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Model Free Flow Simulations in Engine-Like geometries – The Role of HPC Towards Improved Understanding of Cycle-to-Cycle Variations

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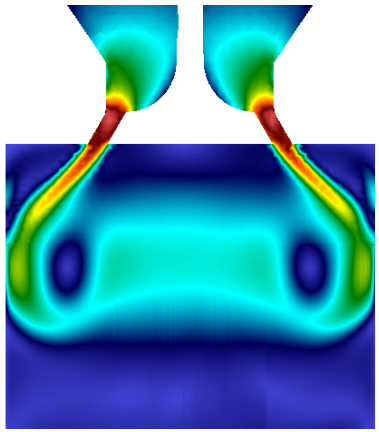
Outline

- Motivation
- Numerical setup
- Experimental setup
- Overview of studies done so far
- Focus on cycle-to-cycle variations
- Conclusions and outlook

Motivation

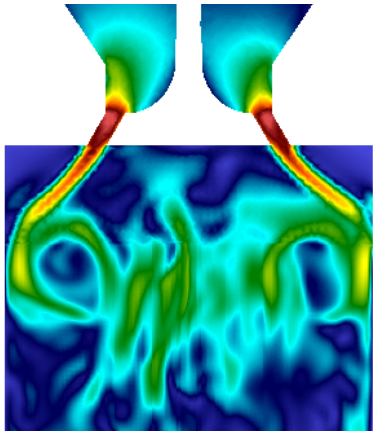
RANS

- Main approach for industrial applications
- Calculation of averaged quantities



LES

- Research tool => emerging in industry
- Able to predict cyclic fluctuations



Results depend on resolution and models

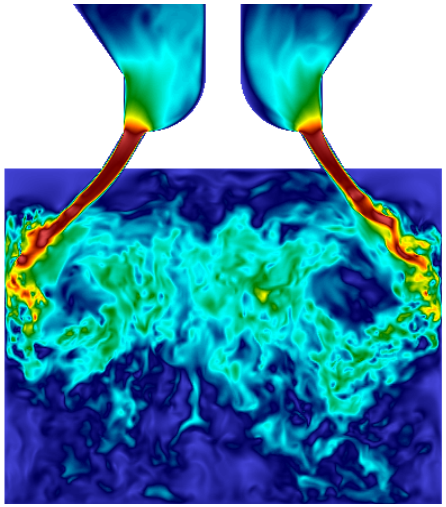
(turbulence, heat transfer, flame speed, etc...)

=> **Validation necessary**

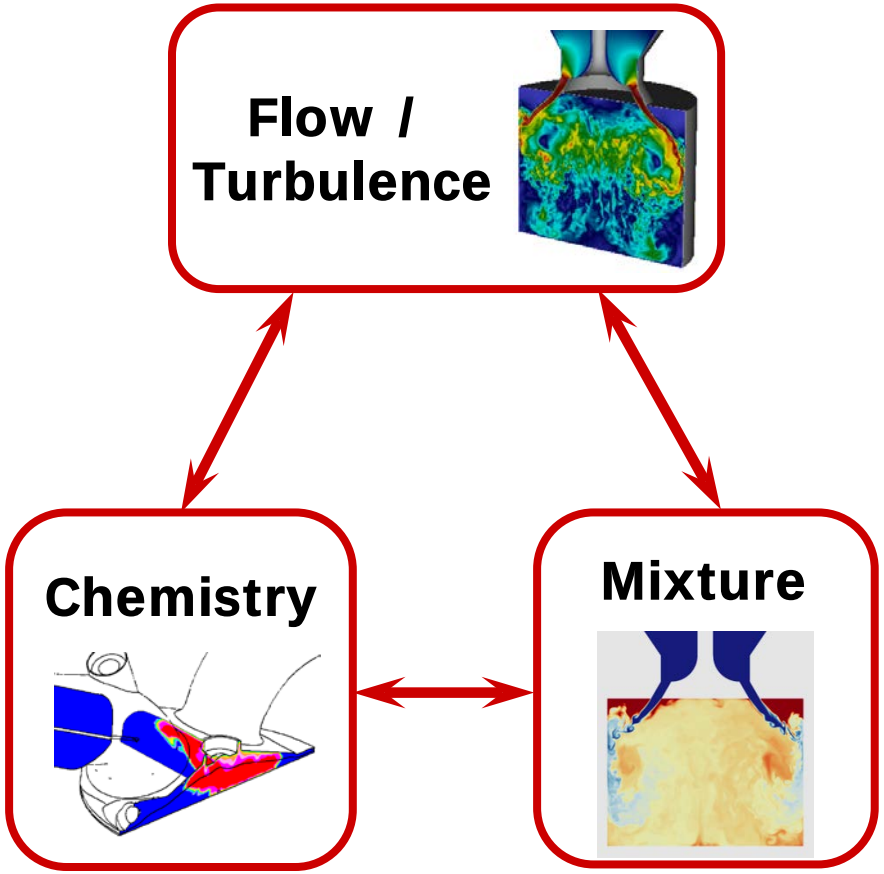
1) Experiments

2) DNS

- Not attempted so far
- Numerical Experiment
- All fields are fully resolved available



Challenges of DNS Calculations in Engines



Physics:

- Wide range of length and time scales:
  - Turbulence/Mixing: µm / ms
  - Chemistry: µm / ns [1,2]
- Large number of species and reactions

Engines:

- Complex geometries (scales cm, s)
- Moving piston and valves
- Large differences in spatial and temporal resolution requirements within the cycle

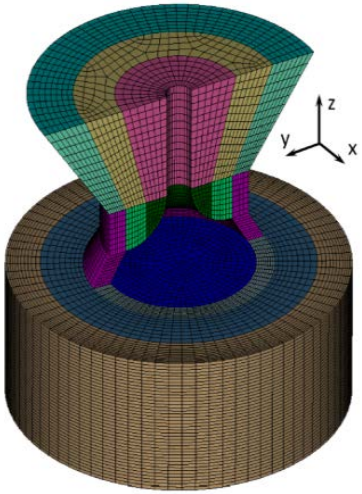
⇒ **Enormous number of DOF**
⇒ **Huge amount of output data**

[1] Maas, U., & Pope, S. B. (1992). Simplifying chemical kinetics: intrinsic low-dimensional manifolds in composition space. *Comb. and Flame*, *88* (3), 239-264
[2] Koch, T. (2002) Dissertation LAV / ETHZ

DNS solver: nek5000 + LAV plugin

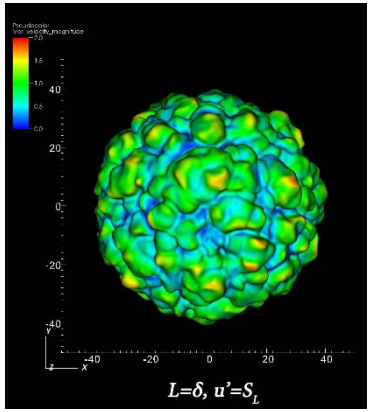
nek5000

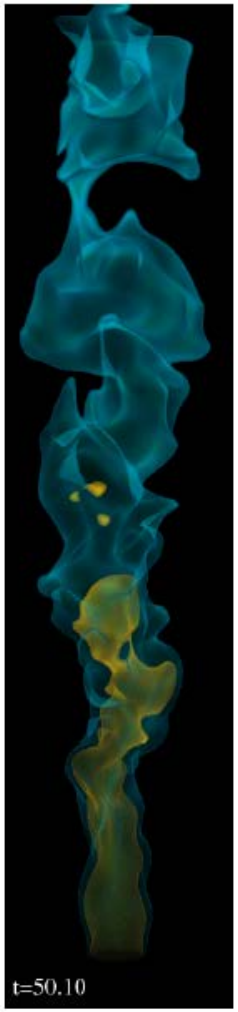
- DNS code based on spectral element method
- Scales to > 524,000 CPUs
- High order accuracy
- Complex geometries
- ALE mesh movement



