1st Daresbury-Jülich Workshop on HPC Applications in Fluid and Molecular Dynamics

Simulation of flows with immersed moving boundaries

Matthias Meinke
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RWTH Aachen University
Germany

People involved:

- Wolfgang Schröder
- Christoph Siewert
- Stephan Schlimpert
- Brito Gadeschi Gonzalo




Outline:

- Raindrop formation
- Combustion instabilities
- The zonal flow solver (ZFS)
- Methods involved
- Parallelization
- Scaling tests
- Conclusions

Some research projects at AIA:

- Base flow rocket aerodynamics
- Hybrid turbulence models RANS-LES
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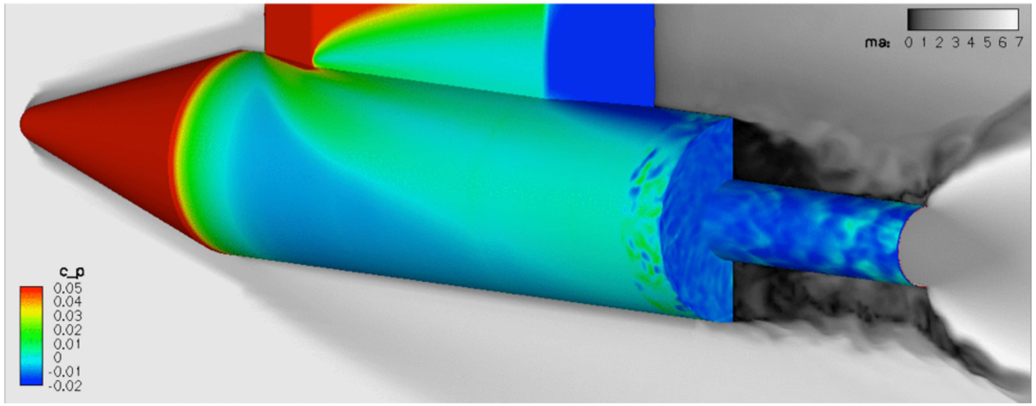
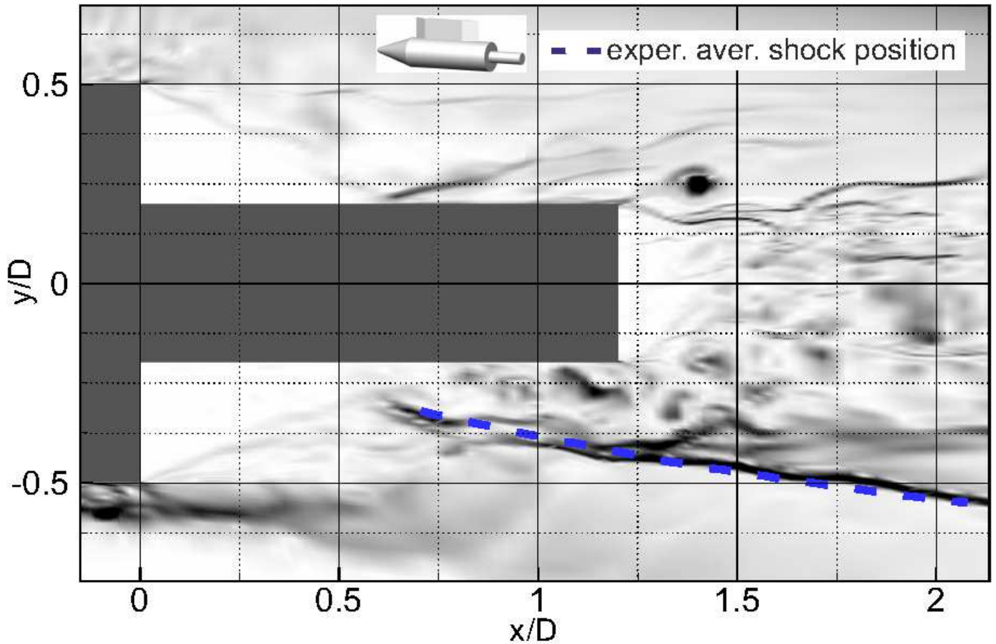
- Aeroacoustics
- Flow analysis in human airways
- DNS of flows in internal combustion engines
- Raindrop formation in clouds
- Combustion instabilities in burners





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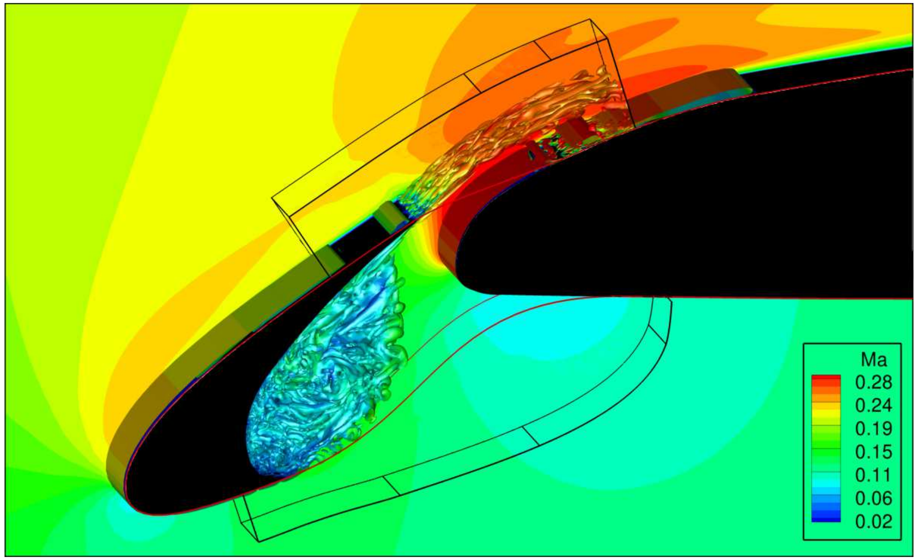

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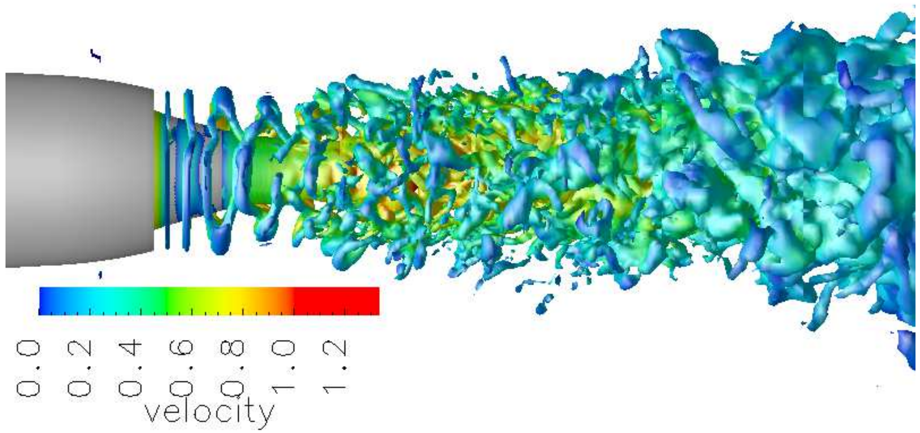

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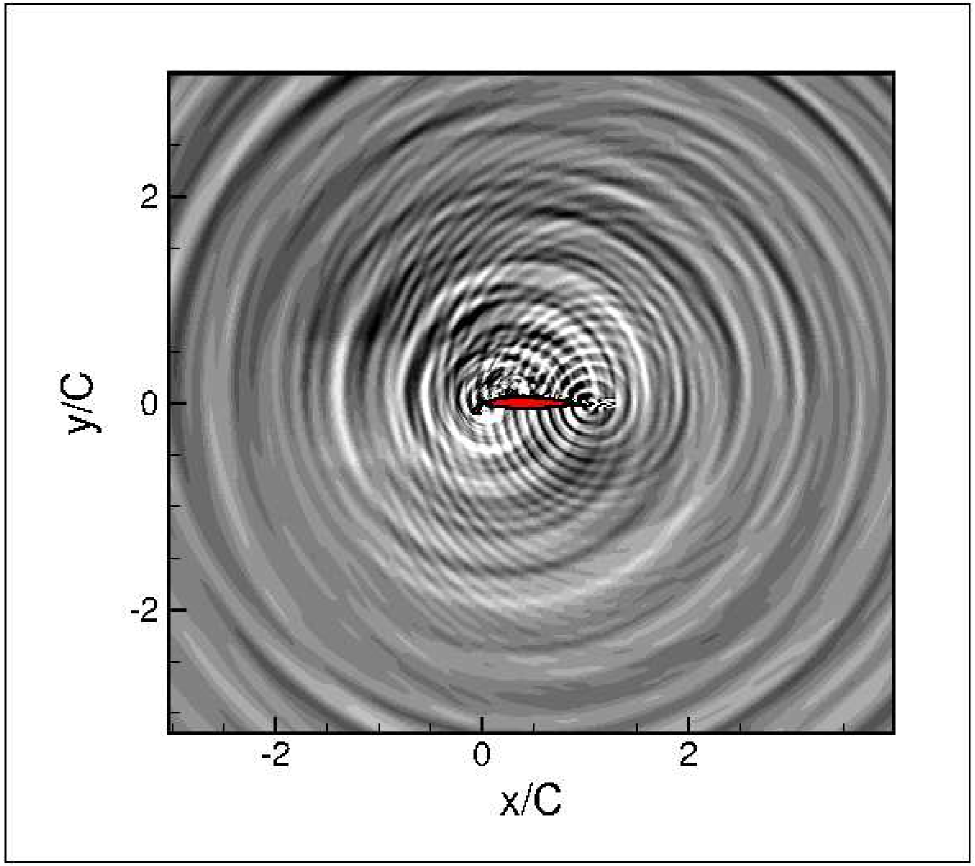

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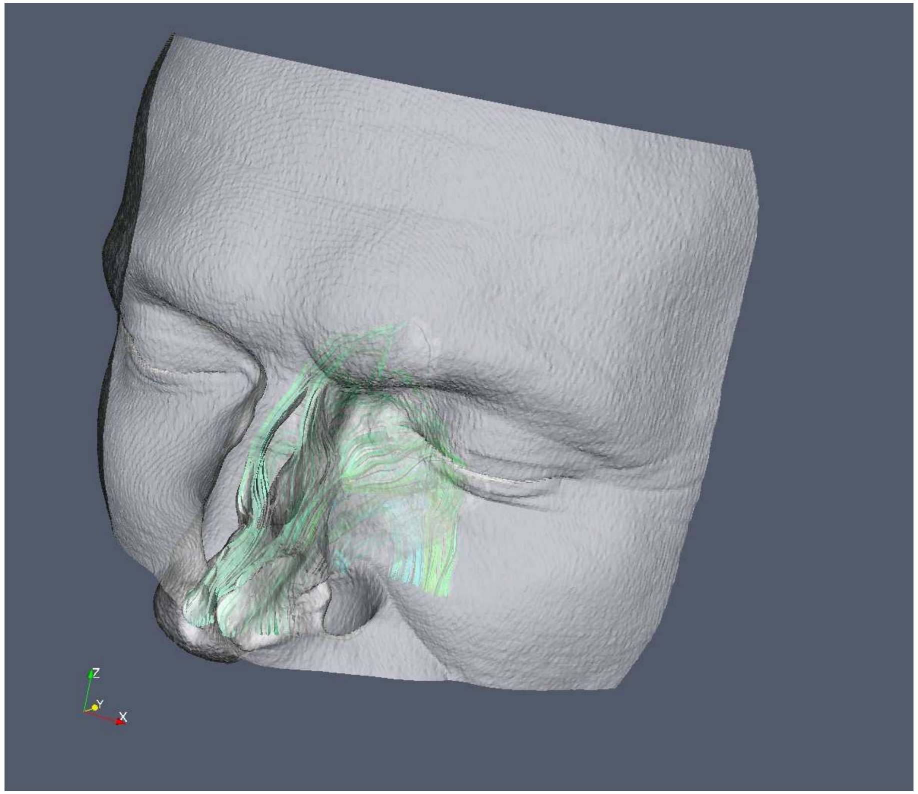

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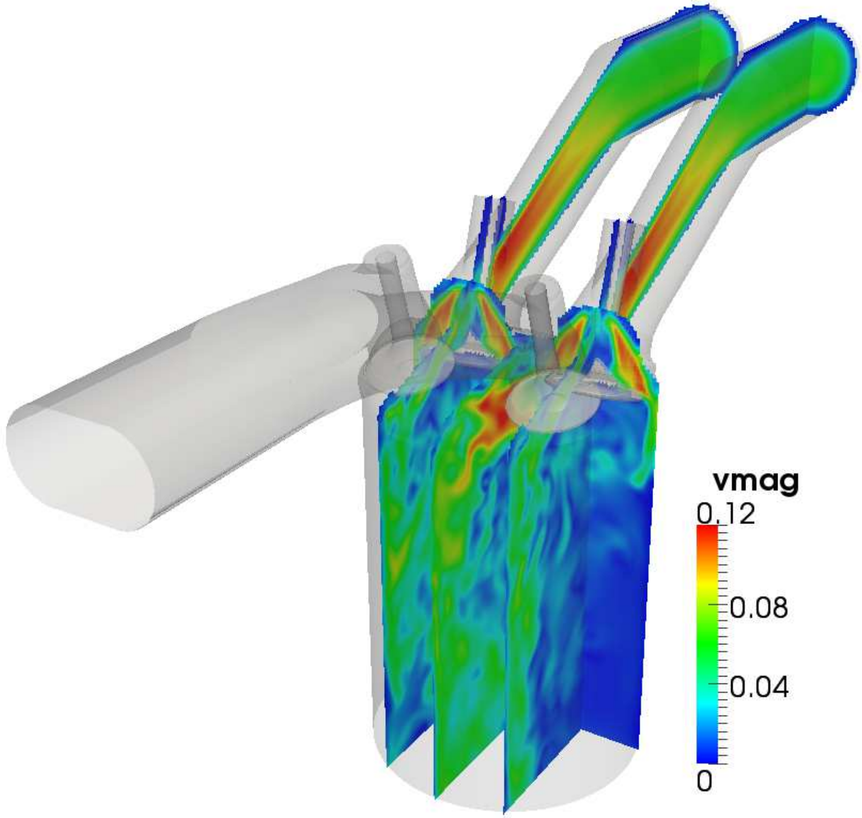

