Recent developments about GPU acceleration in HELYX

1st OpenFOAM – HPC Challenge

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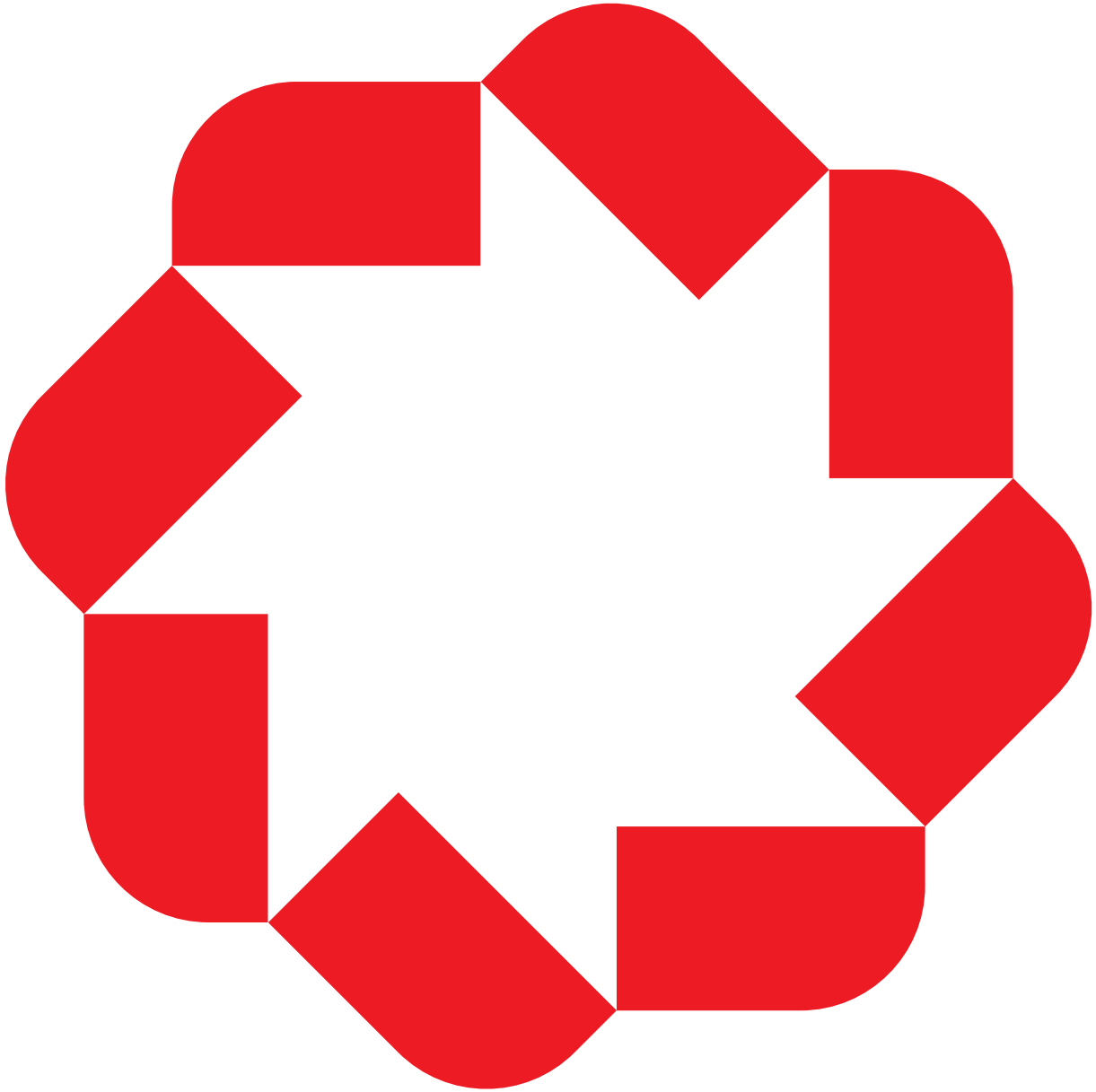
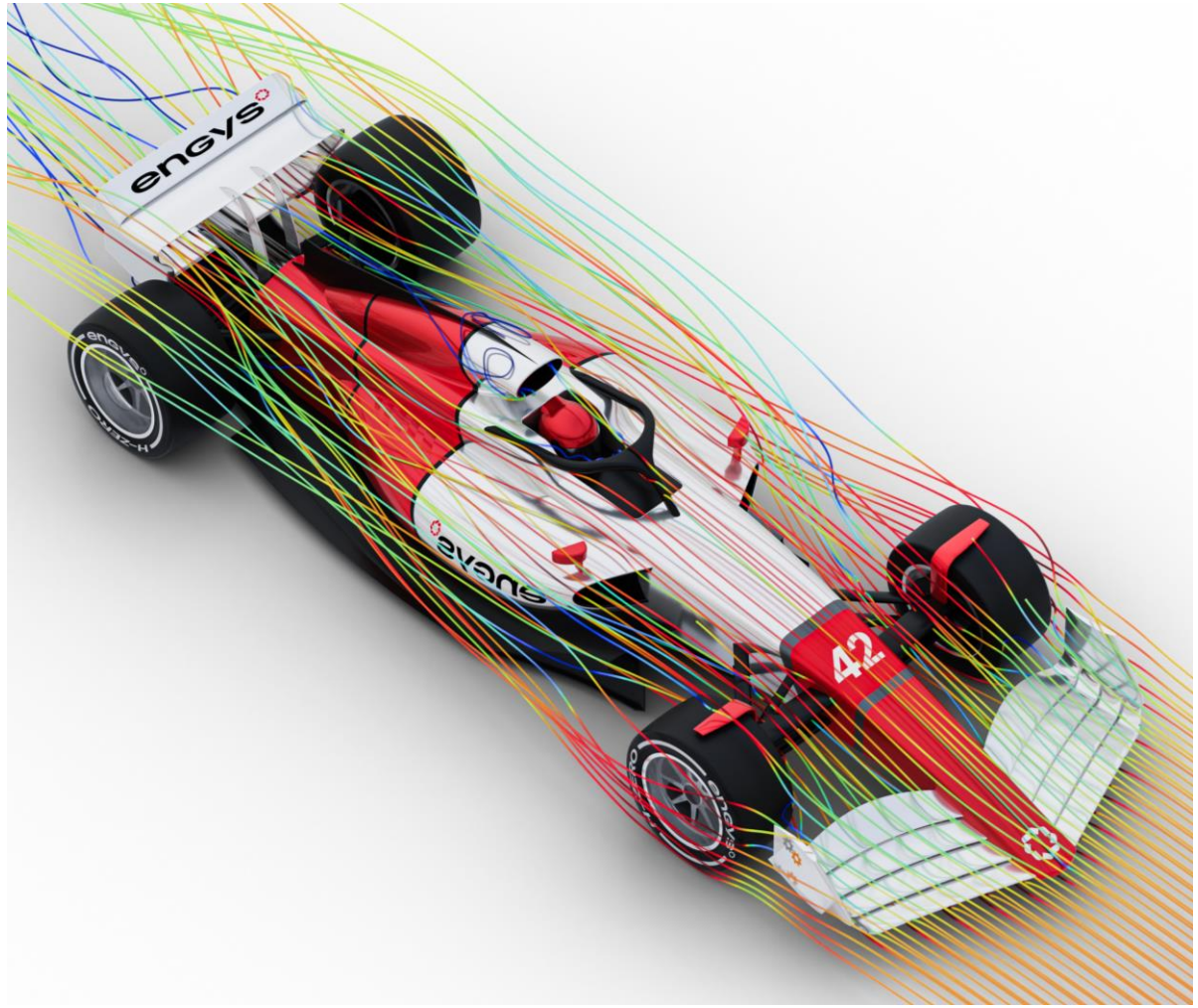