LAV plugin

- Low Mach number reactive flow solver [1]
- Detailed kinetics and transport (CHEMKIN)
- Gas phase & catalytic combustion



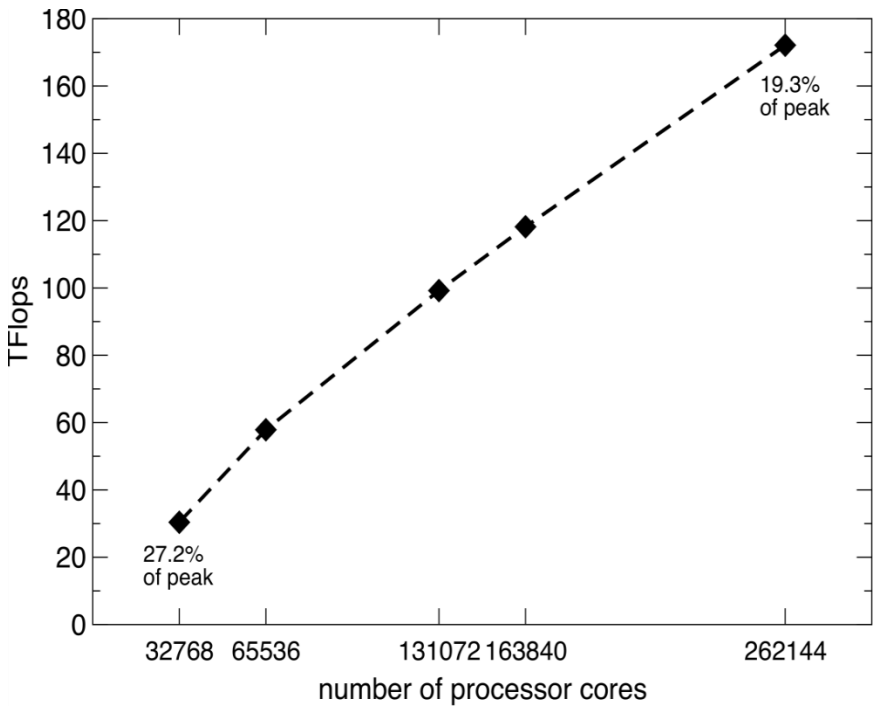


Mixture Fraction [2]

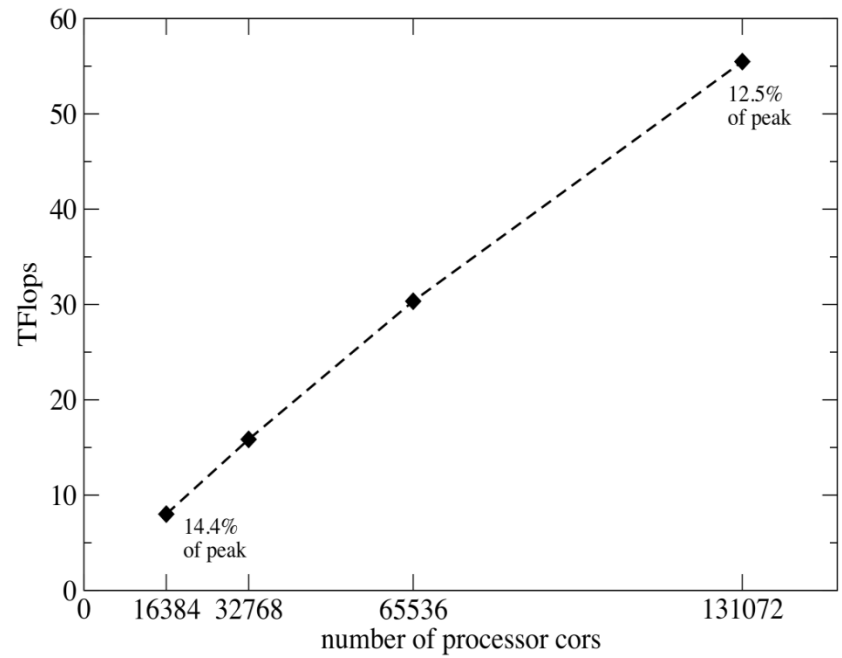
[1] A. Tomboulides et al., JCP (1988), JSC (1997)
[2] S. Kerkemeier, (2010) Autoignition of a hydrogen jet in a hot turbulent co-flow, JFM, 2013

Parallel scaling

Incompressible flow benchmark, Jülich SC



Reactive flow benchmark, ANL BG/P

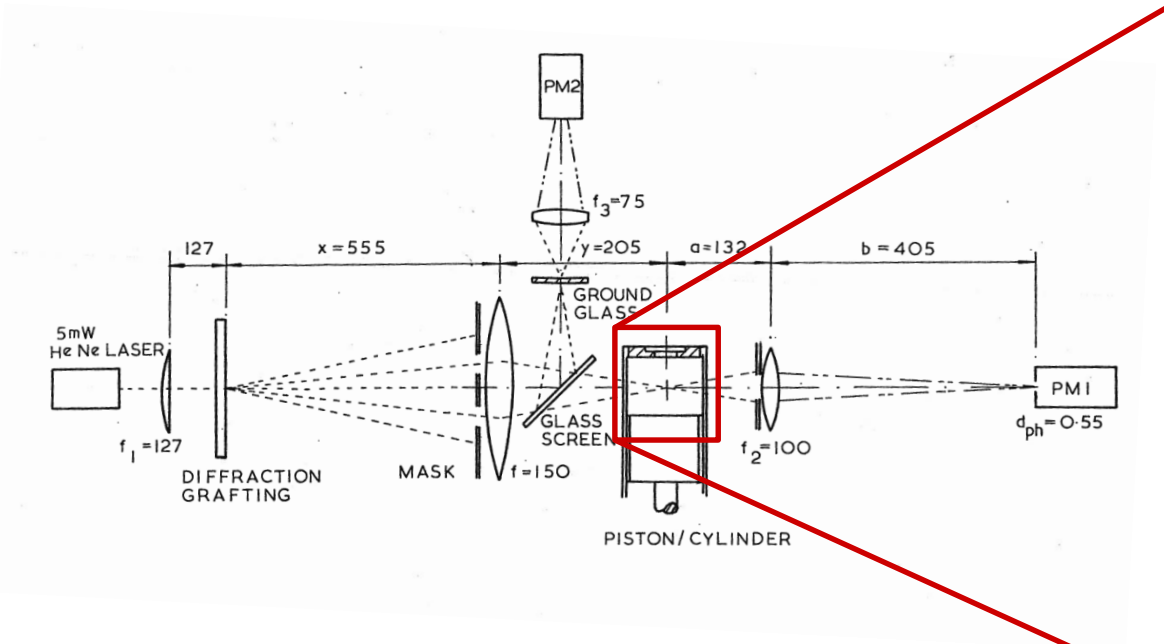


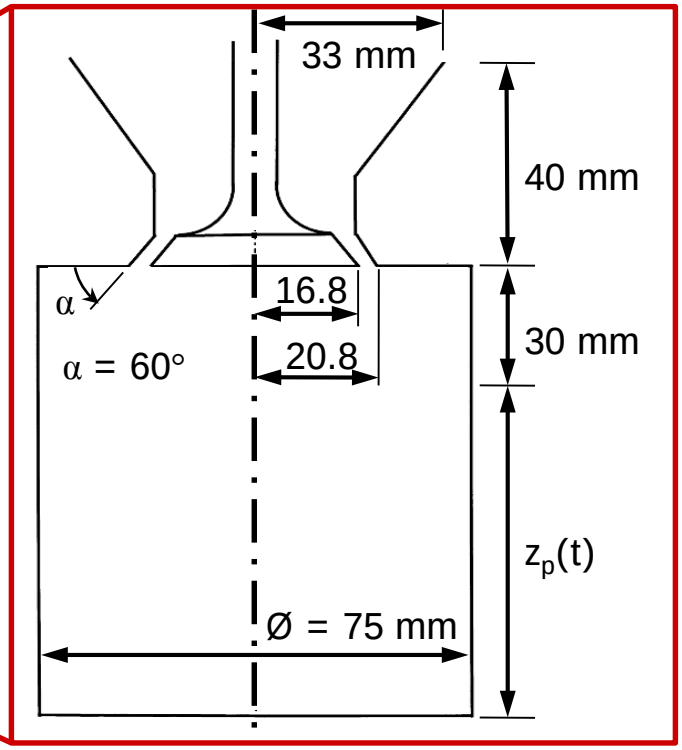
- 7B grid points (E=2.1M, N=15)
- 71% parallel efficiency with ~32,000 grid points/core
- performance up to 0.172PFlops (19% of peak)