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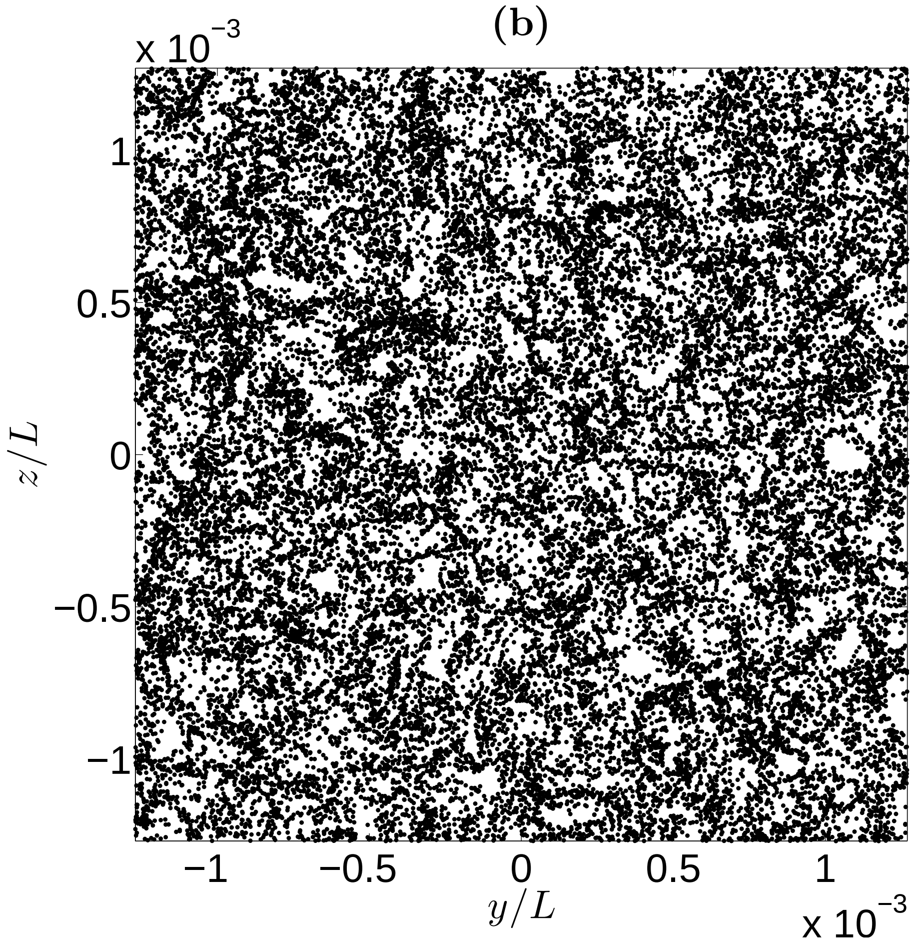

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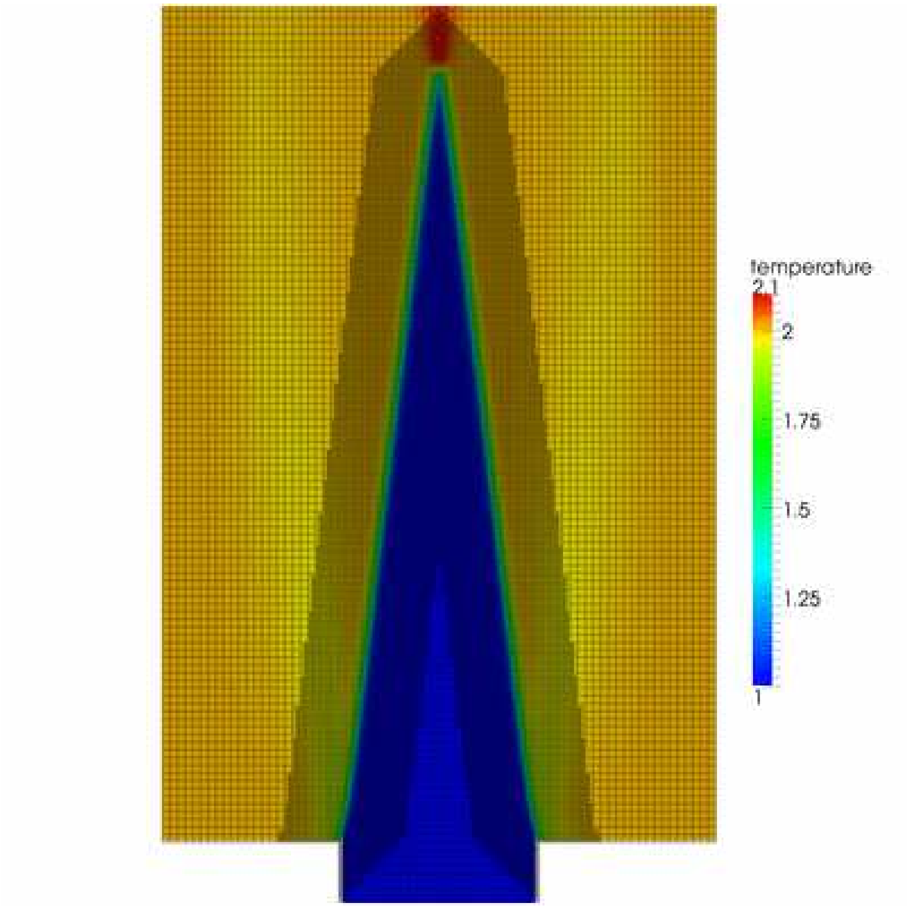
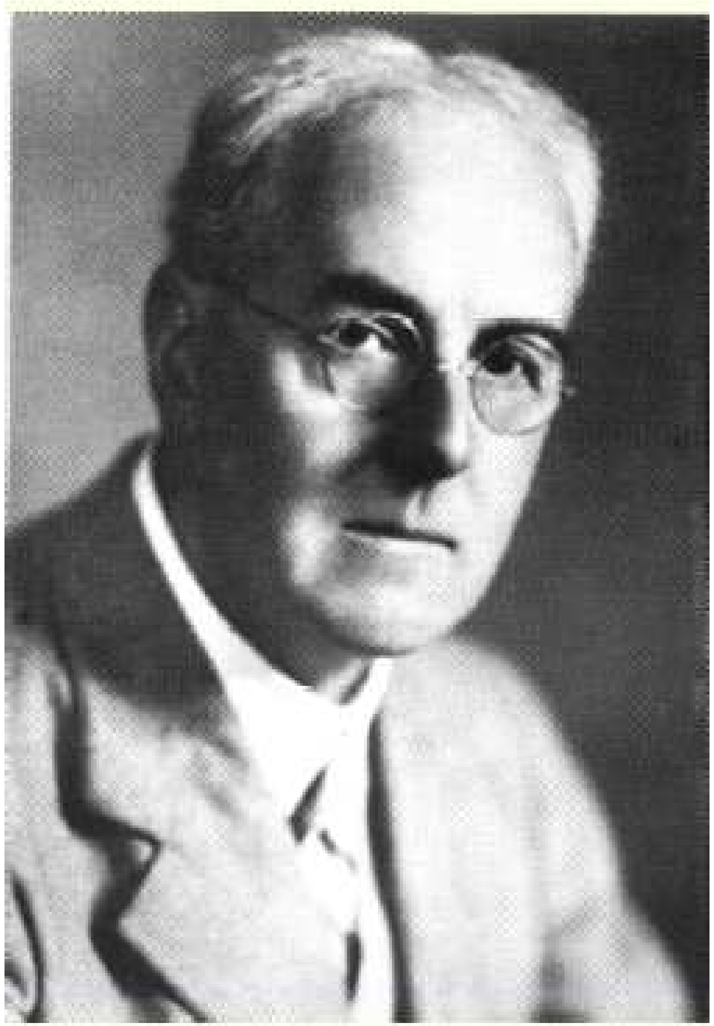


- AIA: Linux Cluster, DELL 1950, 400 Cores (XEON 5160, 3Ghz)
- RZ RWTH Aachen: Bull Cluster, 27700 Cores (Intel), 292 TFlops
- (HLRS Stuttgart: NEC SX-9, 128 Cores, 13.1 TFlops)
- HLRS Stuttgart: Cray XE6, 113,664 Cores (AMD Interlagos, 2.3GHz) 1.1 PFlops
- FZ Jülich: IBM Blue Gene/Q, 458,752 Cores (IBM PowerPC, 1.6 GHz) 5.9 PFlops

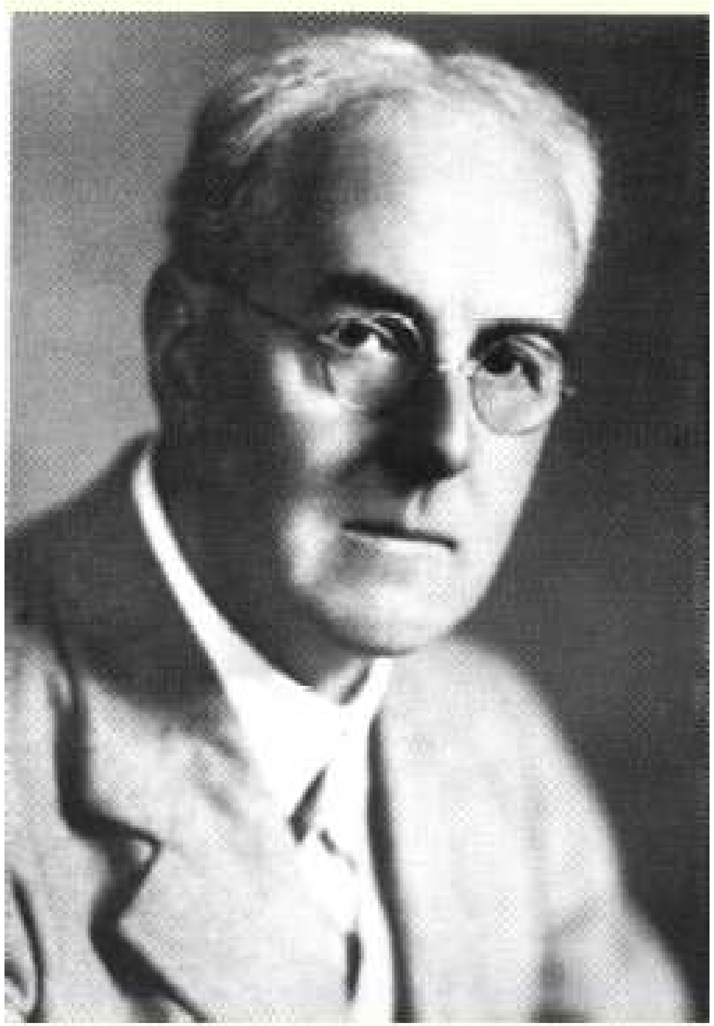
Cray XE6 Hermit @ HLRS

IBM JuQueen @ FZ Jülich



Lewis Fry Richardson
1881-1953

Weather forecasts

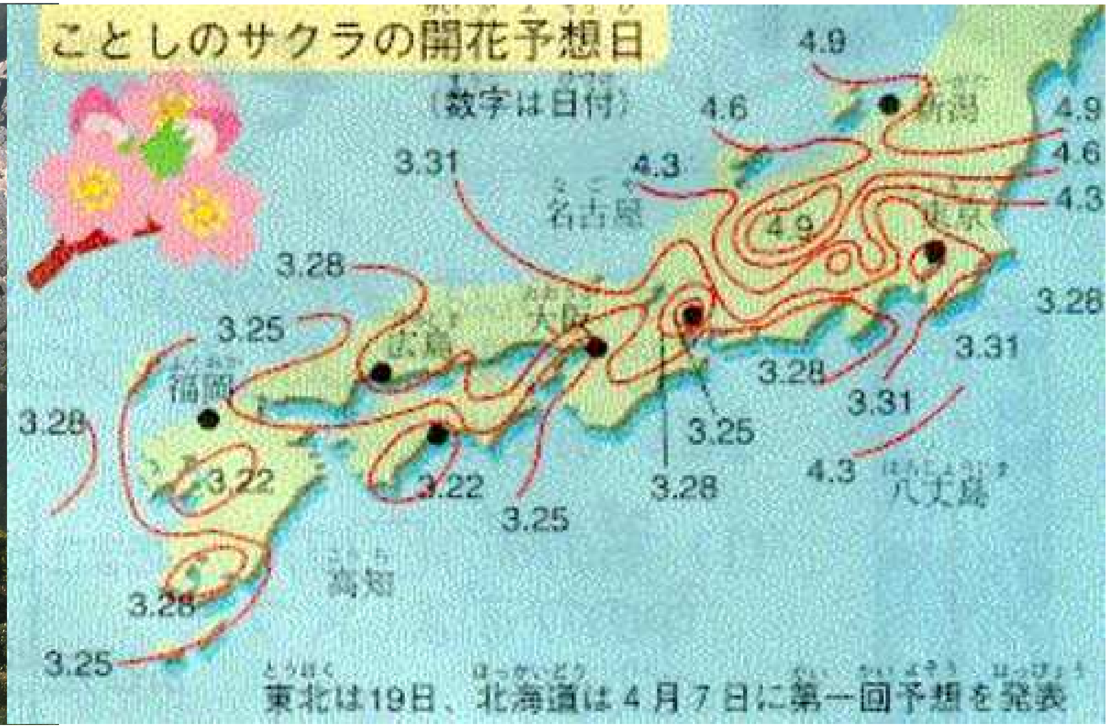


Lewis Fry Richardson
1881-1953

The first numerical weather forecast was carried out by Lewis Fry Richardson in 1920. He described his ideas in *Weather Prediction by Numerical Process*, 1922:

Imagine a large hall like a theatre...A myriad computers are at work upon the weather of the part of the map where each sits, but each computer attends only to one equation or part of an equation. The work of each region is coordinated by an official of higher rank. Numerous little night signs display the instantaneous values so that neighbouring computers can read them. Each number is thus displayed in three adjacent zones so as to maintain communication to the North and South on the map...