Introduction

- Native GPU HELYX core is the ultimate goal
- Completed a prototype to showcase capabilities
- Support from F1 teams consortium



Recent Developments | GPU Status

Prototype native GPU – operational

- Matrix assembly + linear algebra on GPU
  - Most common discretization schemes available
  - Segregated and block-coupled steady/transient solvers
  - Most common linear solvers available
    - ✓ Segregated : PBiCGStab, GAMG with multicolor smoothers/preconditioners (GS, DILU)
    - ✓ Coupled: FGMRES, AMG with block-coupled smoothers (GS, DILU)

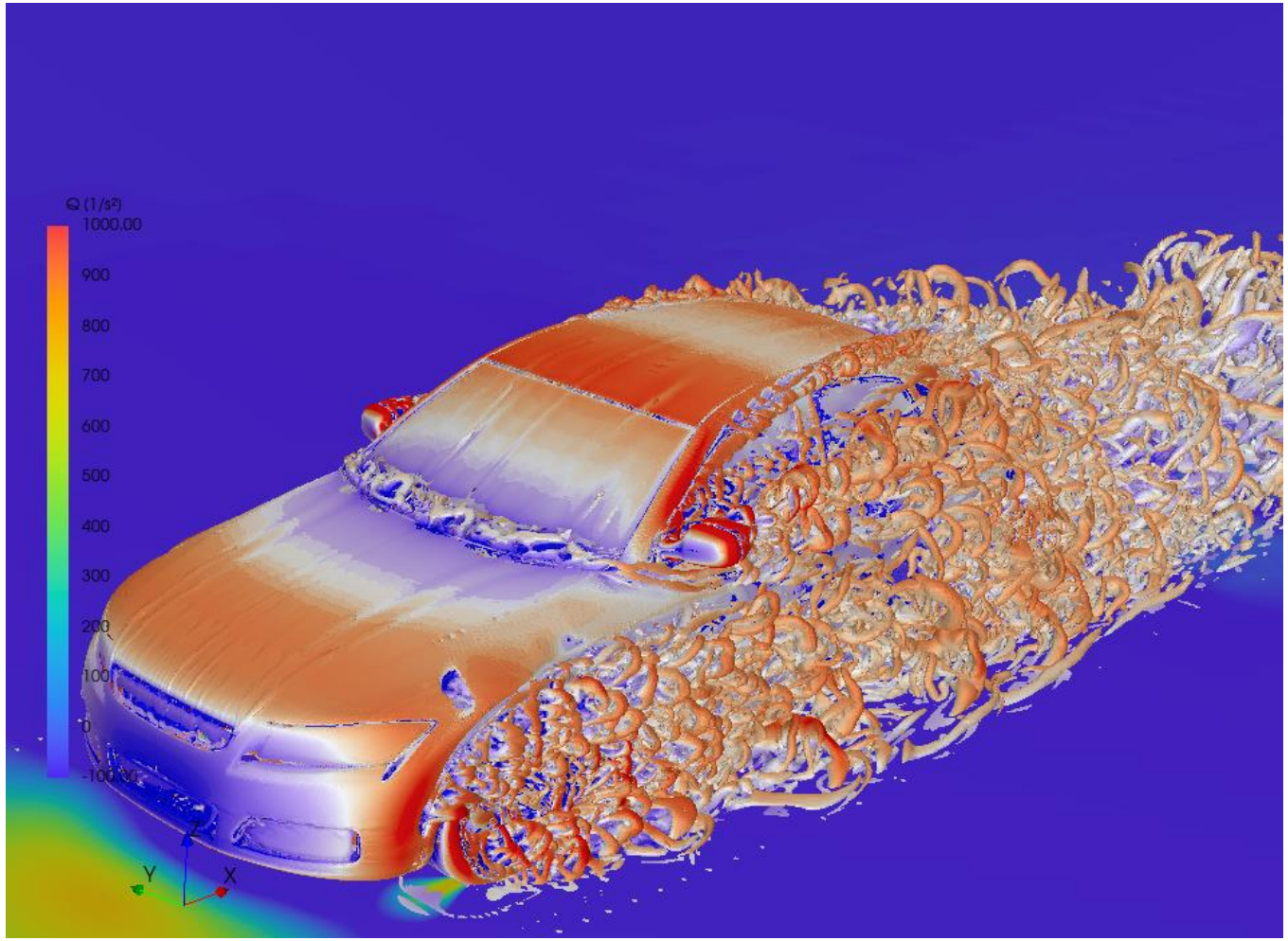
Recent Developments | GPU Status

Turbulence:

- RANS closure (k-Omega SST),
- DES, DDES (k-Omega SST, SA)
- LES (k-Eqn, WALE, Smagorinsky)

Postprocessing:

- Most common ext aero FO (forceCoeffs, probes, fields etc)



Recent Developments | GPU Status

Hardware

- CUDA (Nvidia hardware)
- Compiled and tested also on AMD – looking into performance gap

OFHPC Challenge - Results

Grids:

- Used fine grid from committee (236M)

Methods:

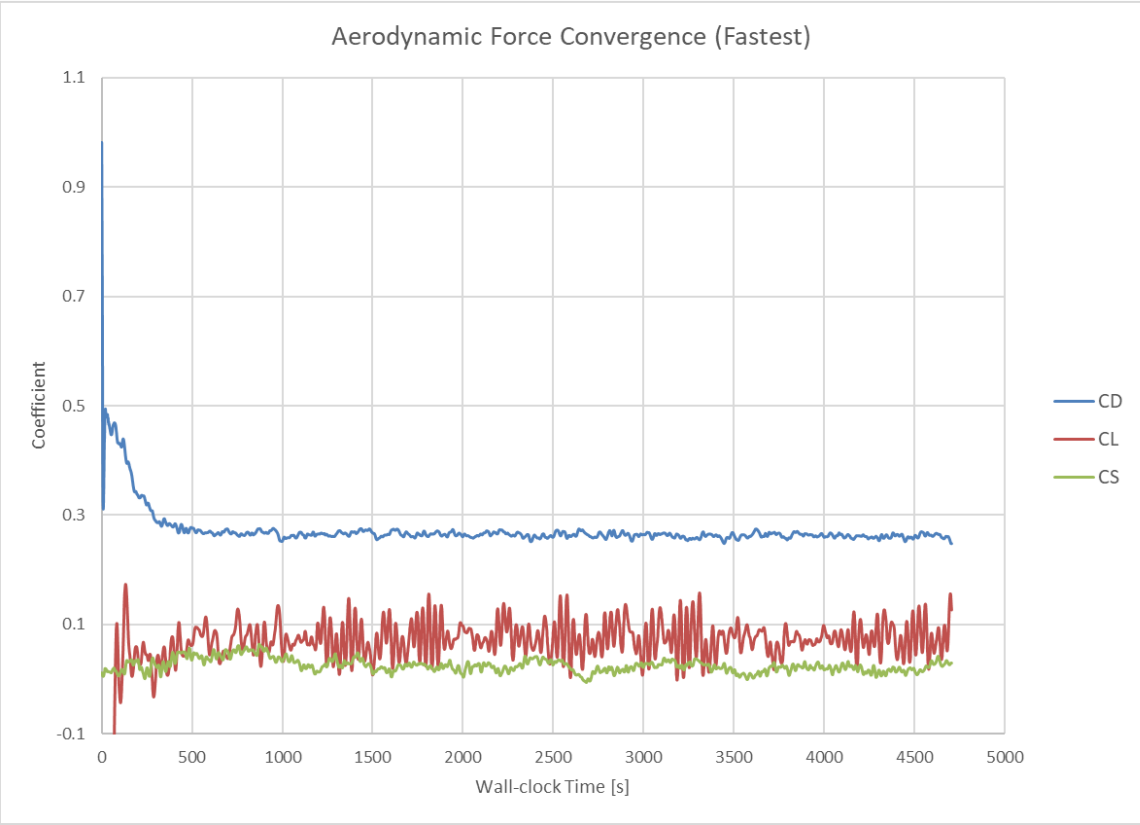
- Software Track, simulations run with standard HELYX and HELXY-GPU
- Setup is the same as specified for the Hardware track (fvSchemes, fvSolution, FO, initialization etc)
- Convergence assessment with meanCalc