- 0.73B grid points (E=1M, N=9)
- 89% parallel efficiency with ~5,500 grid points/core
- performance up to 55.5TFlops (12.5% of peak)

Imperial College experiment [1]

- Valve-piston assembly
- Turning speed = 200 rpm, Compression ratio = 3
- Mean and RMS velocities extracted from Laser Doppler Anemometry (LDA) measurements (ensemble based statistics)
- Setup used in previous RANS/LES studies [2]





[1] Morse, A.P., Whitelaw, J. H. & Yianneskis, M. 1979,. *J. Fluids Eng.* 101, 208–216.
[2] Liu, K. & Haworth, D. C. 2010 *Flow Turb. Combust.*, 85, 279–307.

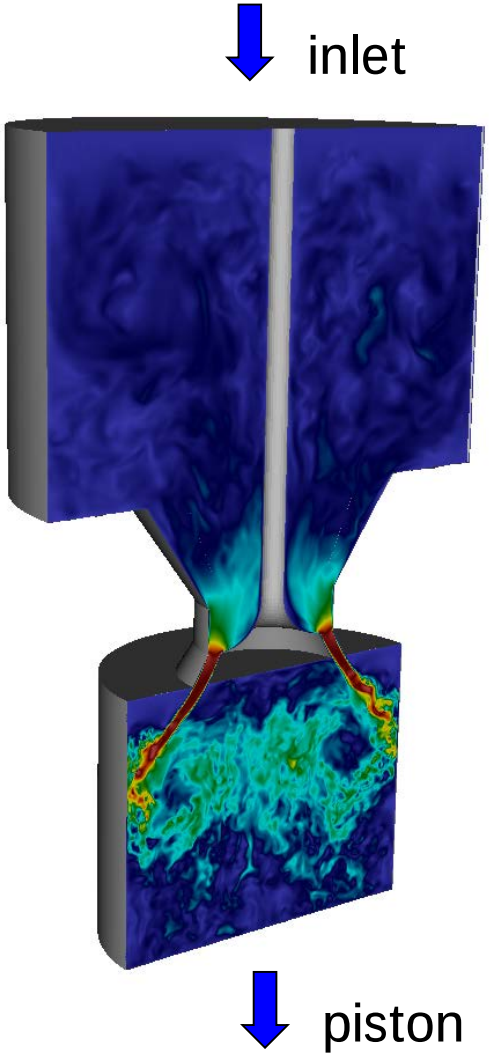
Solver and Simulation setup

Boundary Conditions:

- Velocity at piston and inlet
- Zero velocity on other boundaries
- Thermal boundaries fixed at 500K
- Zero flux species boundary conditions

Numerics:

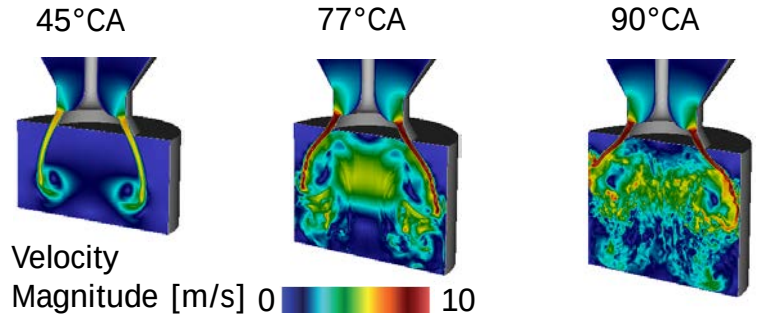
- Spectral element solver: nek5000 (ANL)
- LAV plugin for low Mach number combustion
- 7th order spatial discretization
- 3rd order time integration



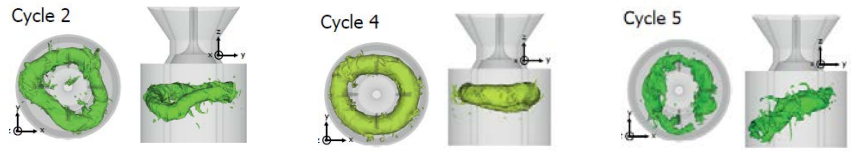
Studies carried out so far

Calculate intake / exhaust stroke (total 8 cycles) [1]

- Validation with experiment (LDA)

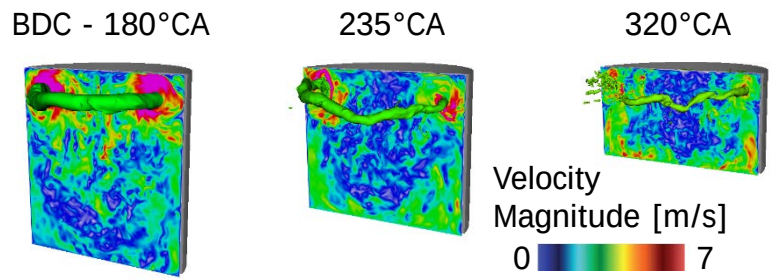


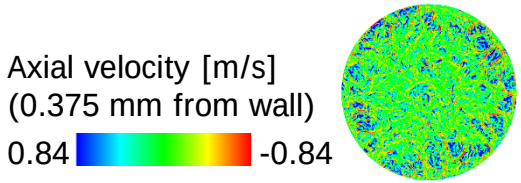
Investigate cycle-to-cycle dynamics (total 11 cycles) [2]

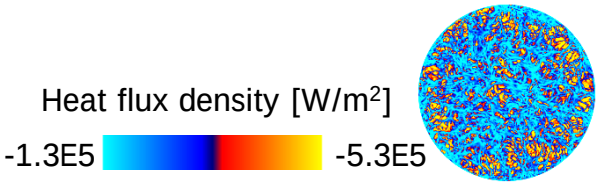


Close valve at BDC and simulate the compression (total 8 cycles)

- flow, mixing, reactions
- wall heat transfer [3]