Forecasts can be a diffcult task:



In Japan the state weather forecast had to predict the beginning of the cherry blossom (sakura zensen) until 2010

Weather forecasts

Accurate weather predictions are

- important for society, agriculture, air traffic, etc.
- methods for weather forecasts contain various models for physical processes
- increasing the accuracy of forecasts is of fundamental interest

9 days

3 days

1 day

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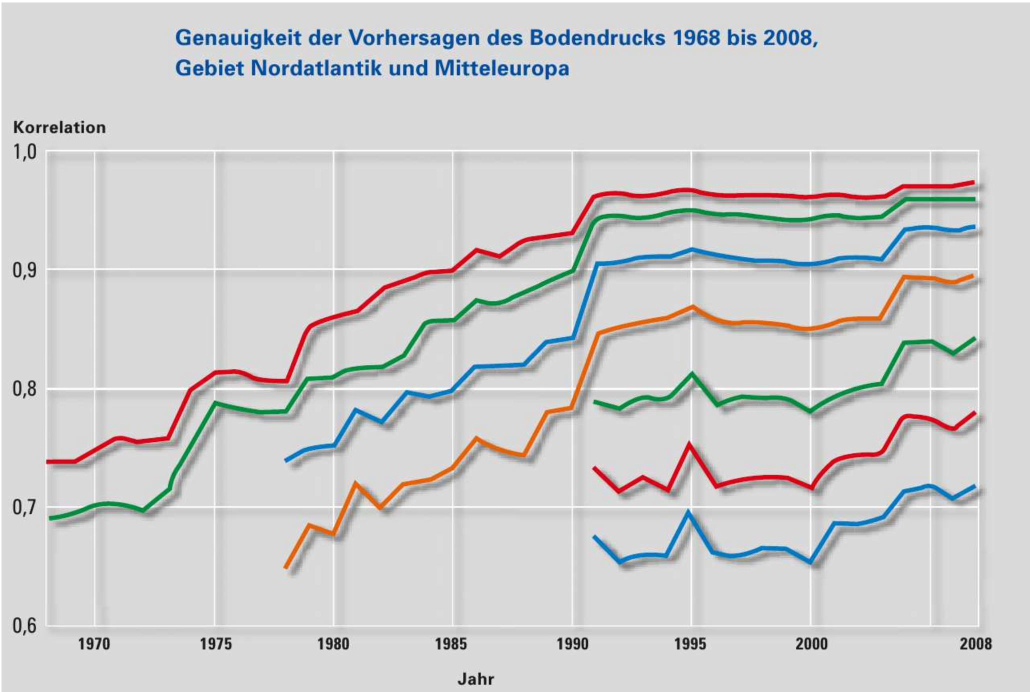

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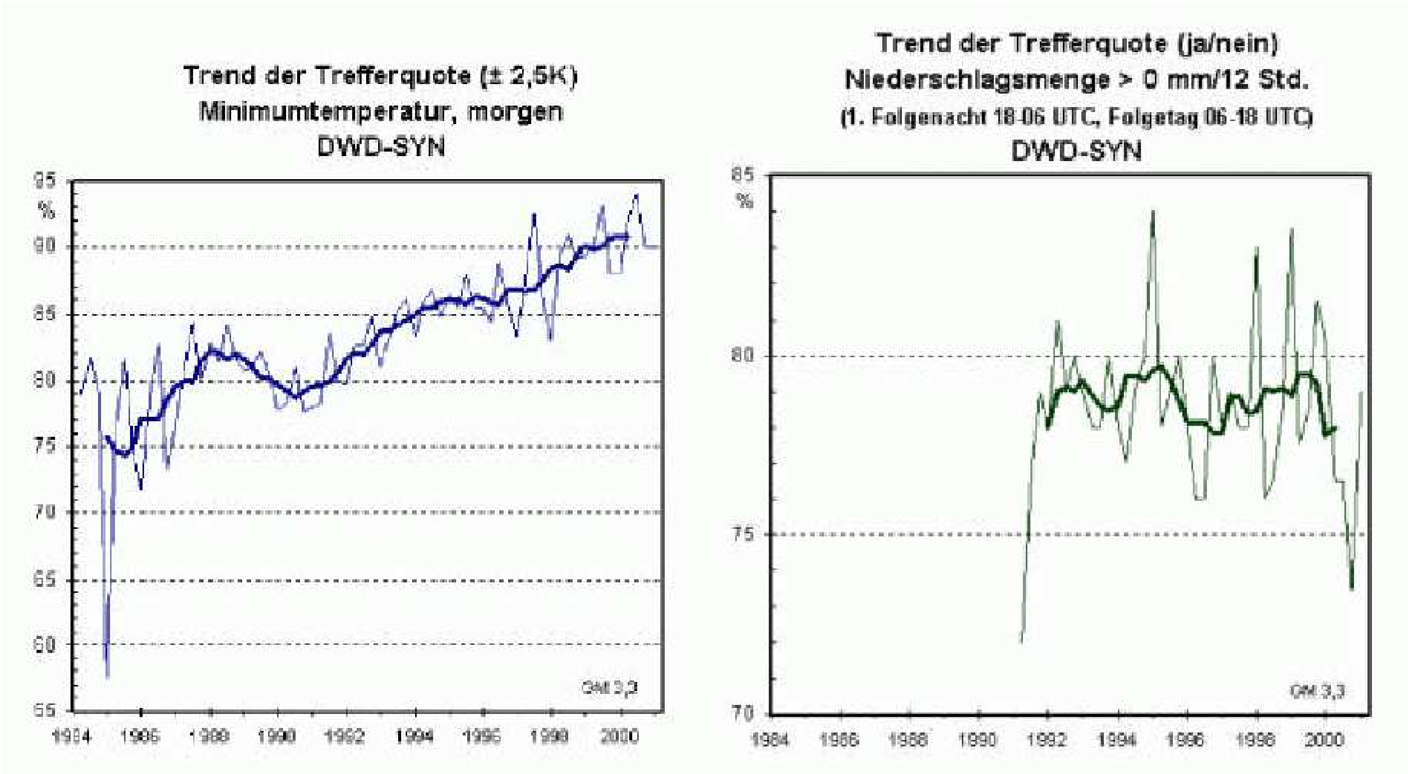


Classical model for raindrop formation

step	mechanism	drop radius
1	aerosol particle absorb water vapor	up to 5 μm
2	condensational growth	5-20 μm
3	growth due to particle-particle collisions	50-5000 μm

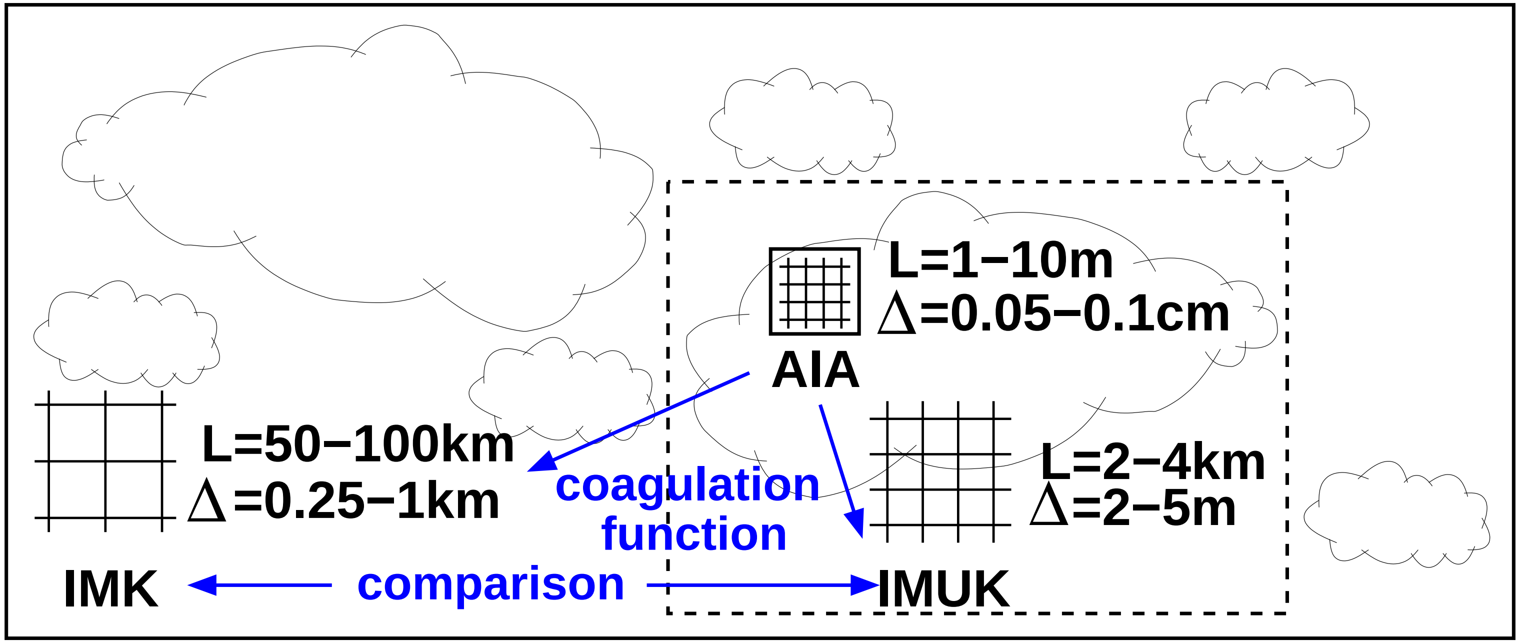
Particle collision are assumed to occur due to different speeds of the particles with different droplet radii because of the different terminal velocities while falling under the influence of gravity

raindrop formation is faster than predicted by the classical theory![1]

$\rightarrow$ Investigation of the influence of the turbulent flow field on the collision rates

[1] Devenish et al., 2012. Droplet growth in warm turbulent clouds. Q. J. R. Meteorol. Soc.

Interaction of project partners



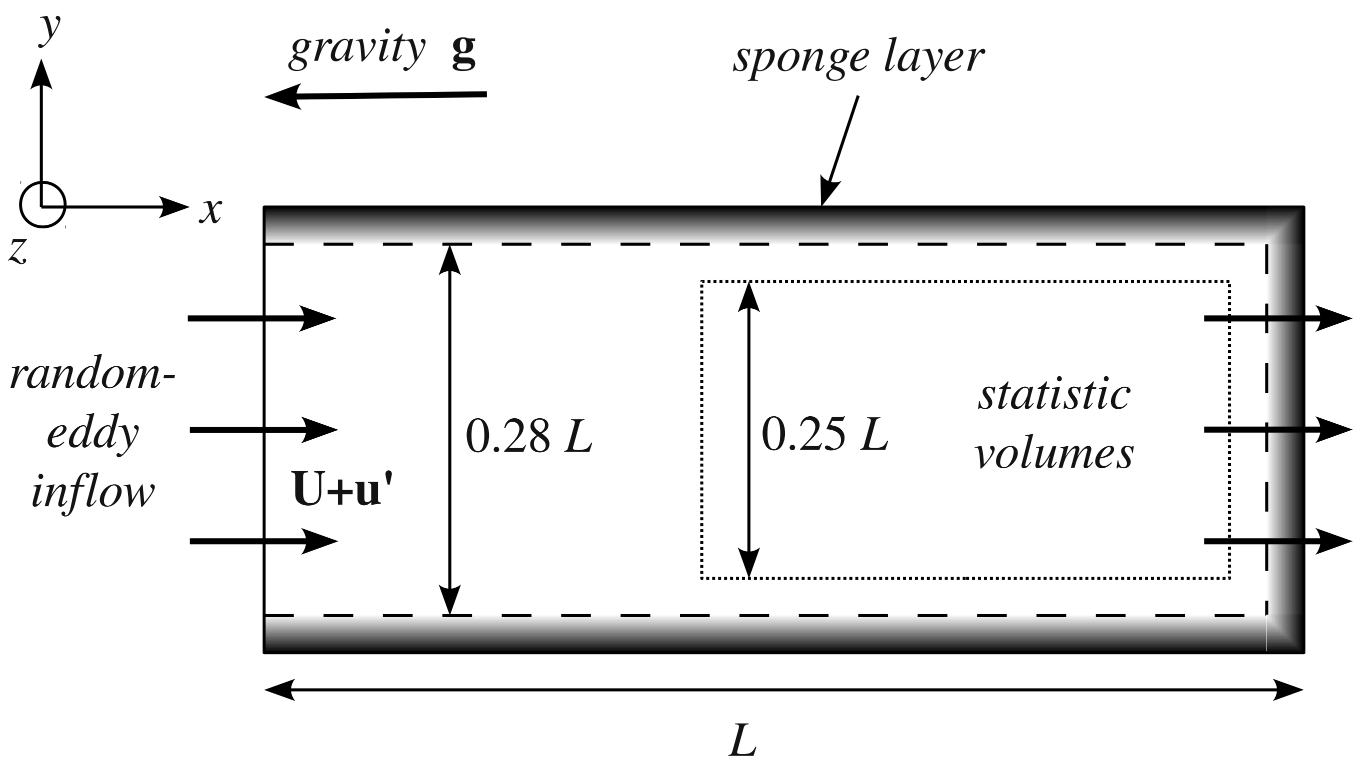
range of length scales:

physical scale	length
regional cloud system	100 km
single cloud	5 km
rain drop	1mm
smalles scale of turbulence	0.5 mm
cloud droplet	20 μm
condensation nucleus	1μm

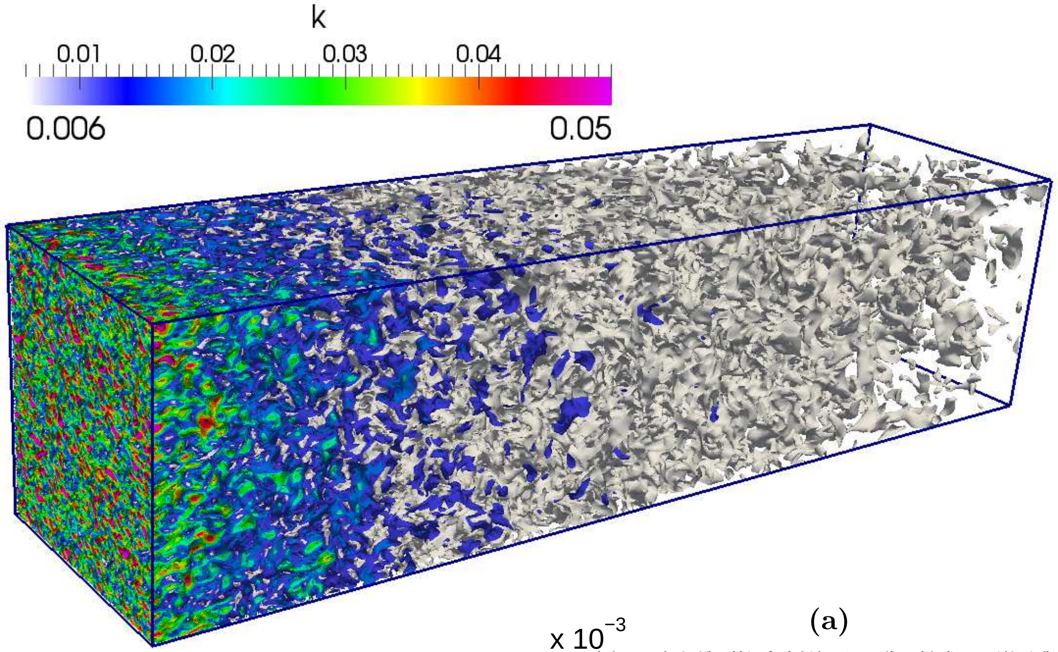
DNS of a turbulent flow field (Reynolds number $\mathrm{Re}_L = 80.000$)