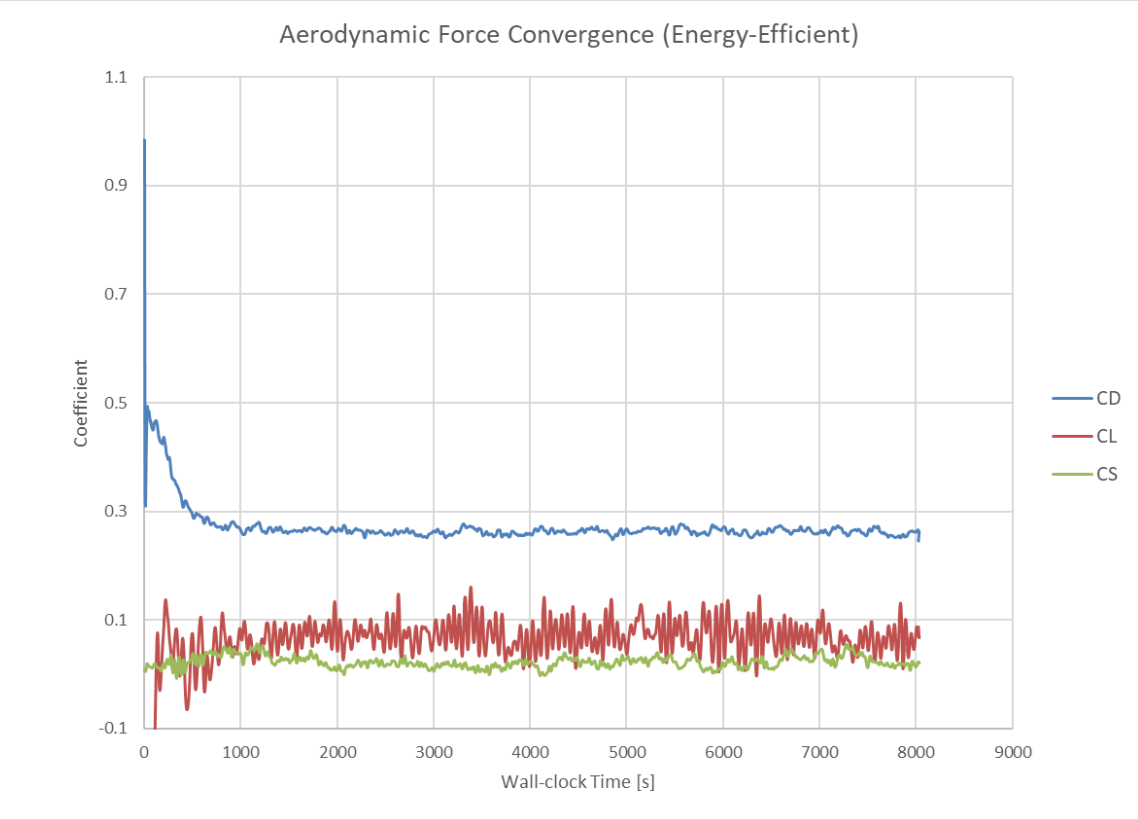
Hardware:

- Simulations run on Leonardo (CINECA) – Booster partition.
- Nodes used at full capacity