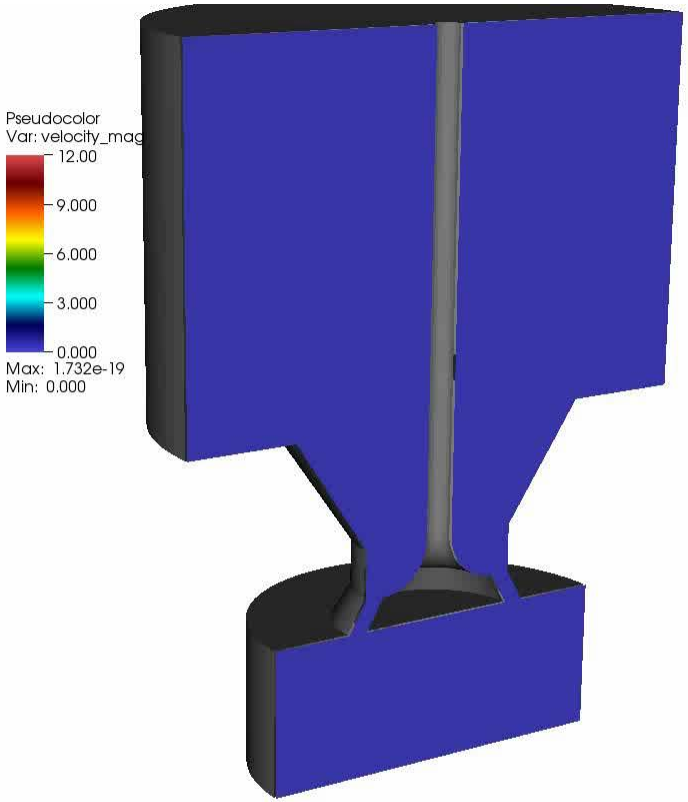


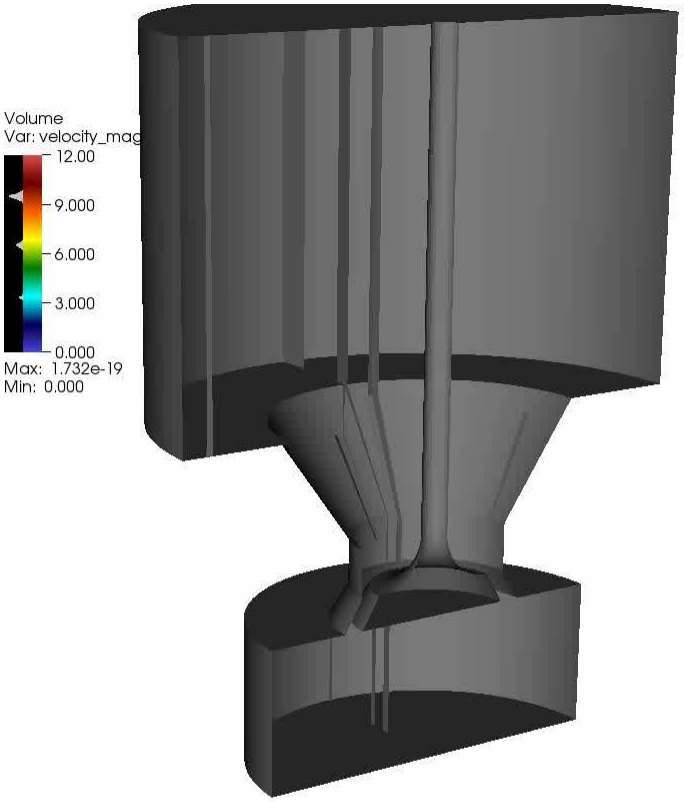




[1] Schmitt et al., *Phys. Fluids 26* [2] Schmitt et al., *accepted to Phys. Fluids* [3] Schmitt et al. *Proc. Combust. Inst. 35*

Instantaneous velocity magnitude





Time= 0.00500

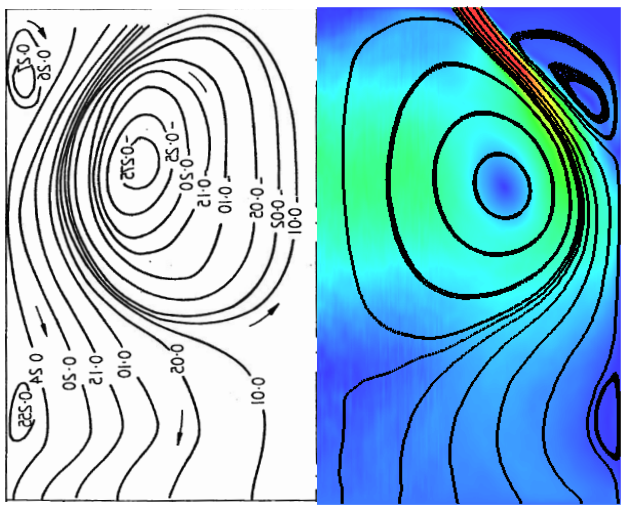
Comparison Simulation - Experiment

144°CA

Streamlines:

90°CA

Experiment Simulation

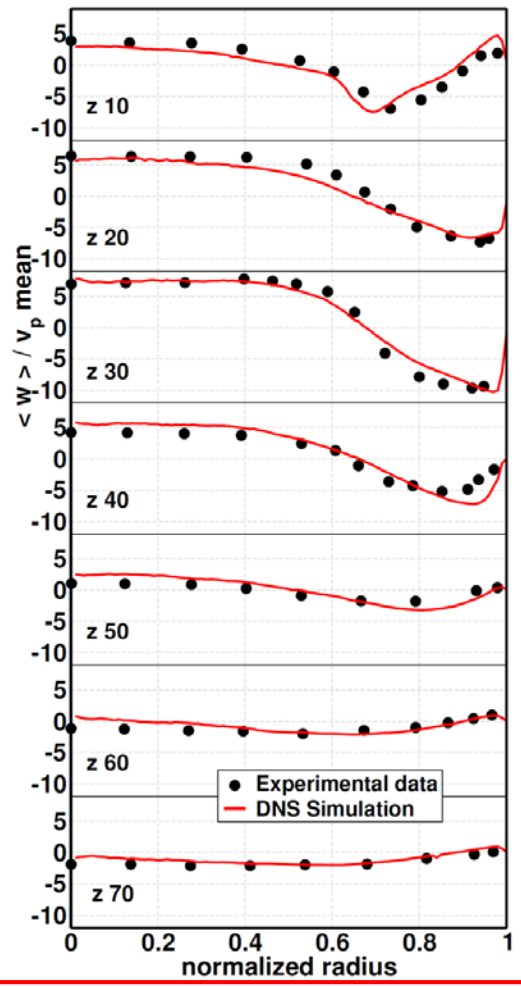


Vel. mag. [m/s]

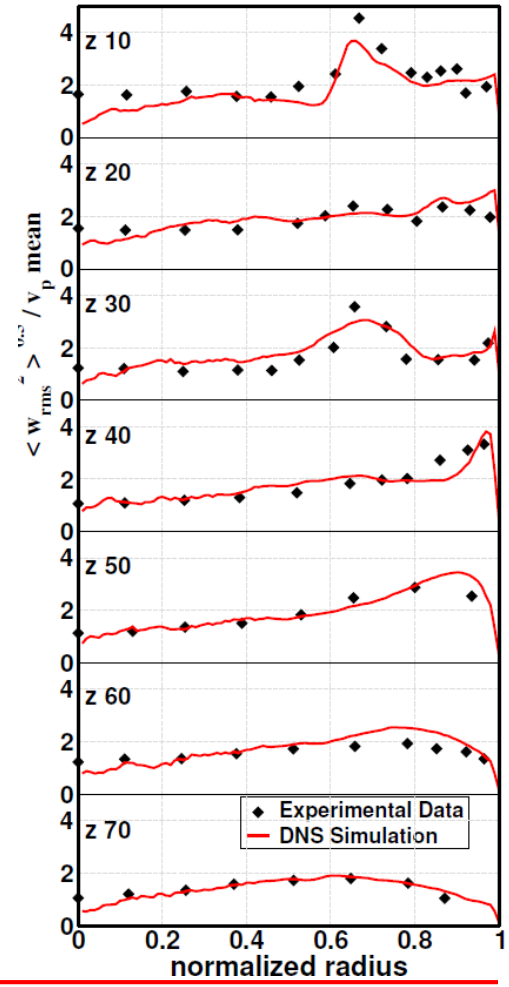
10

0

Axial Mean Vel.