- resolving the smallest turbulent scales
  - smallest scale: Kolmogorov length $\eta_k \approx 0.5$ mm
  - largest scale $L \approx 1$ m
- generate synthetic turbulence at the inflow boundary

53 million cells
45 million particles



Flow field and particle distribution

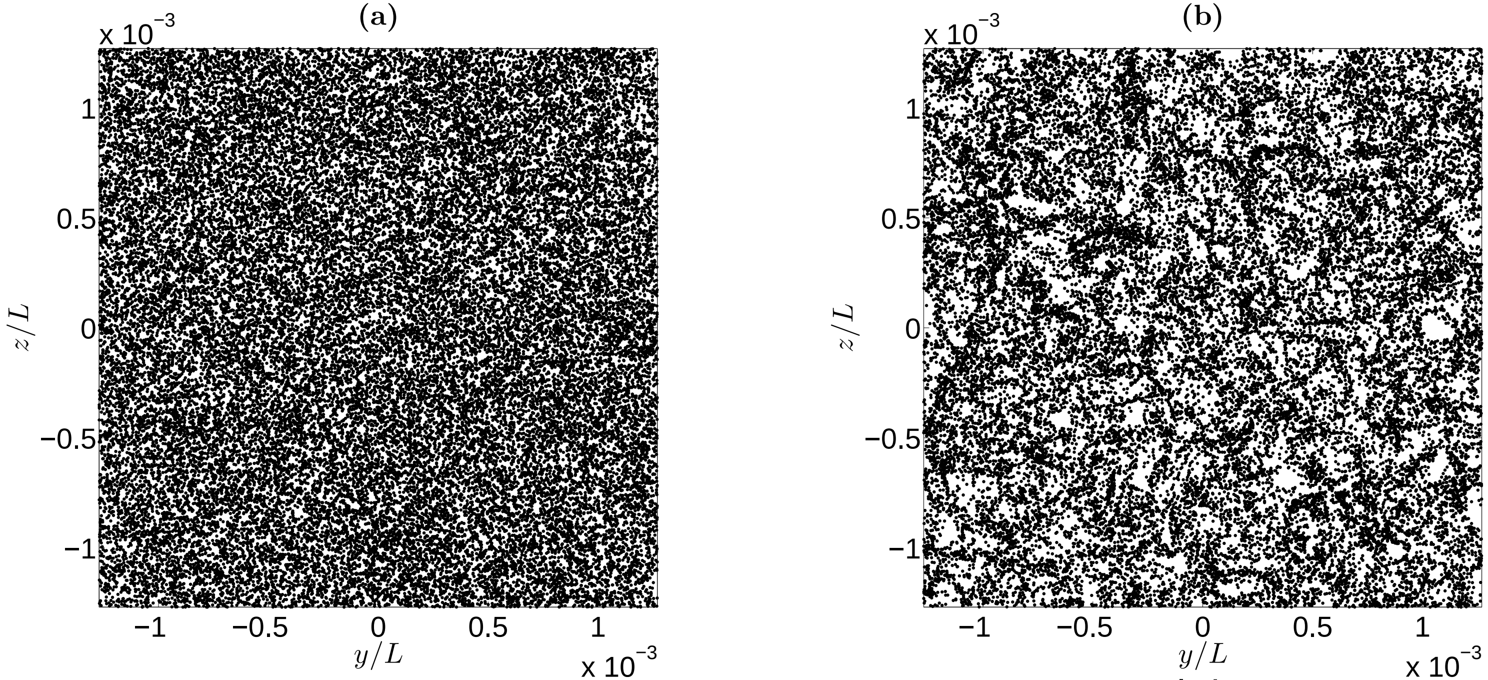


5 turbulent kinetic energy contours (left)

particle distributions for two Stokes numbers St=$\frac{\tau_p}{\tau_\eta}$

St $\ll$ 1 (bottom left)

St $\approx$ 1 (bottom right)

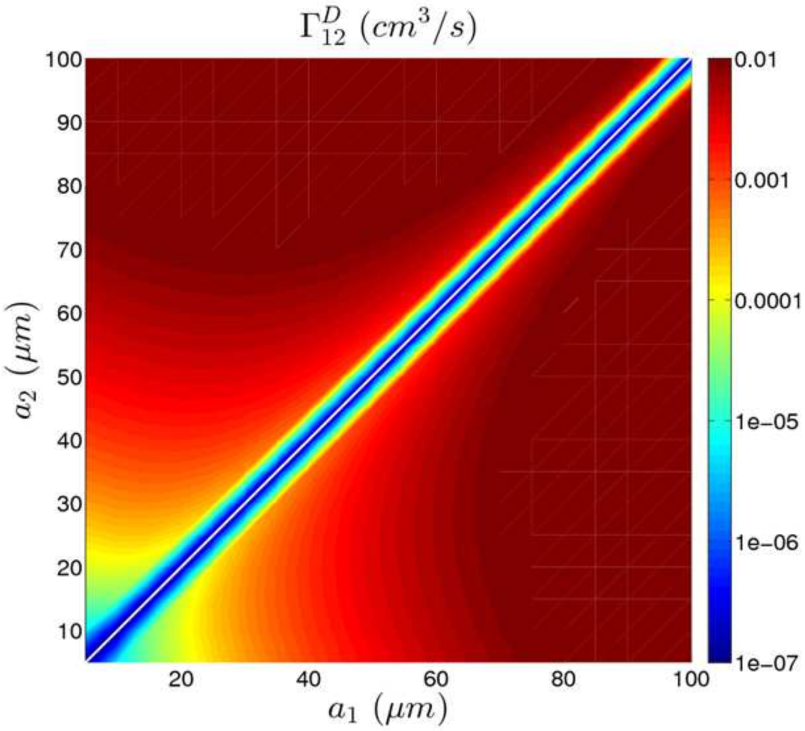


Particle collision statistics

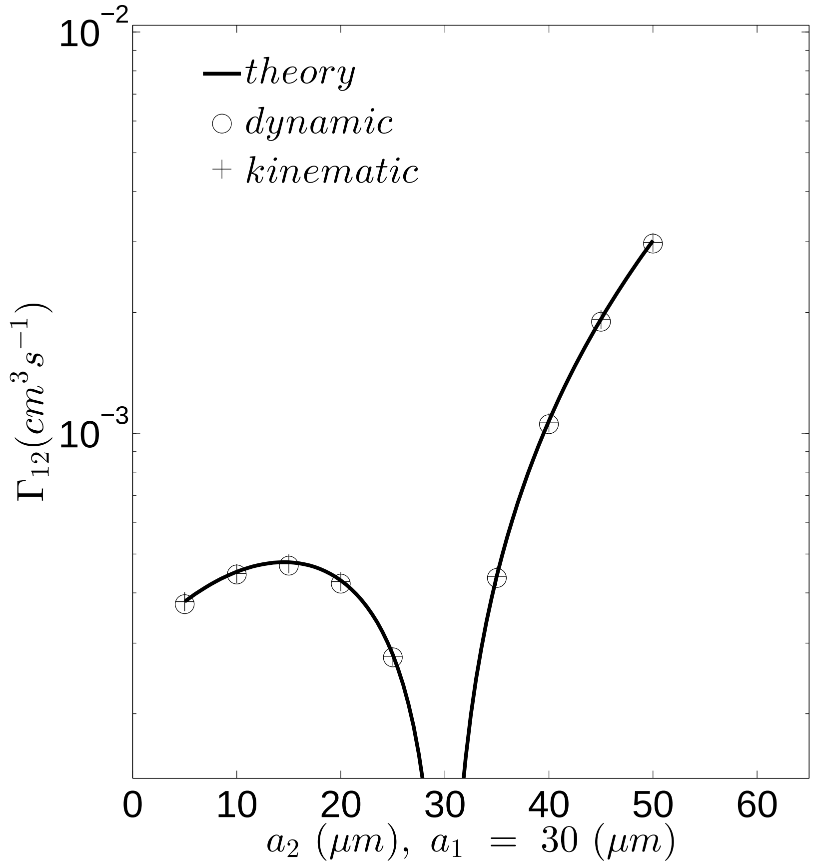
collision rate: $\dot{N}_{12} = \Gamma_{12}\, n_1\, n_2$

n_1, n_2: particle concentrations, Γ_{12}: collision kernel

Results for laminar flow:



analytic solution



numerical results

Particle collision statistics

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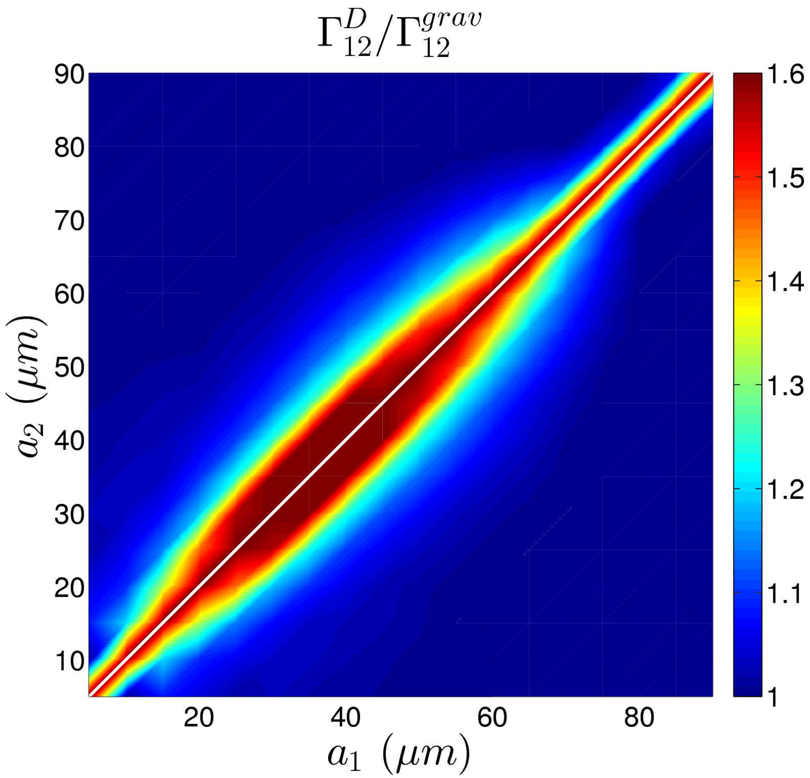
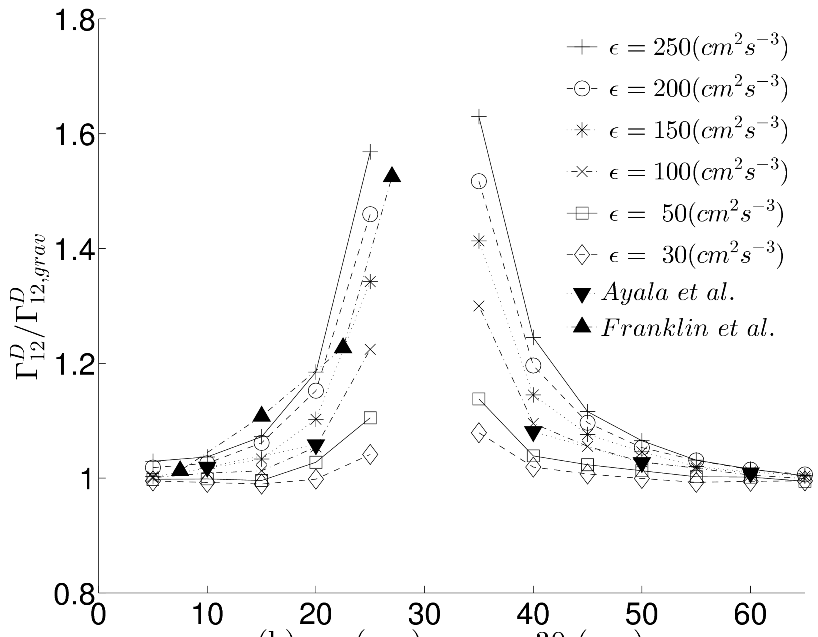
Results for turbulent flow:





(b) a_2 (μm), $a_1 = 30$ (μm)

parametrization $\Delta\Gamma(R, \tau, \epsilon) = 0.00035\,(1 + \tanh(R/12 + \epsilon/240 - 4))$

Reduction of Emissions

Generation of energy and transportation requires extensive burning of fossil fuels emitting large quantities of CO_2, but also NO_x, unburned hydrocarbons, etc.