No Focus on Pre-processing

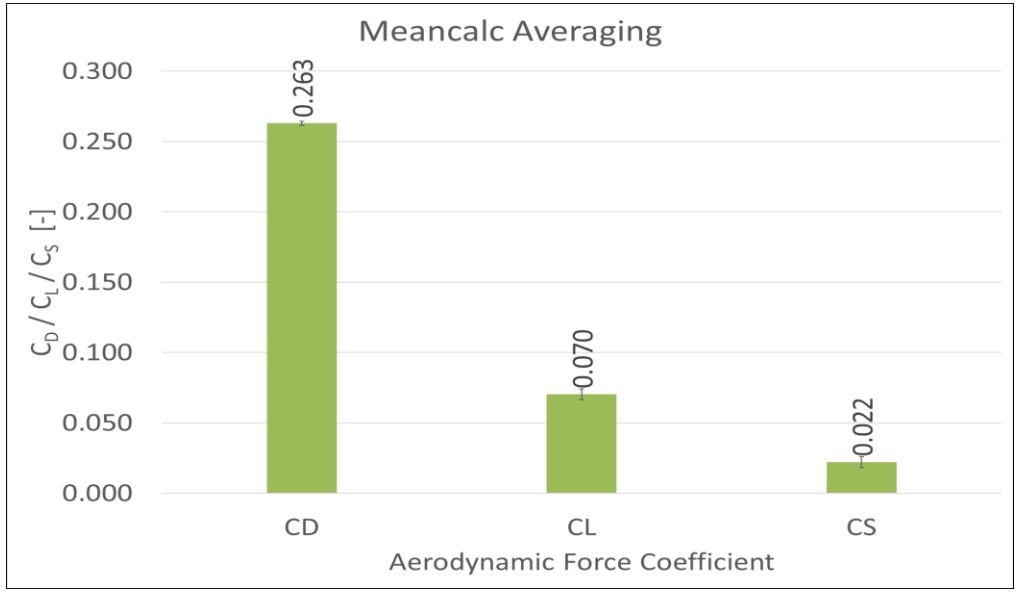
OFHPC Challenge - Results

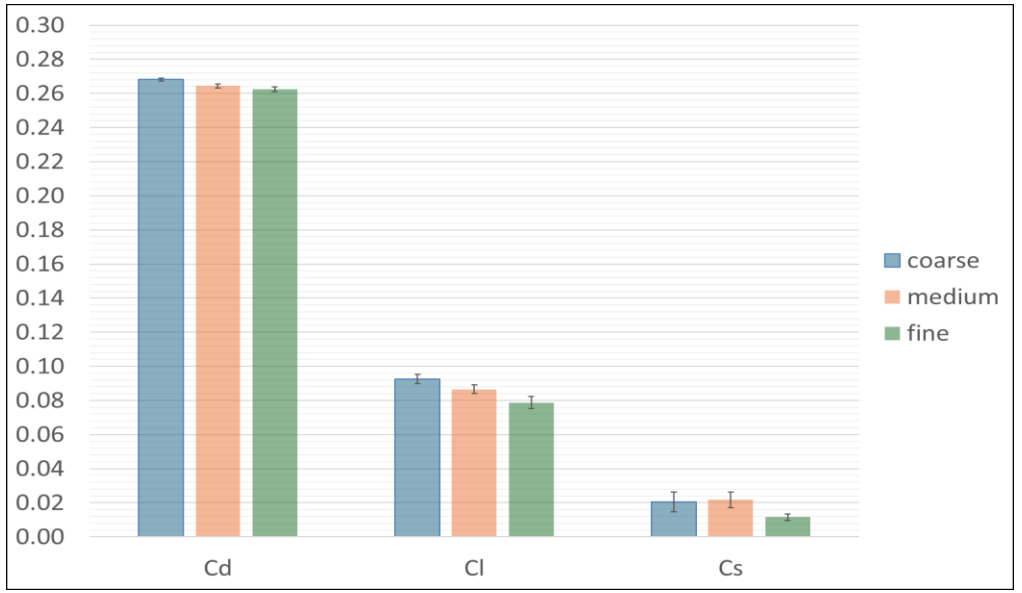




OFHPC Challenge - Results

- Drag coefficient is in good agreement with vanilla OpenFOAM
- Lift coefficient convergence is more sensitive to simulation settings (e.g. schemes and linear solver tolerances/multigrid setting)
- Side coefficient is more similar to coarse/medium grid
- All coefficients are in good agreement with data from AutoCFD workshop





