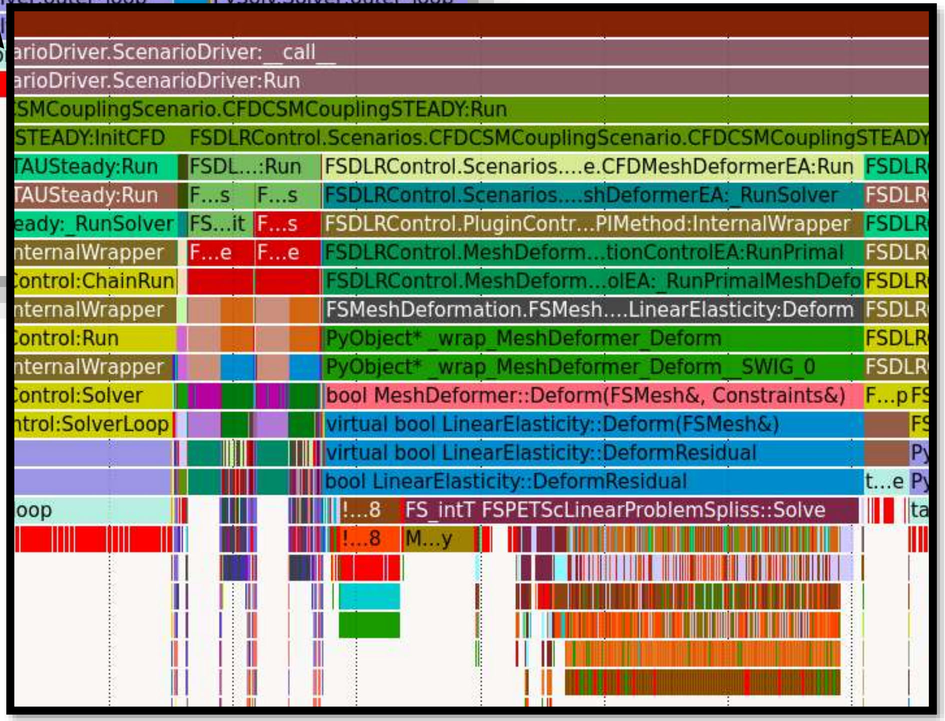


Trace size: 138 MB

Overhead: 1%

Traces with Cpp instrumentation





Trace size:	5 GB
Overhead:	6%
	depends on filter

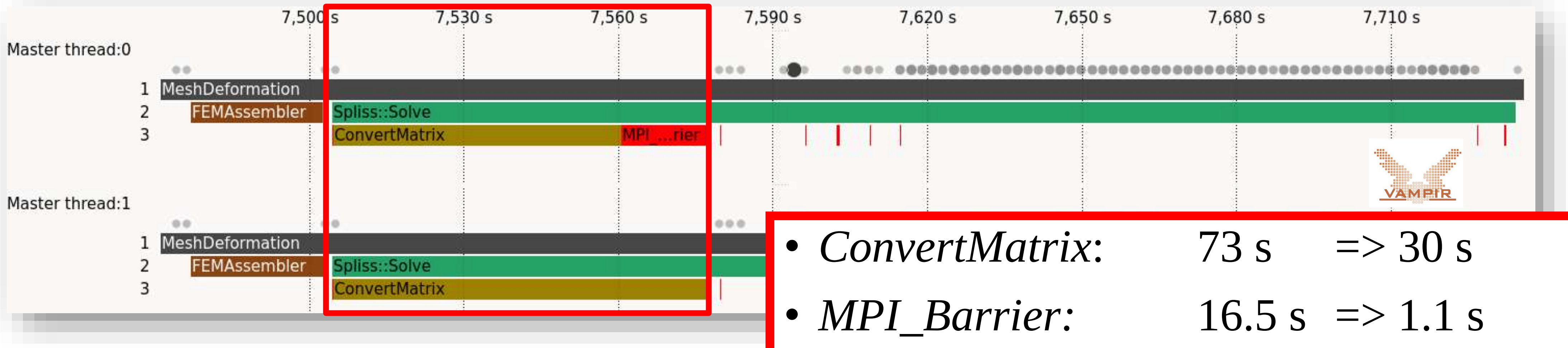
Mesh deformation (2 MPI x 4 OpenMP)

Focusing on *MeshDeformation*

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

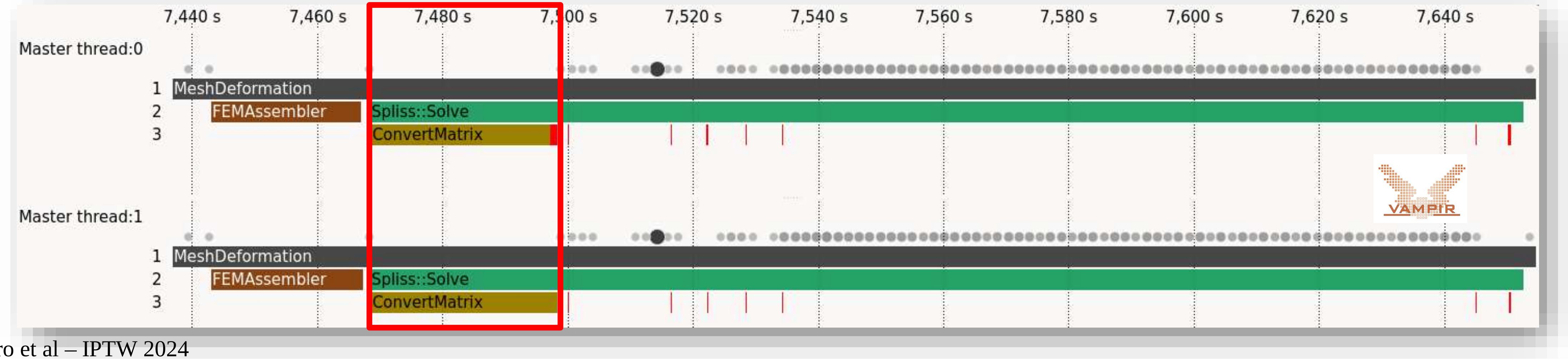
Matrix conversion algorithm improvement (2 MPI x 4 OpenMP)

Original algorithm



- *ConvertMatrix*: 73 s => 30 s
- *MPI_Barrier:* 16.5 s => 1.1 s
- *MeshDeformation*: -18%

Improved 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

Acknowledgments

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