- efficiency increase reduces the amount of emitted CO_2, which is, however, often connected with higher combustion temperatures

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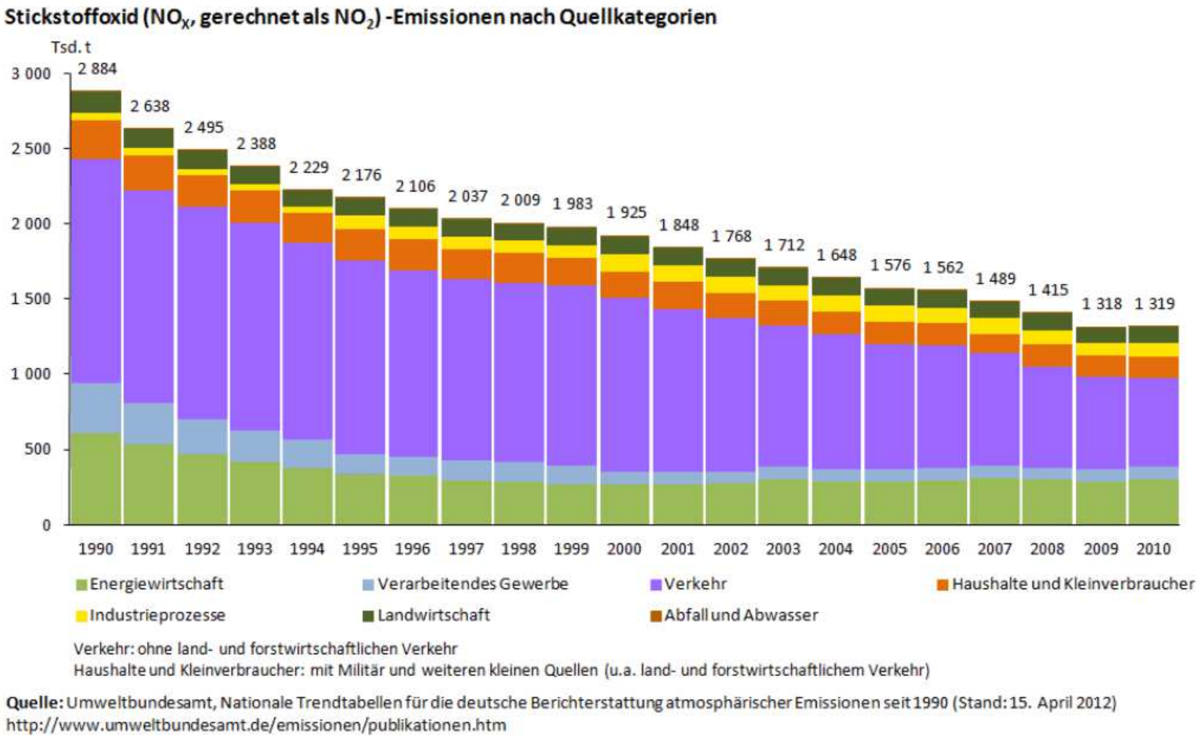

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- higher combustion temperatures enhance the production of NO_x
- Lower combustion temperatures can be achieved by lean combustion, i.e. using a higher air/fuel ratio than stochiometric conditions

Reduction of Emissions

Further aspects for emissions from air transportation

- Aircraft traffic will increase considerably in the next years
- 2001 the Advisory Council for Aeronautics Research in Europe (ACARE) has set reduction targets of 50% in CO2 and of 80% in NOx for 2020
- Politics in EU has decided to charge aircraft traffic according to emissions

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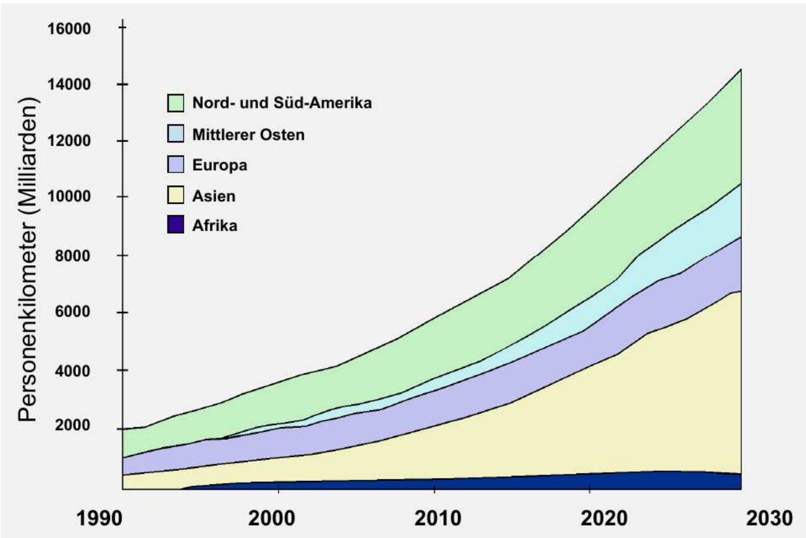
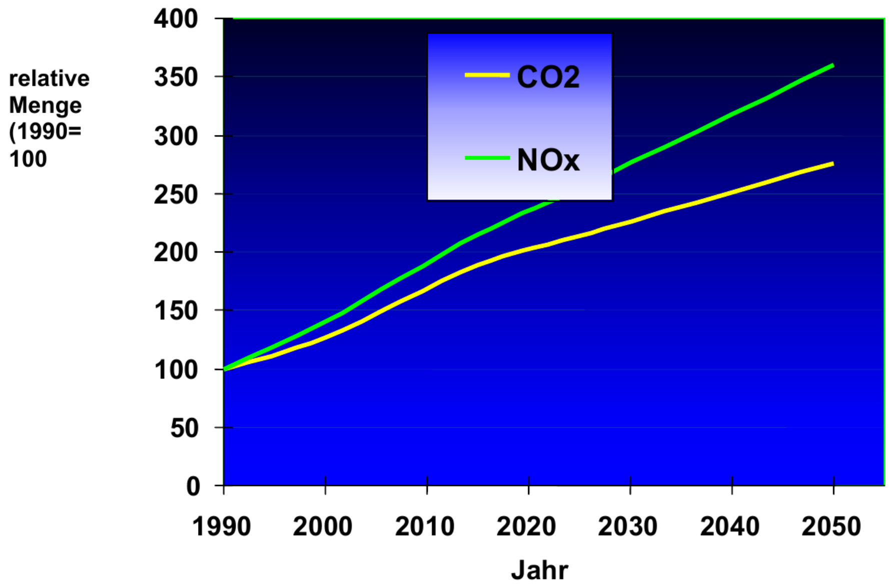
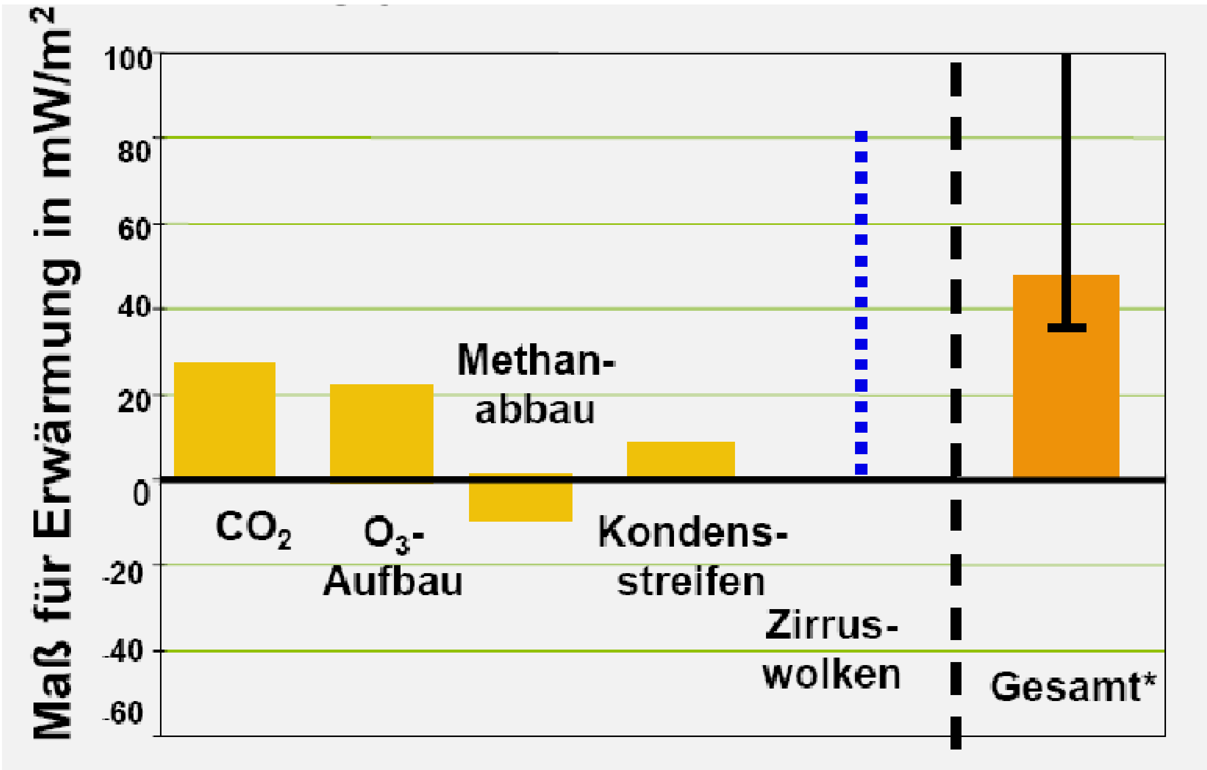




Reduction of Emissions

- Some uncertainty how NO_x in the upper tropospehre/lower stratospehre affects global warming over Ozon budget



Reduction of emissions and increasing efficiency for burning chambers by

- lean premixed combustion, leading to lower flame temperature, and thus less NO_x and soot
- enhanced mixing of fuel with air leads to homogeneous temperature distributions and thus to lower CO and unburned carbon hydrogen emissions

For lean premixed combustion the following problems are observed:

- combustion instabilities occur generating acoustic waves with large amplitude (up to 150db), which can damage the structure of the burning chamber
  $\rightarrow$ devices to reduce oscillations are frequently added still nowadays when the combustion facility is taken into service
- increased mixing can cause flashback of flames into the injector with the possibility of destruction

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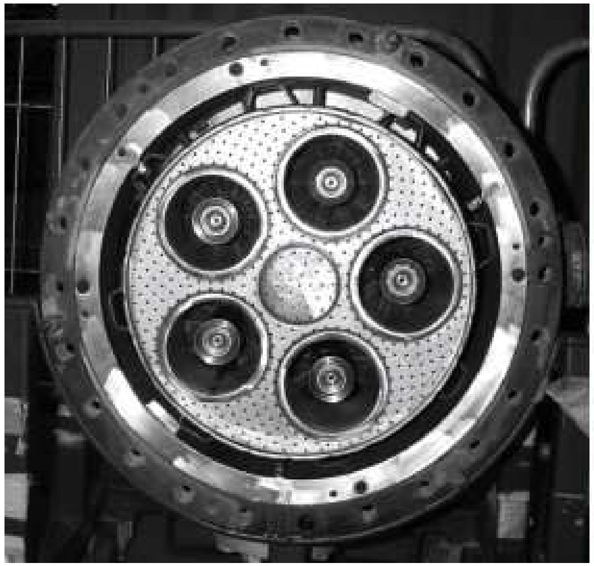

Burner asembly

Burner assembly damaged due to combustion instabilities

Goy et al., Chapter 8 by T. Lieuwen, Progress in Astronautics and Aeronautics, 210, pp. 163-175, 2005

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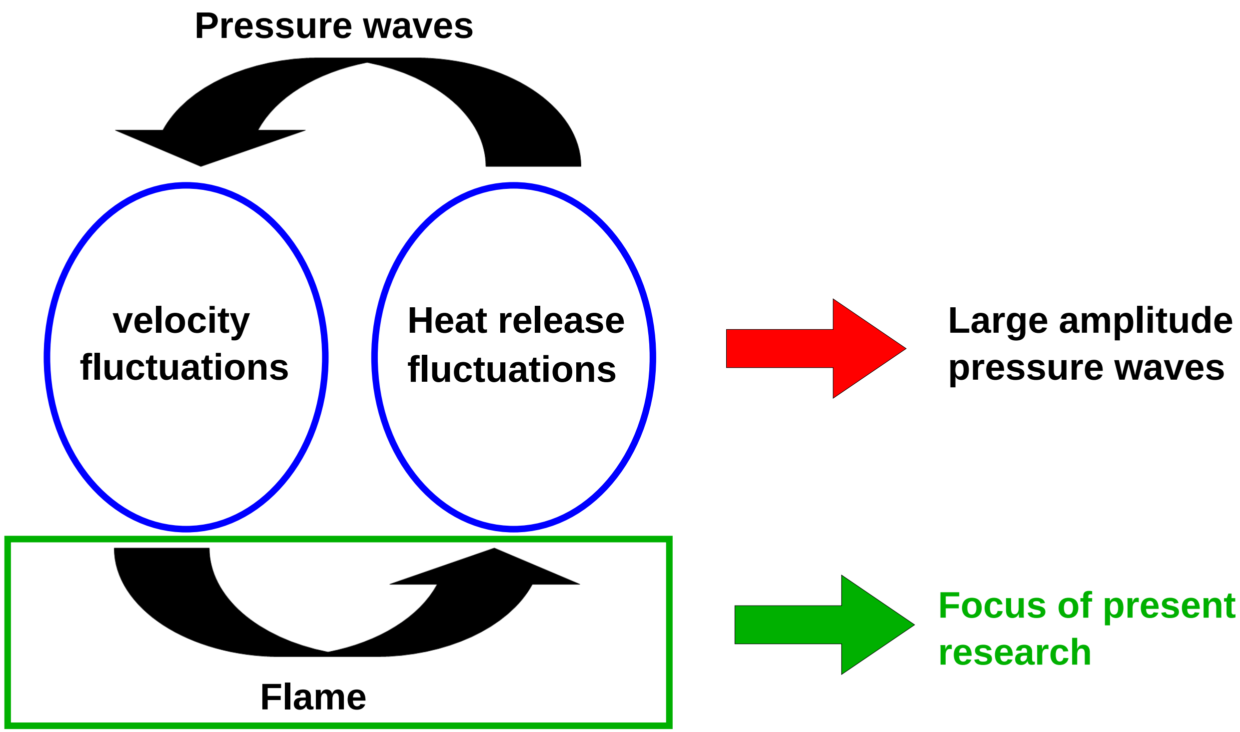


Colloborative Research Centre (SFB) 686 at RWTH Aachen and Univ. Bielefeld

Goal: stabilization of the combustion process can be obtained by an active control strategy

- different active control strategies are available: e.g. sound waves, fuel/air mass flux, etc.
- predictive active control has to work in real time, i.e. CFD solutions are not applicable
- reduced or simplified models are required which model the flame response to various excitations

Perform detailed CFD simulations including combustion to develop and calibrate reduced order models

Zonal flow solver (ZFS)