OFHPC Challenge - Results

ENERGY EFFICIENT

FASTEST

Software	Simulation #1	Simulation #2	Simulation #3
Solver Type:	FVM	FVM	FVM
Compressibility:	Incompressible	Incompressible	Incompressible
Pressure/ Density Based:	Pressure	Pressure	Pressure
Segregate/Coupled:	Segregated	Segregated	Segregated
Velocity convection scheme:	linearUpwindV	linearUpwindV	linearUpwindV
Order of accuracy (space/time):	2nd	2nd	2nd
Steady-State/Transient:	Steady State	Steady State	Steady State
Time for pre-processing [s]:	0	0	0
Wall-clock time to completion excl. pre-processing [s]:	8042	4705	24271
Wall-clock time per timestep/iteration [s]:	2.01	1.18	6.07
TDP of system (CPU+Accelerator) [W]:	3700 W	7400 W	4000 W
Total energy to completion [kW*h or J]:	7.15 kWh	8.36 kWh	27.0 kWh
Decomposition Method:	Scotch	Scotch	Scotch
Renumbering Method:	RCM	RCM	RCM
Hardware:			
Server Type:	GPU	GPU	CPU
Hardware Spec (CPU):	Intel Ice Lake Xeon Platinum 8358	Intel Ice Lake Xeon Platinum 8358	ntel Ice Lake Xeon Platinum 8358
Hardware Spec (GPU):	Nvidia A100 custom 64GB	Nvidia A100 custom 64GB	/
# of nodes used:	2	4	16
# of CPU cores used:	8	16	512
# of GPUs used:	8	16	0
Memory type:	HBM2e	HBM2e	DDR4-3200
Memory capacity per node:	256 GB	256 GB	512 GB
Last-level Cache (LLC):	40 MB	40 MB	48 MB
Network Interconnect:	NVLink 3.0 + Mellanox HDR Infiniband	NVLink 3.0 + Mellanox HDR Infiniband	Mellanox HDR Infiniband
Storage Device:	SSD	SSD	SSD
Storage File-system:	Lustre	Lustre	Lustre
Network Topology:	Dragonfly	Dragonfly	Dragonfly

OFHPC Challenge - Results

- In terms of runtime: 1 A100 ≈ 195 Intel Xeon Platinum 8358 cores
- In terms of energy consumption: 8 A100 are almost 4 times more energy efficient than 512 Intel Xeon Platinum 8358 cores
- Cost (from AWS) : 8 A100 are 3 times cheaper than 512 Intel Xeon Platinum 8358 cores
- In terms of memory bandwidth: 1 A100 ≈ 300 Intel Xeon Platinum 8358 cores → lots of room for improvement (theoretically!)
- Moving from 8 to 16 GPUs the parallel efficiency is only 85 % → has to be improved (mainly due to poor resources utilization at coarse grid levels for multigrid)

Need to explore new algorithms/ techniques to achieve speedup ≈ MB ratio

Conclusions

- Prototype of HELYX native GPU solver has been shown
- GPU offload can help reducing turnaround time and energy consumption
- Testing on a broader spectrum of hardware is ongoing
- Significant work still needed to improve performance (especially linear algebra)
- Multigrid solvers tend to scale worse compared to other parts of the code