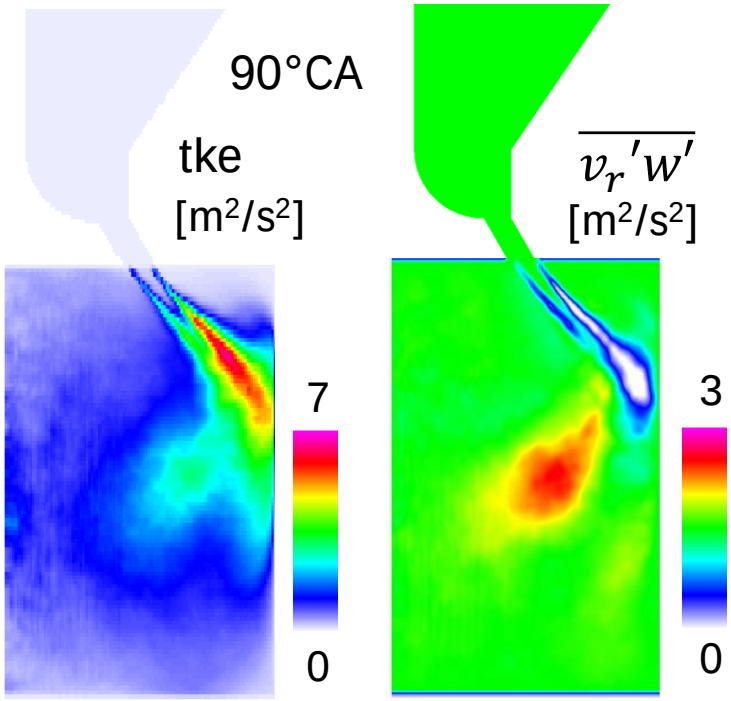
Axial RMS Vel.



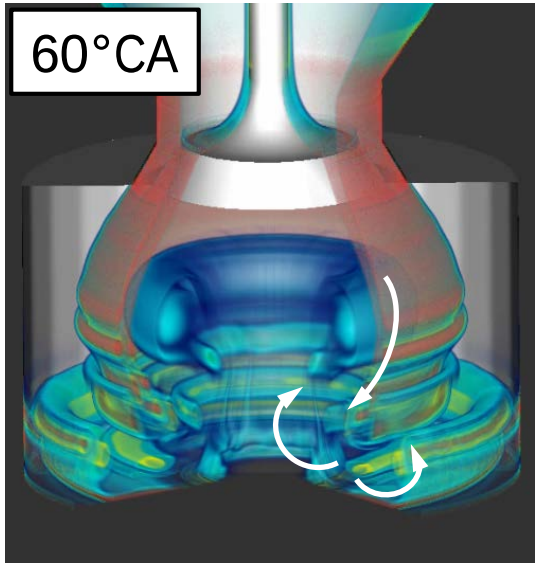
Very good agreement for all available experimental data

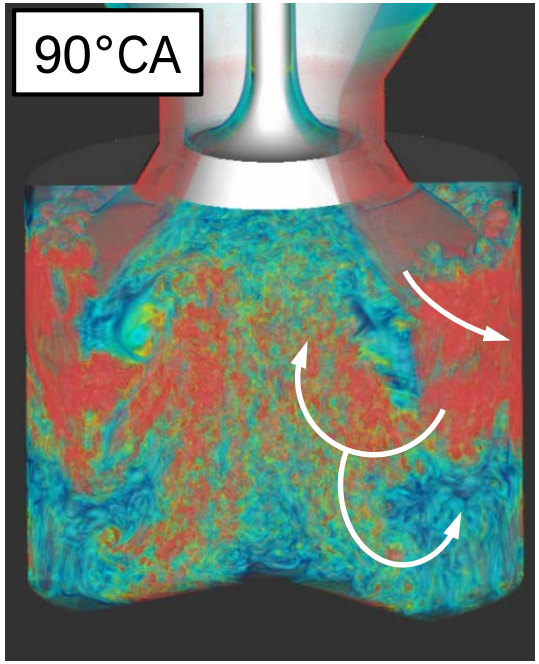
How to use the DNS data?