Solver for compressible flows [1,2]
- 2nd order accurate in space
- low dissipation AUSM method
- 2nd order Runge−Kutta method

velocity field

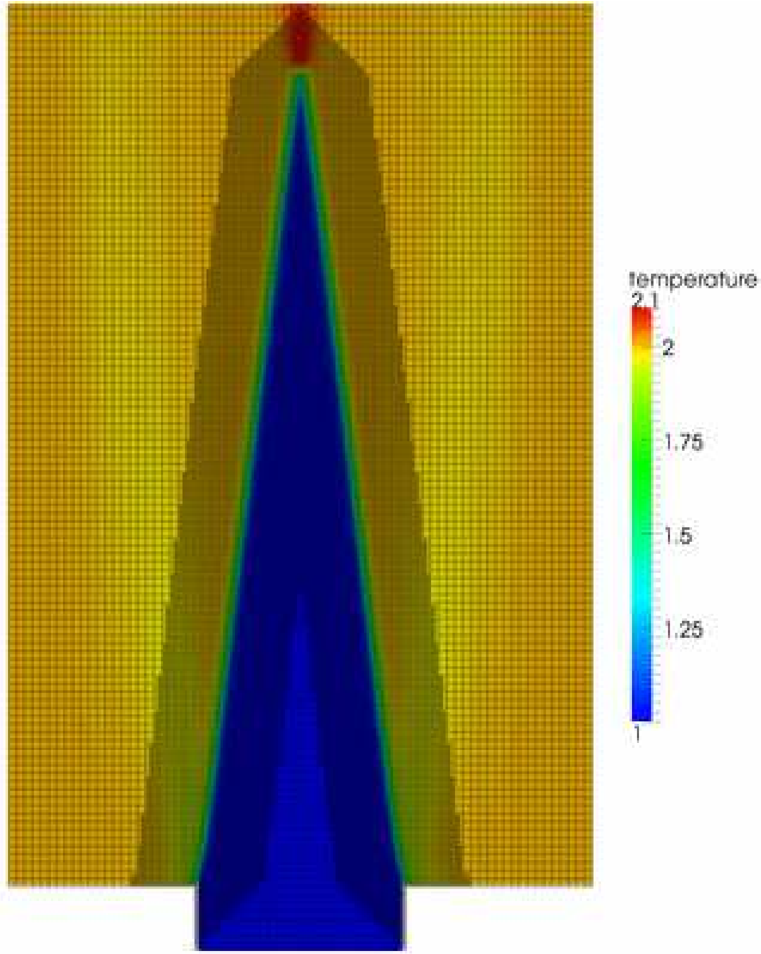
Level−Set solver [1,2]
- 5th order central scheme
- 5th order central scheme
- 3rd order TVD Runge−Kutta method
- 5th order WENO scheme
  for constrained reinitialization
- adaptive refinement at flame front

position of flame front
local flame speed

Combustion model
- progress variable approach [3]

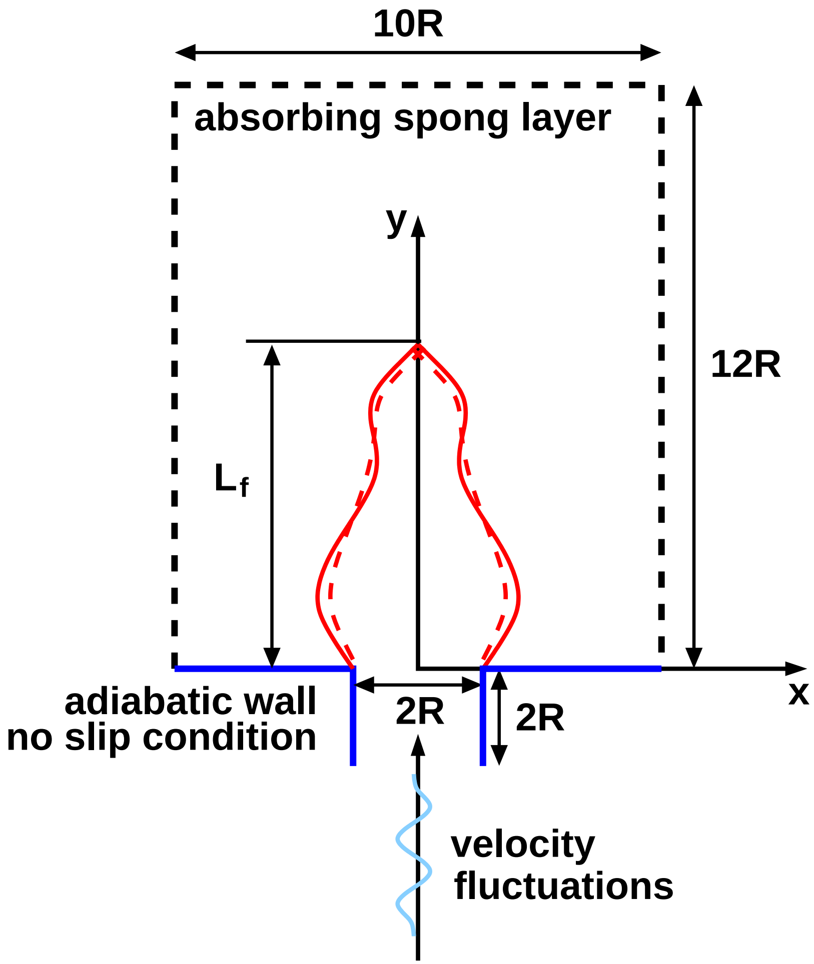
flow field

heat release



[1] D. Hartmann, M. Meinke, W. Schröder, J. Comp. Phys. 229, 1514-35, 2010.
[2] D. Hartmann, M. Meinke, W. Schröder, Combust. Flame 158, 1318-1339, 2011.
[3] V. Moreau, B. Fiorina, H. Pitsch, Combust. Flame 156, 801-812, 2009.

Computational Setup and Results



$$v(x,t) = v_o(x)(1 + \frac{v'}{v_o}\sin(\omega_f t))$$

Flow parameters: Re=592, M=0.0714, s_{L0}=0.00857, $\frac{v'}{v_0}$=0.1

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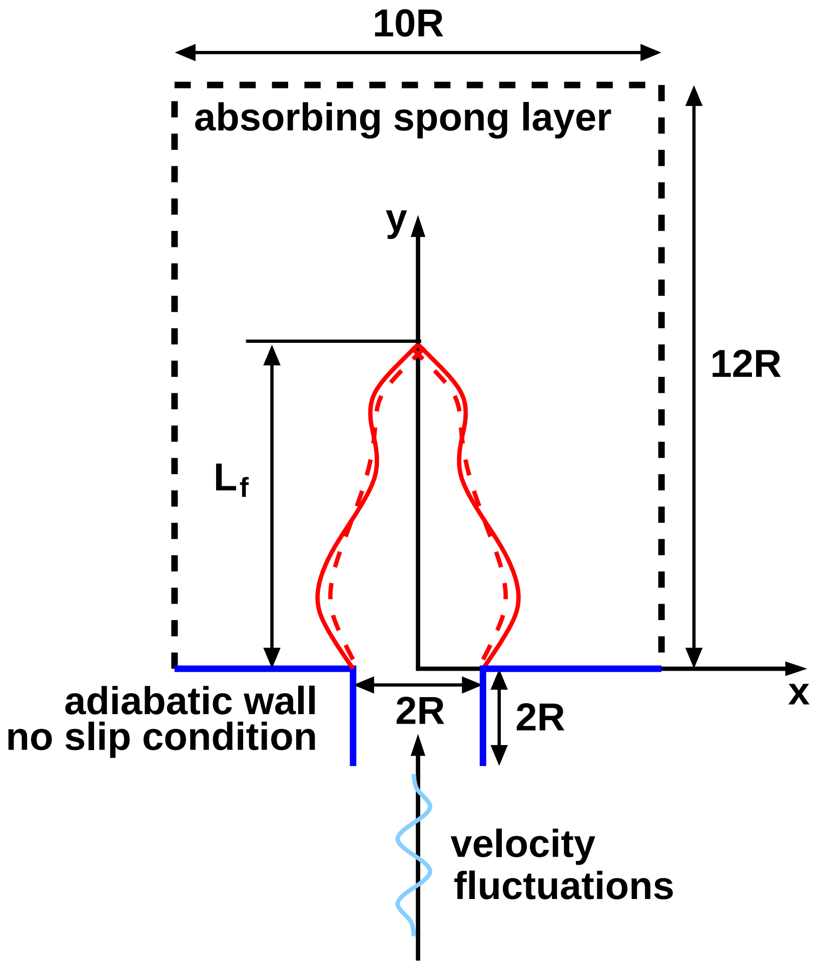

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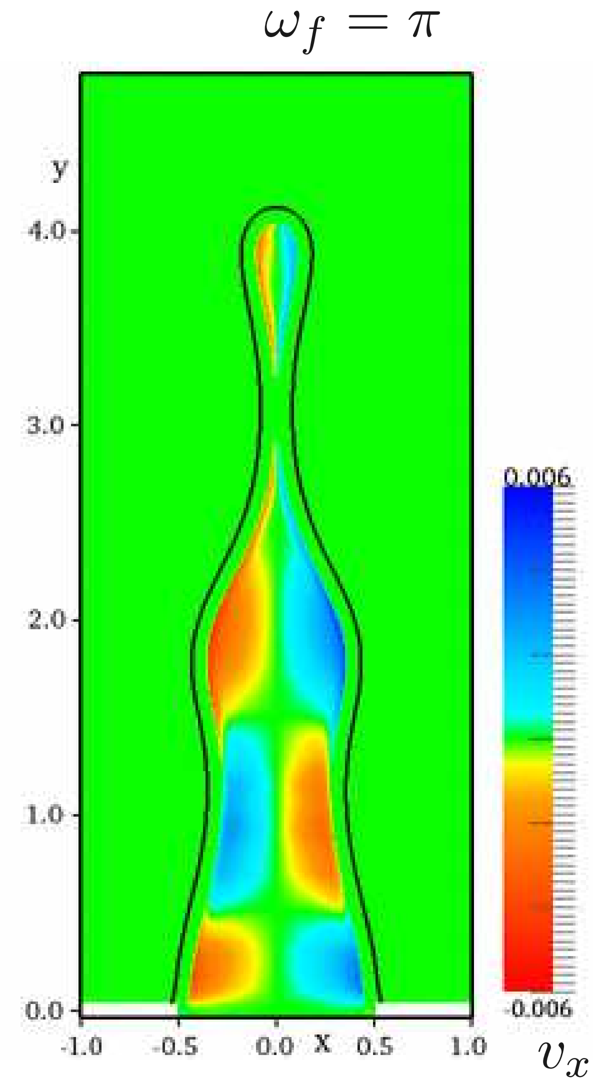

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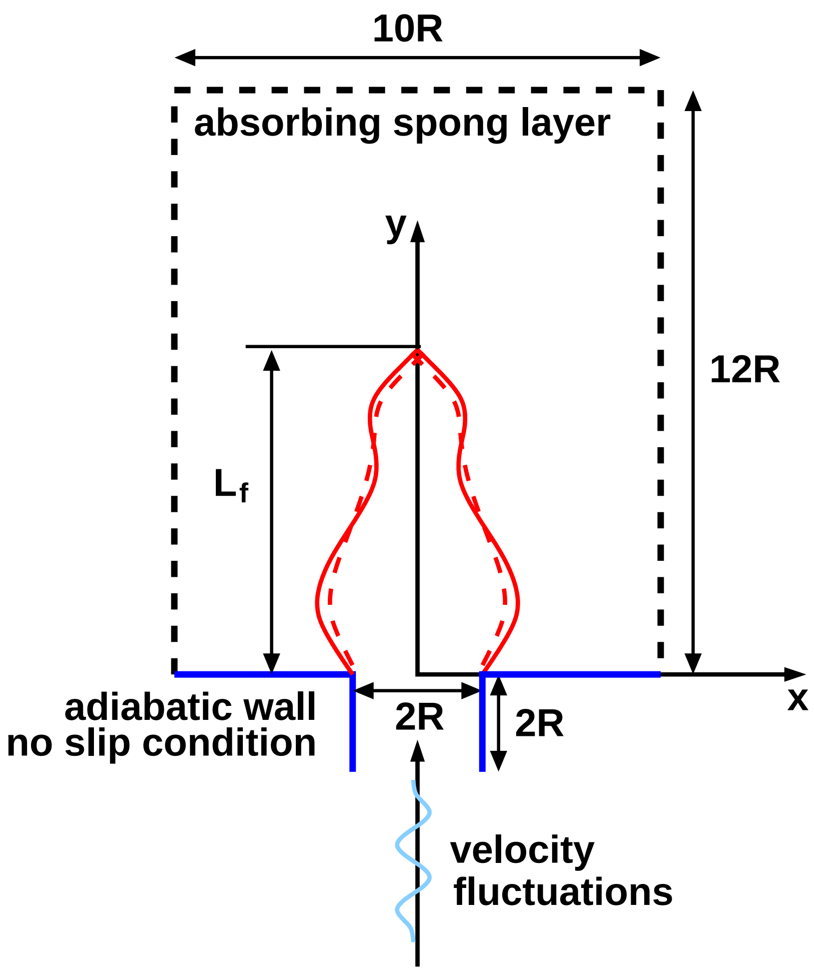

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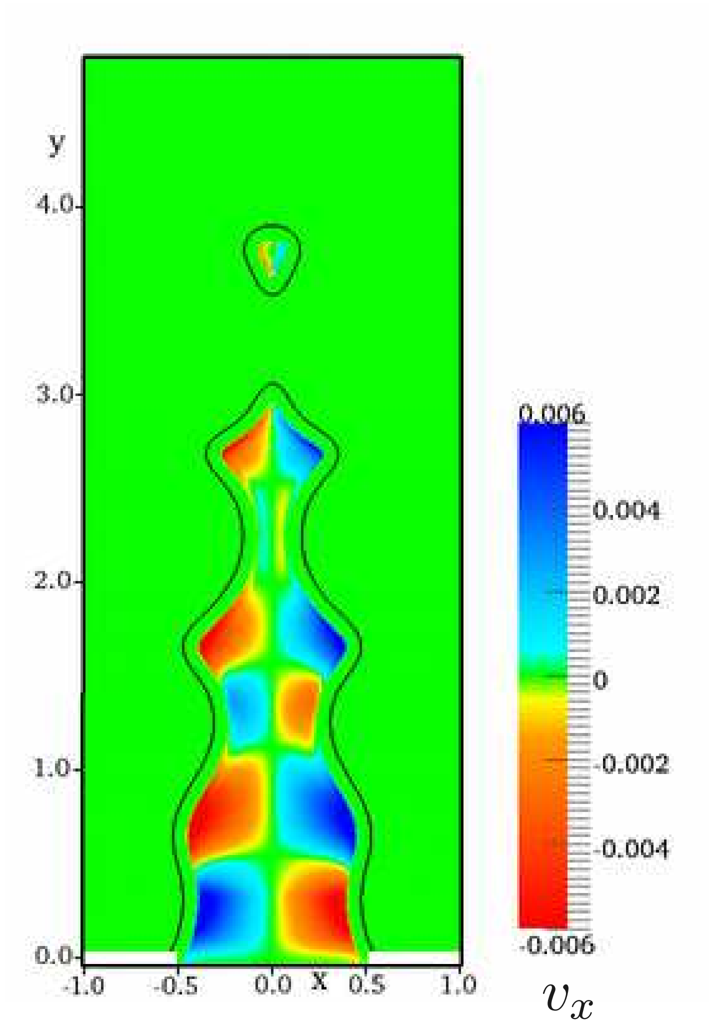
$\omega_f = 2\pi$