Acknowledgements

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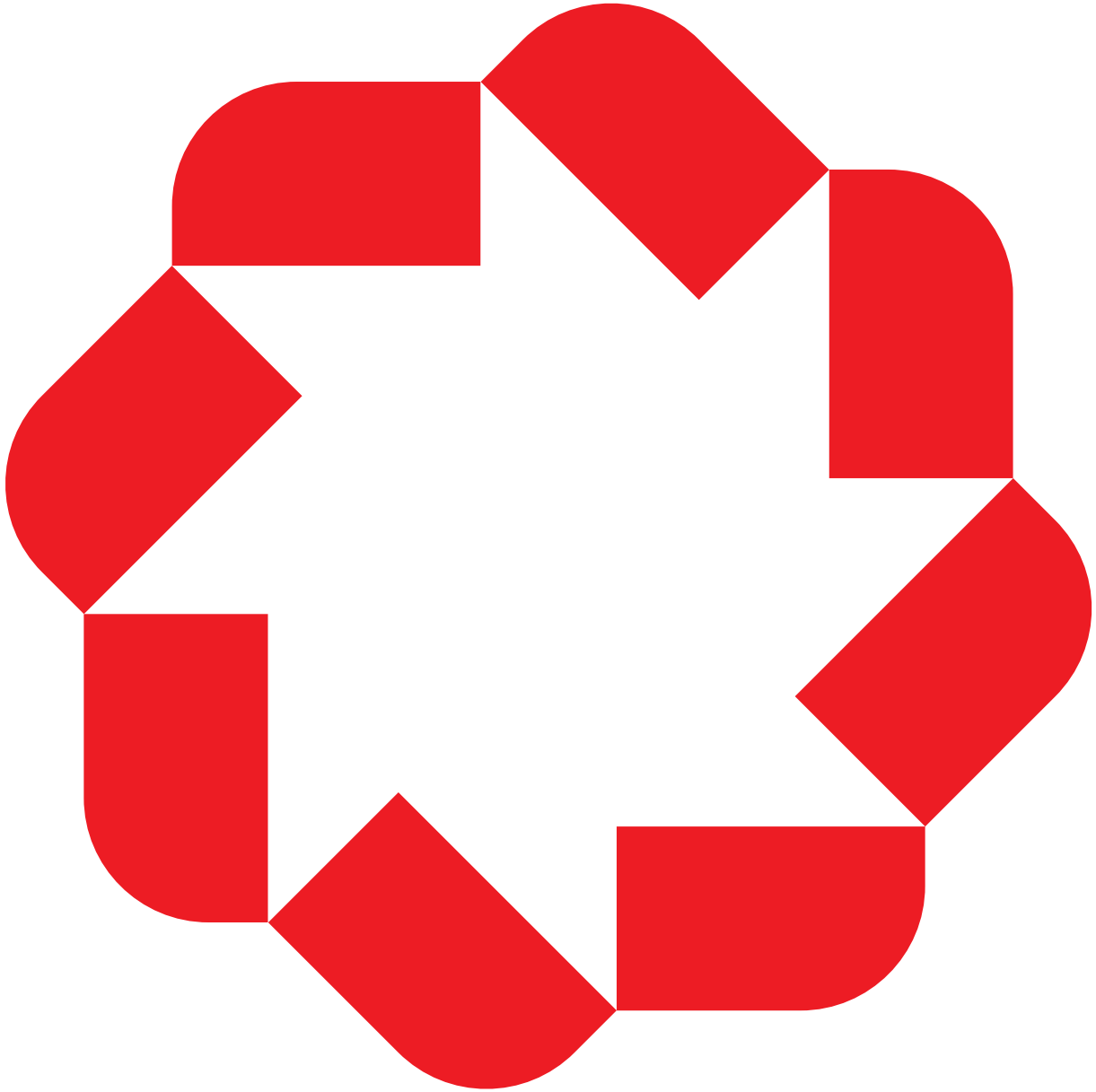
SPECTRAL COMPUTE

NVIDIA

EuroHPC Joint Undertaking



Thanks for the attention!

engys
Innovation through CFD

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