1) Validation data

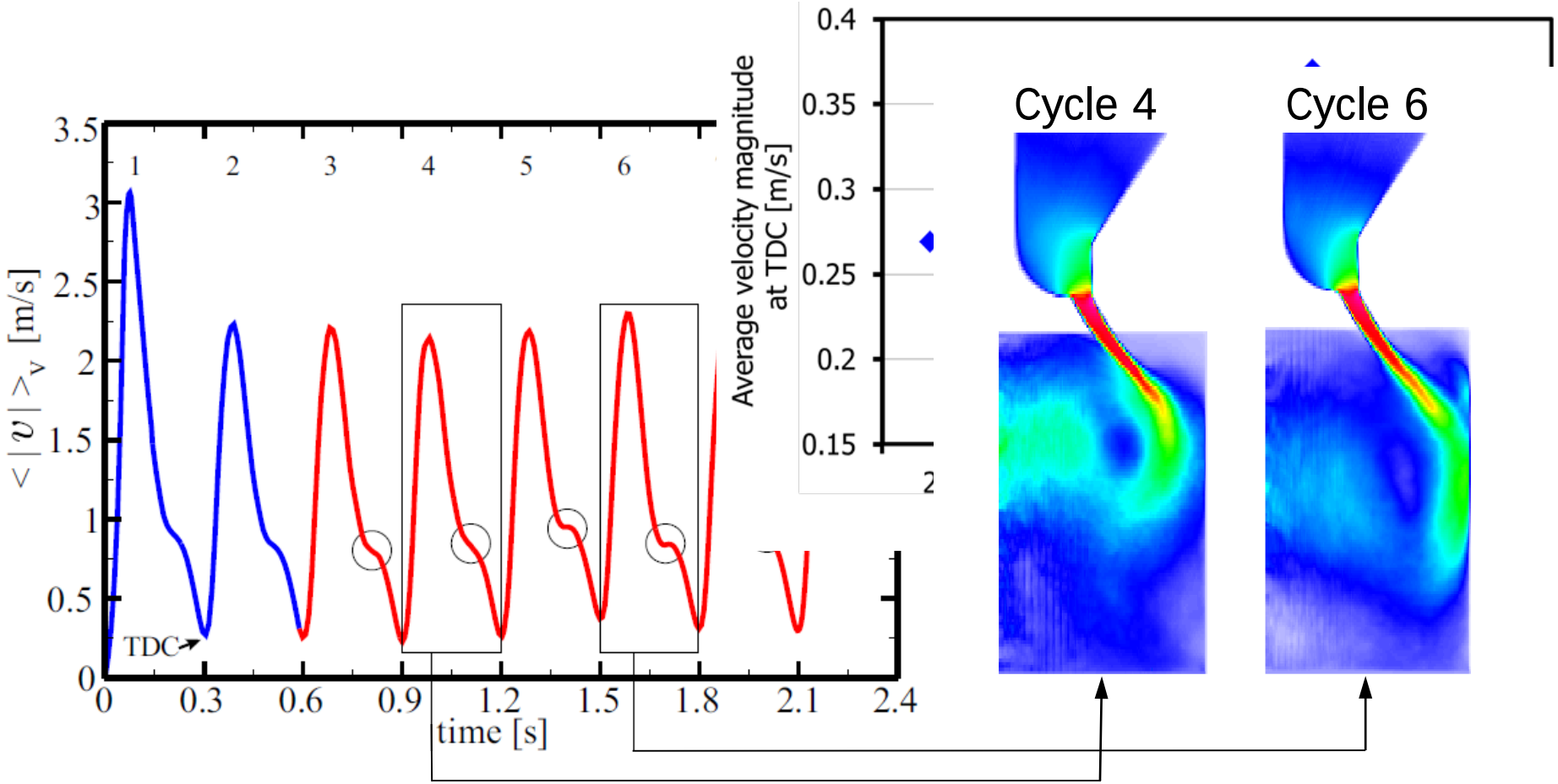


2) Understanding of the physical processes

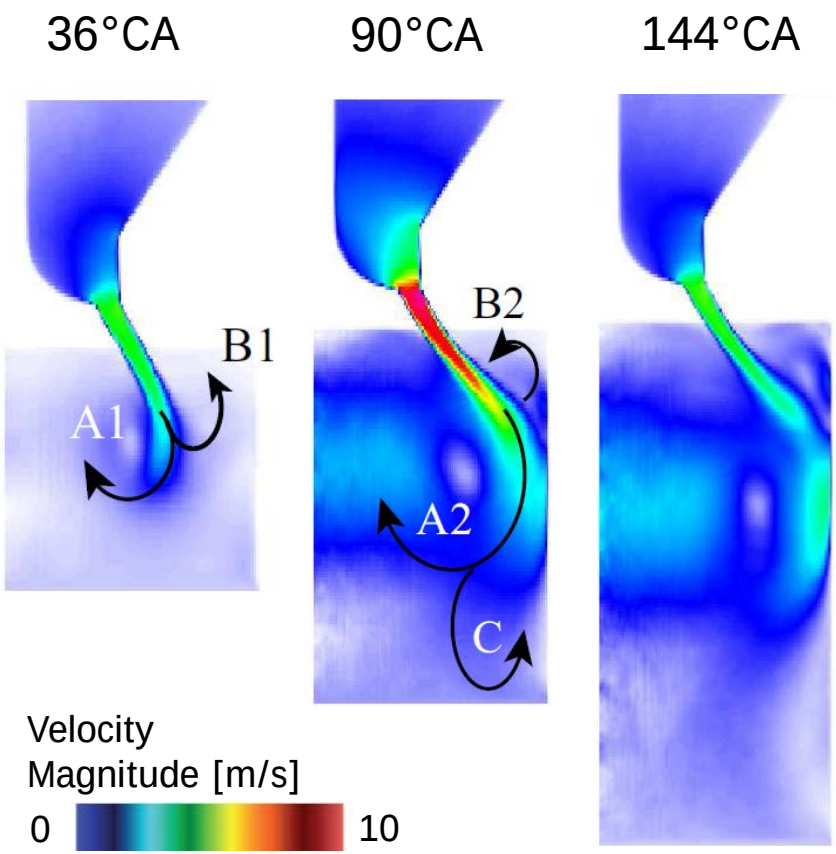




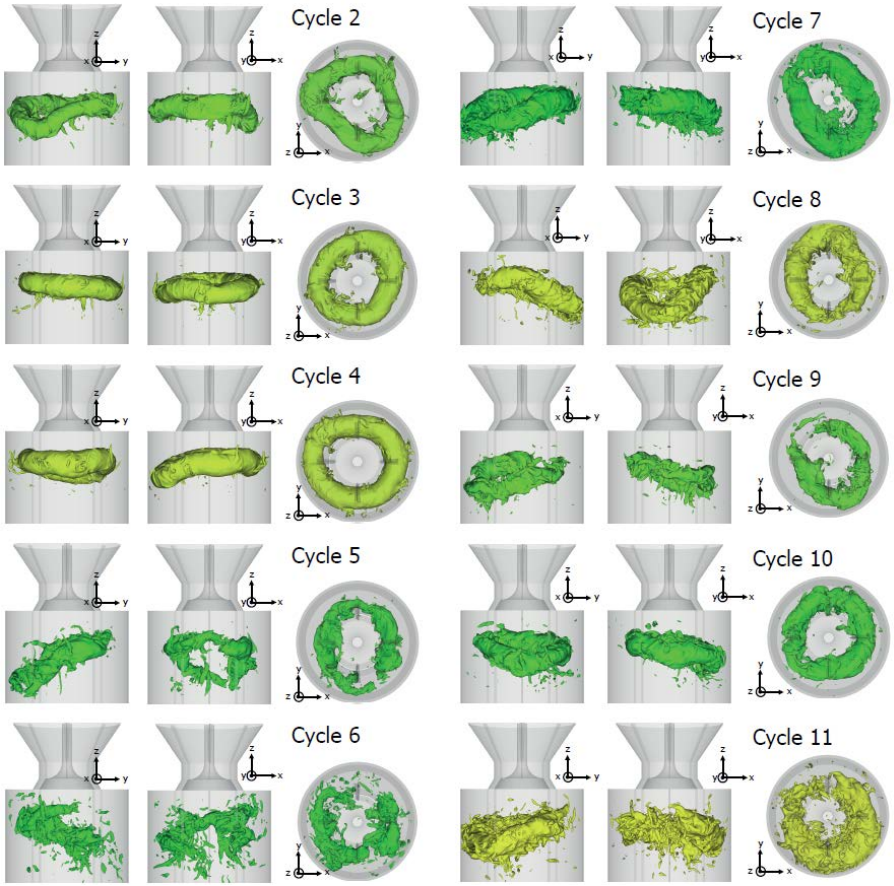
Cycle-to-Cycle Variations (CCV)



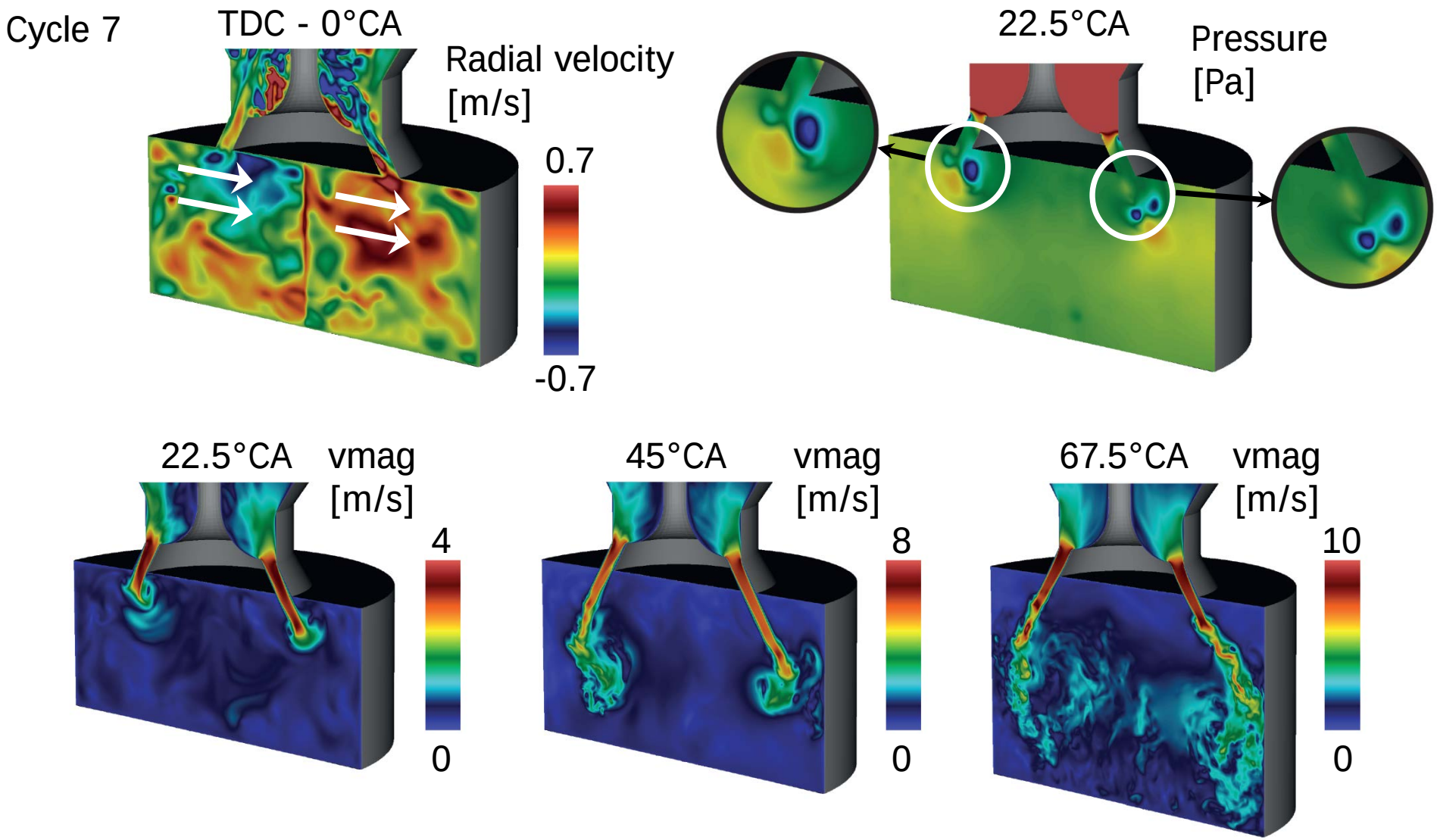
Intake process and vortex ring formation