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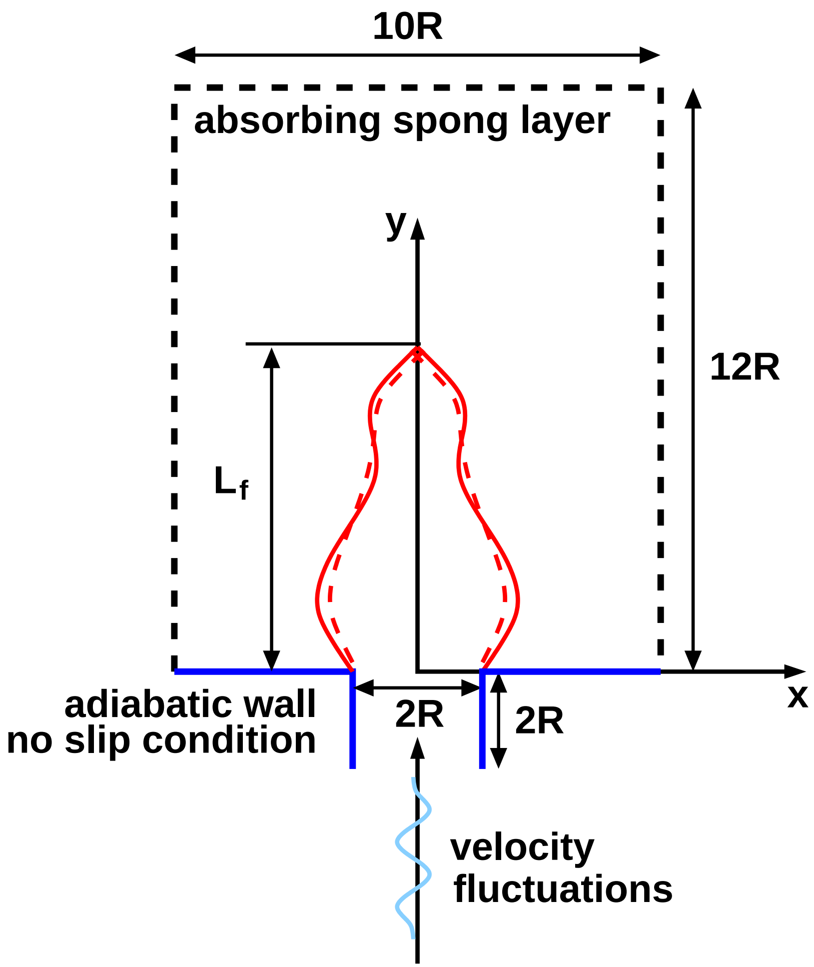
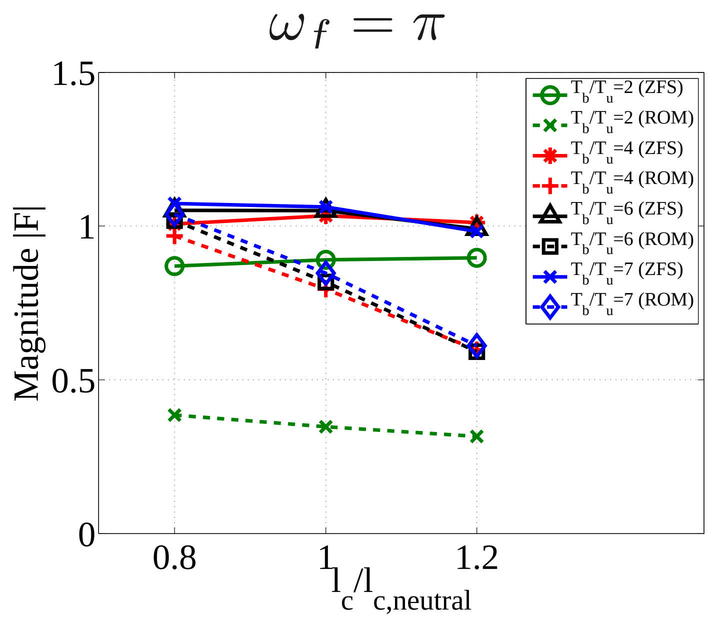
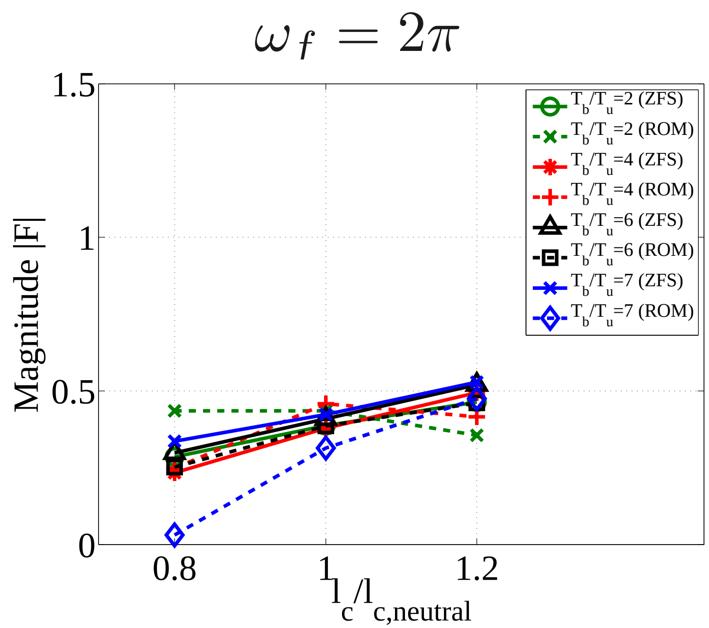
Flame Transferfunction



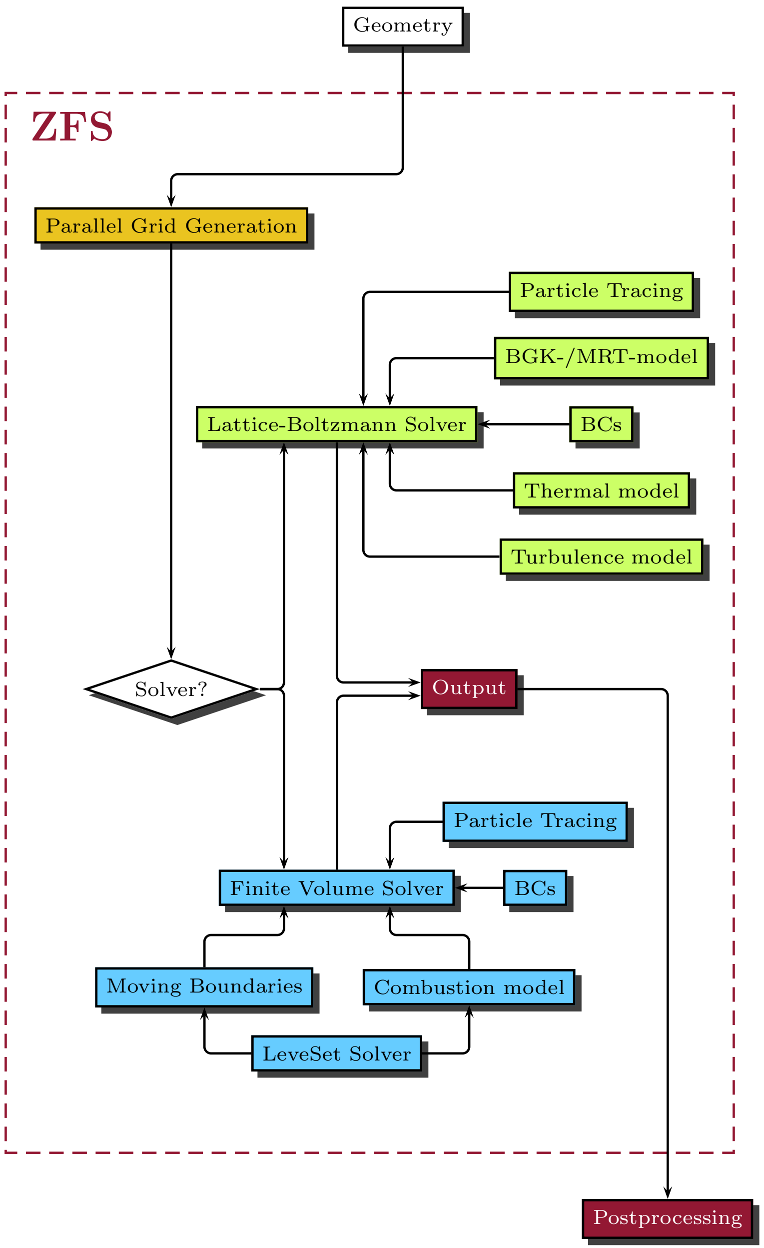


Flame transfer function

$$F = \frac{q'(\omega_f)}{q_0}\frac{v_0}{v'}$$



Zonal flow solver (ZFS)



Solve

- Navier-Stokes equations
- Boltzmann equation

using unstructured hierarchical cartesian meshes

ZFS main features:

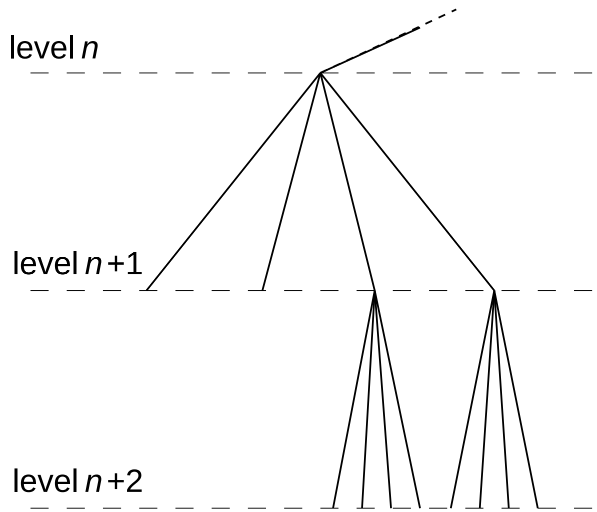
- automatic parallel mesh generation based on STL input data
- solution adaptive meshes
- Lagrange model for particle tracking
- level-set method for moving boundaries
- thermal Lattice Boltzmann model
- fully conservative cut-cell method
- multiple species and premixed combustion model
- parallelization by domain decompositioning

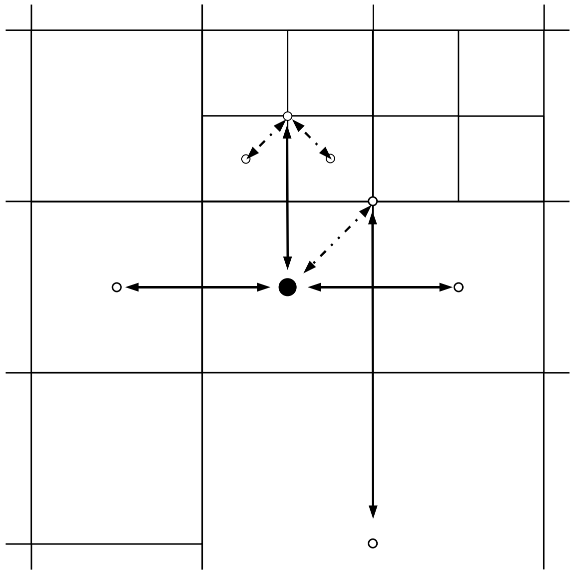
Numerical Method

Hartmann et al. Comp. Fluids 37 (2008) 1103-1125

Solution of the Navier-Stokes equations based on Cartesian refined meshes

- 5-stage explicit Runge-Kutta time stepping
- AUSM with modified pressure splitting, MUSCL scheme
- least-squares gradient reconstruction
- A hierarchically consistent tree data structure is used to organize the cells
  - parent-child pointers for vertical tree connections
  - neighbor pointers for horizontal tree connections
    only pointers to neighbor cells at the same level of refinement
    $\rightarrow$*enables the application of multigrid methods*