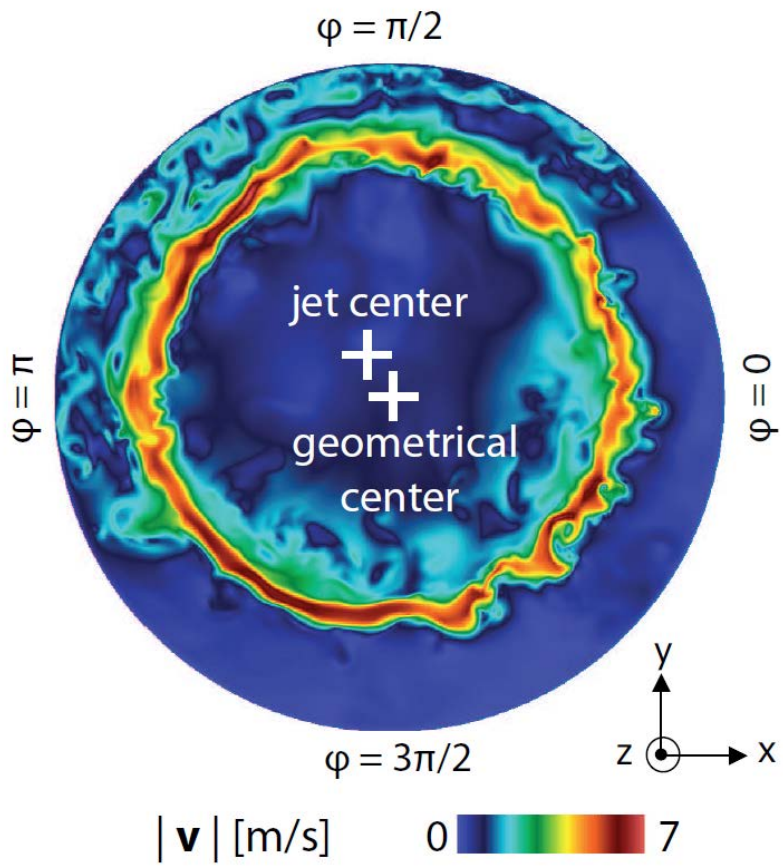
Vortex ring at 180°CA

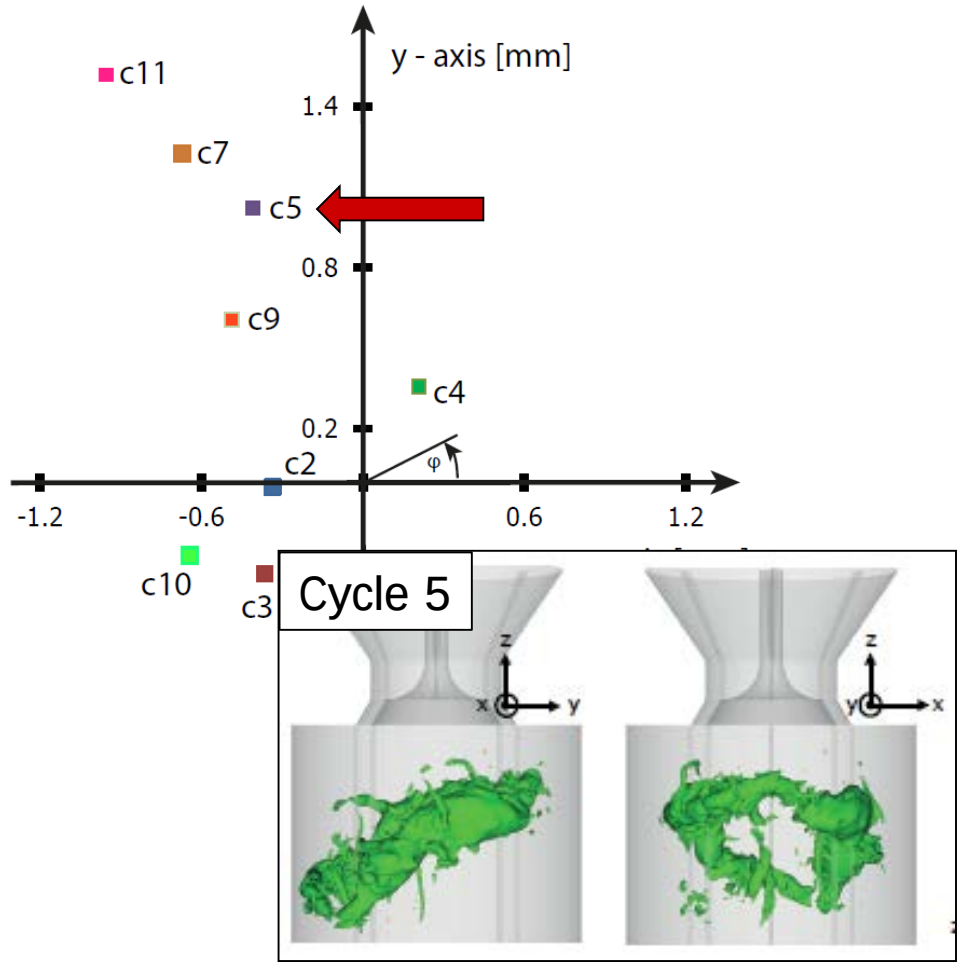


Initial Conditions vs. Jet Flow

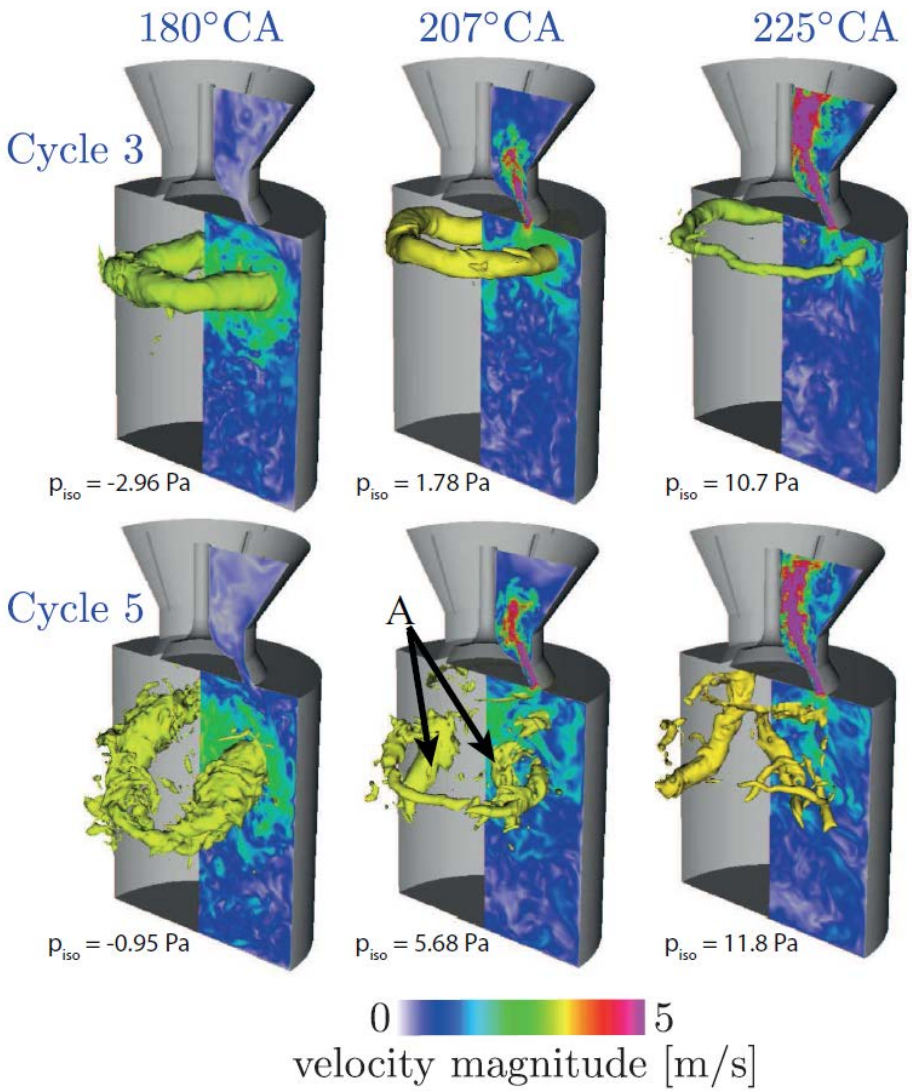


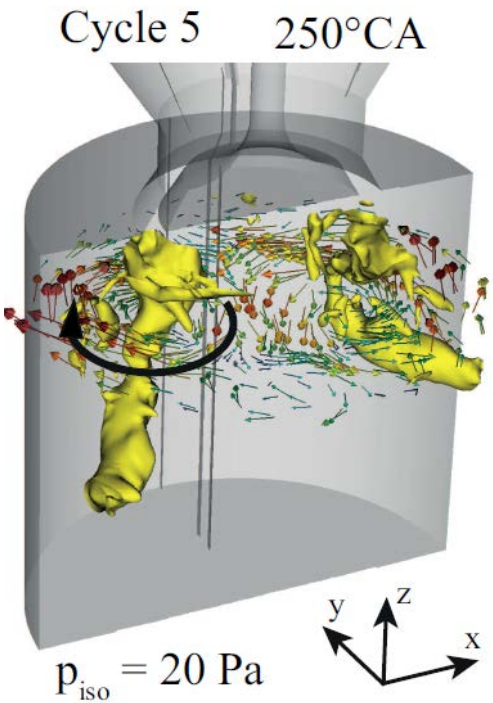
Jet Center Position





Impact on next cycle



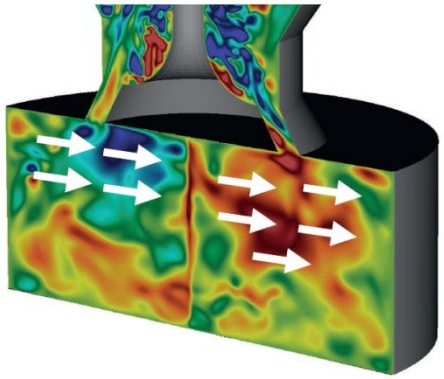


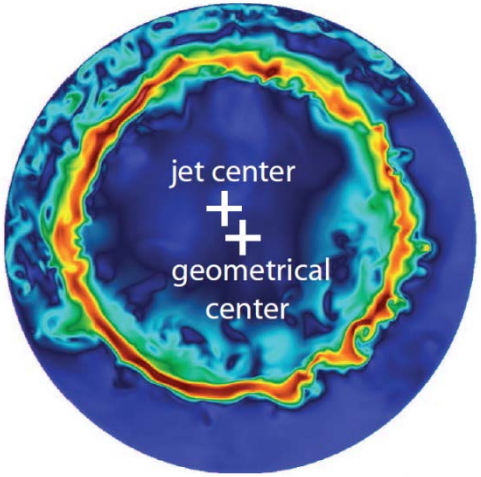
Summary - CCVs

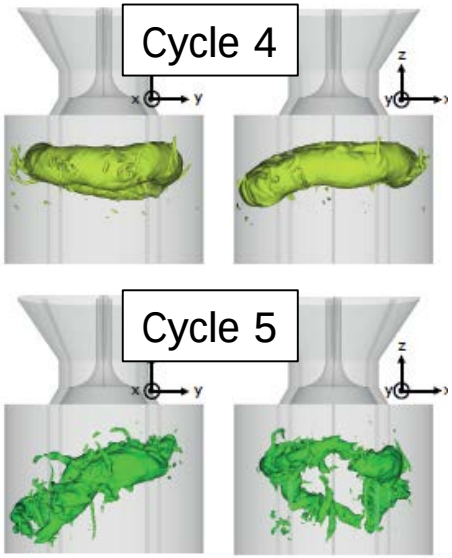
Radial velocity at TDC

Jet center at 45°CA

Vortex ring at BDC



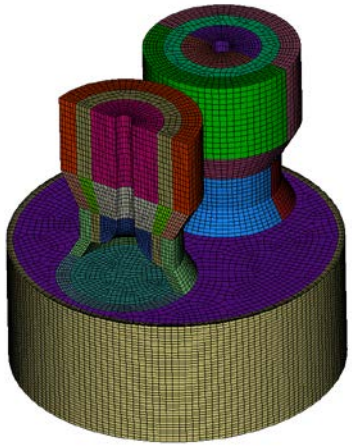




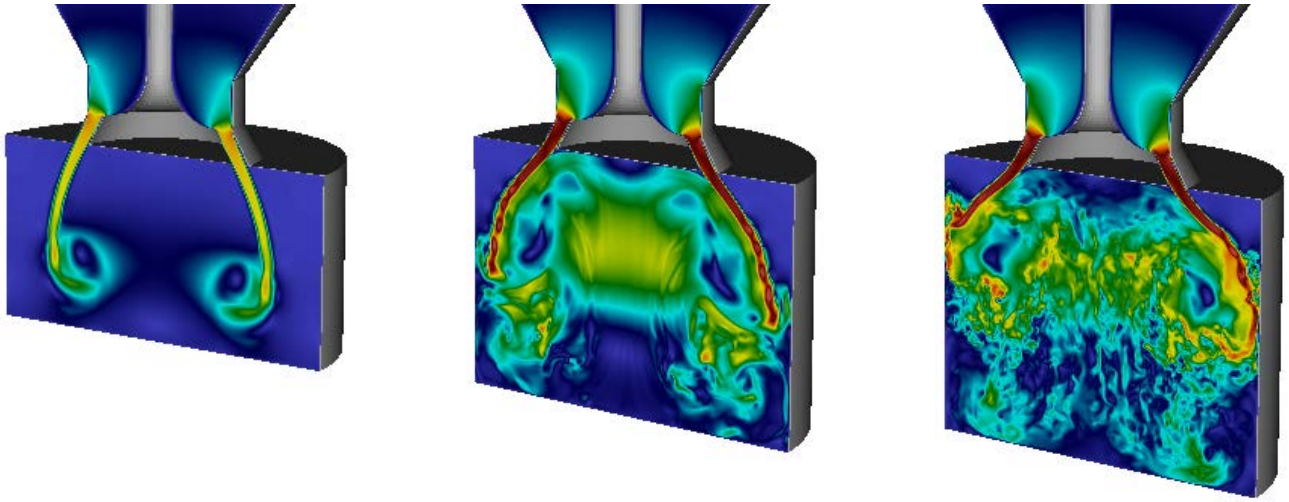
Conclusions and outlook

- DNS performed of engine-like geometry (11 consecutive cycles)
- Dynamic system identified which is responsible for the CCVs in this simplified geometry
- Results cannot be applied one to one to real engine configurations, but:
  - First description of cause-effect-relationships of CCVs in engine-like geometry
  - Results are a base for investigating CCVs in realistic engine geometries
  - Some findings are likely to apply also for more realistic engine geometries
- Excellent platform for the validation of LES simulations to capture CCVs (cause and effect relationships can be directly tracked)

- **Ongoing and future work:**
  - Compression stroke, wall heat transfer, combustion
  - Higher engine RPM, more realistic configurations
  - Establish database for model validation purposes



Thank you!



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