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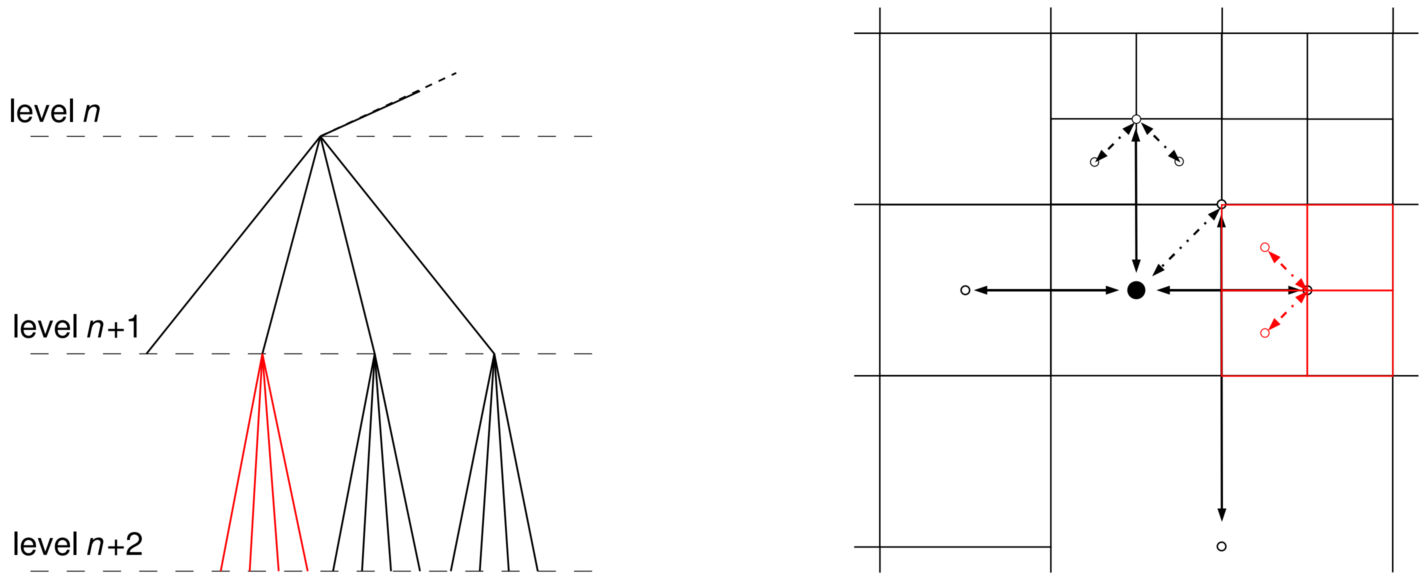
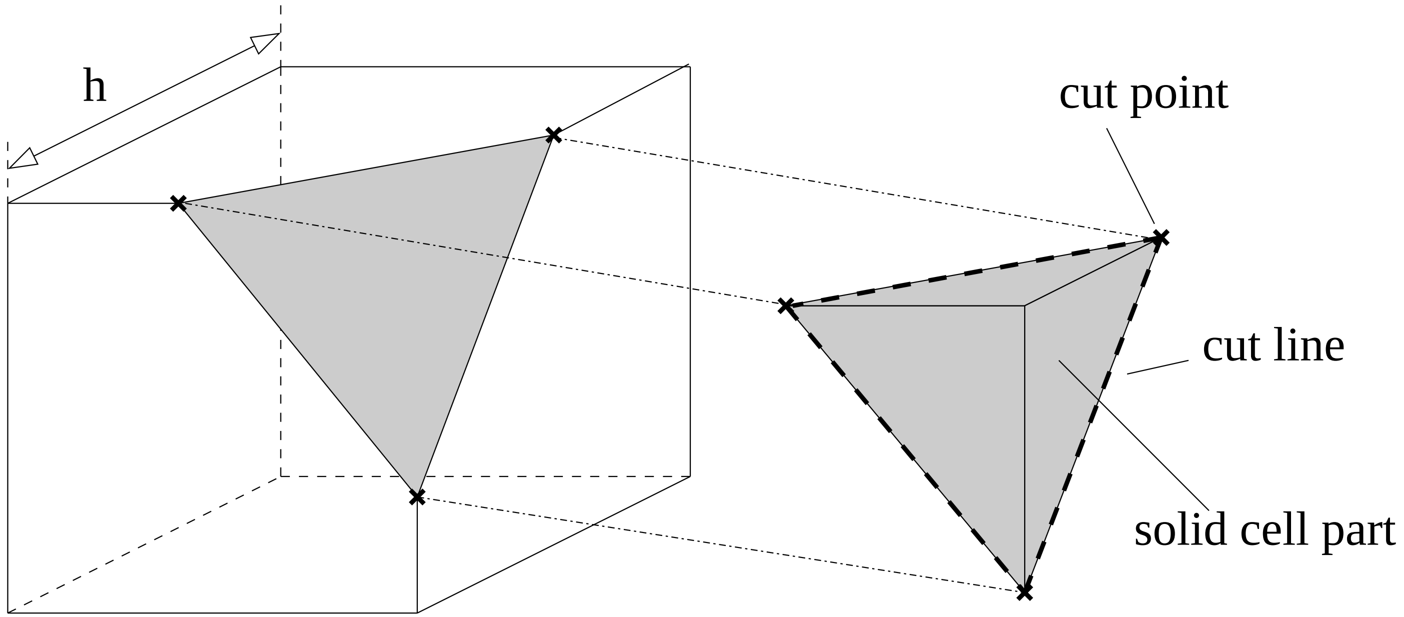


Reshaping of cut cells:

- cut points are determined from the geometry information
- cut cells are reshaped, solid cell part is discarded
- moving geometries require a new determination of cut cells at each time level
- for fixed boundaries: use cell-merging technique to avoid small cells (Hartmann *et al.*, 2011)



Objectives:

- For premixed combustion flames are typically thin surfaces in which chemicial reactions occur
- Flames are difficult to resolve since they connected to small spatial and time scales
- Use a combustion model coupled with a tracking of the flame surface

Level Set Method (Hartmann et al. J. Comp. Phys. 2008 & 2010)

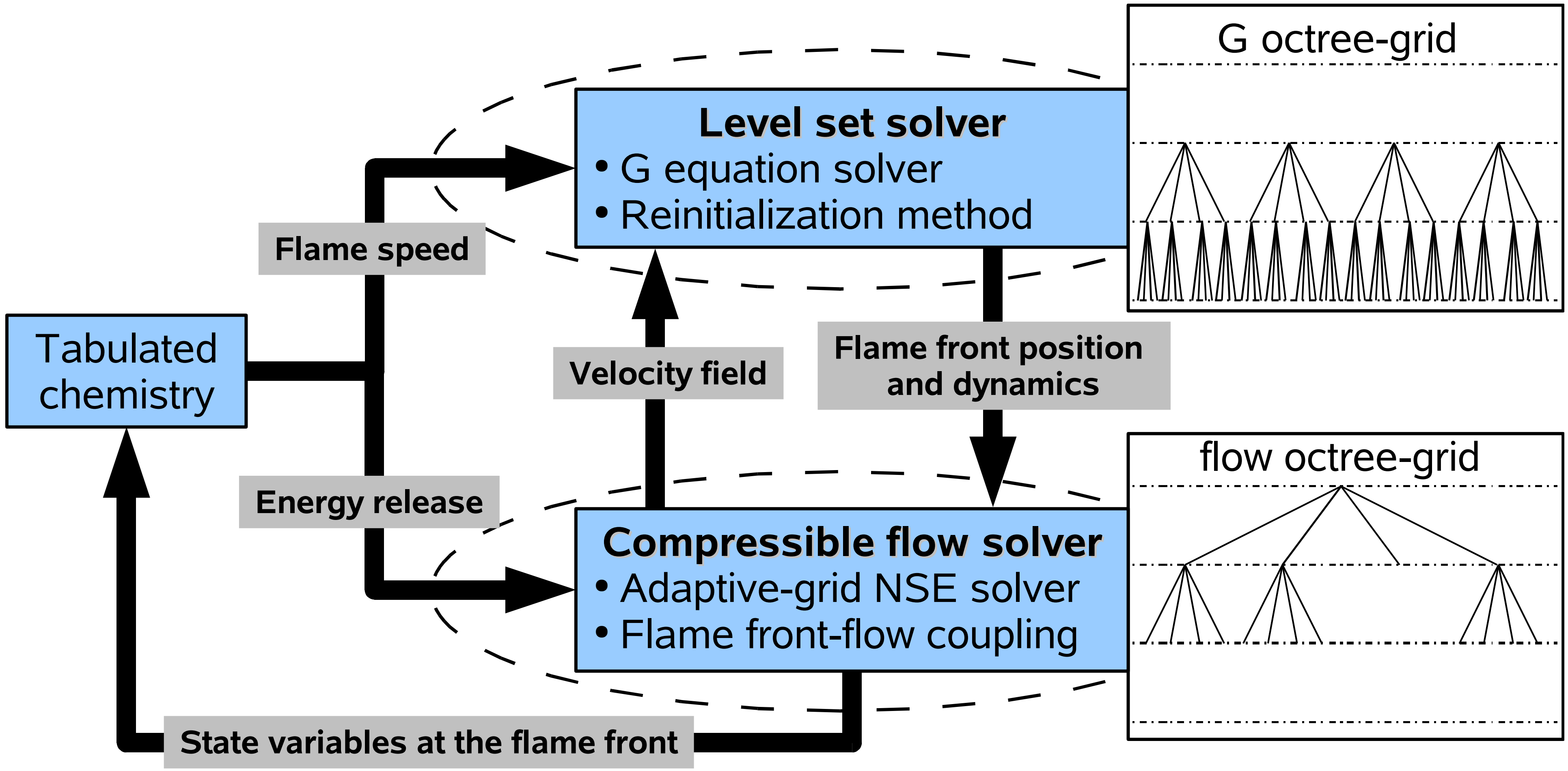
- can be used to implicitly represent moving surfaces by its zero level G_0=0:

$$\partial_t G + \mathbf{v} \cdot \mathbf{\nabla} G = 0$$

- Also used for moving geometries since the cut cell information can be generated more efficiently based on the level set method than by using STL data.

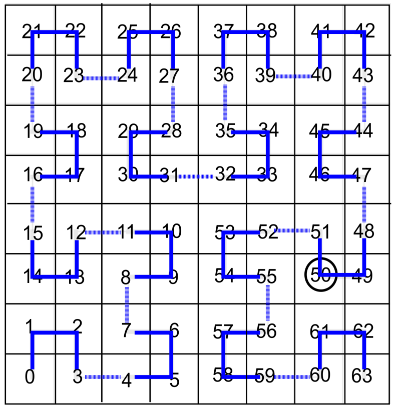
Numerical Method: Dual-mesh approach

- Flow cells and G cells are organized in two connected hierarchical octree data structures.
- The flow grid and the G grid can be independently refined and coarsened.

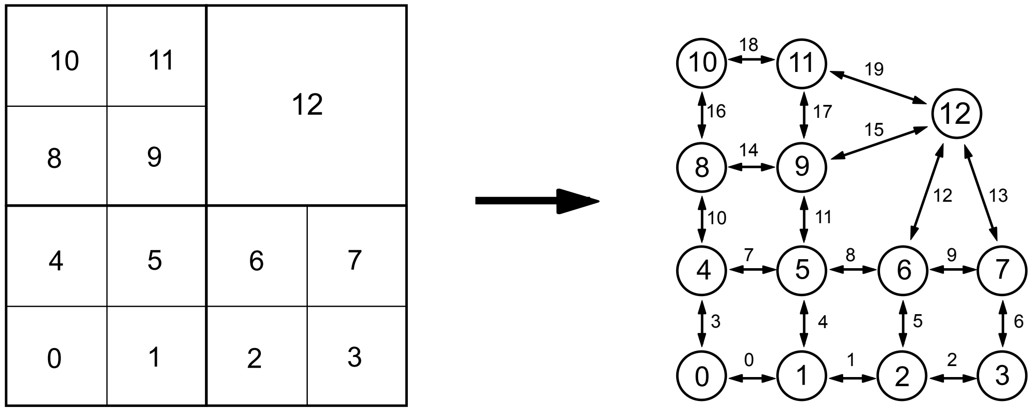


Hierarchically consistent MPI parallelization

- Domain decompositioning by space filling curves or Metis subdomain.

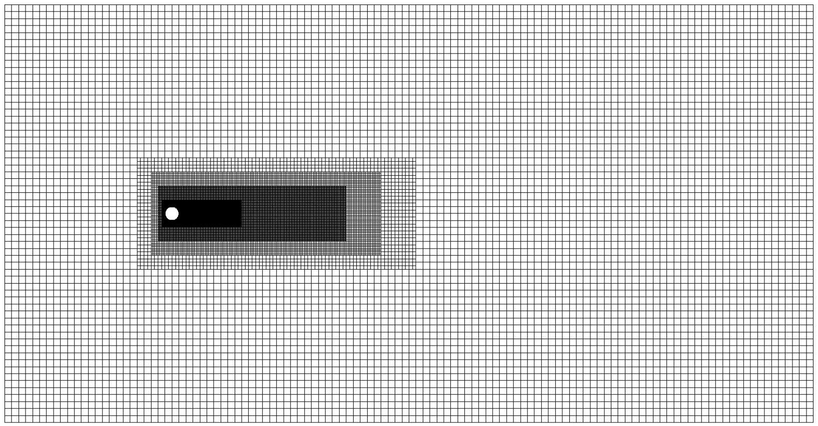


Hilbert Curves

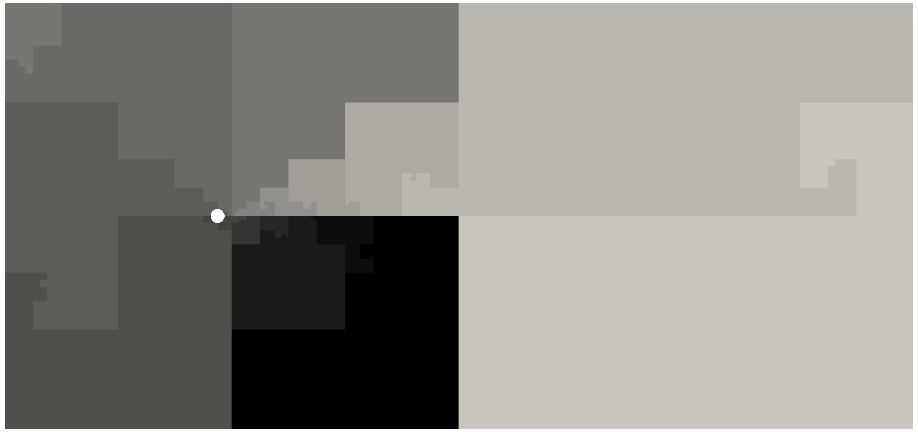


Graph Partitioning (Metis)

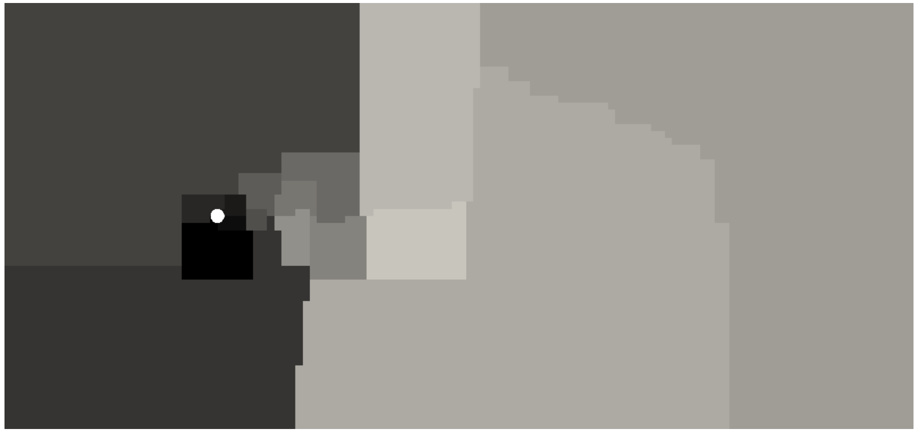
- Domain decompositioning by space filling curves or Metis subdomain.



refined mesh

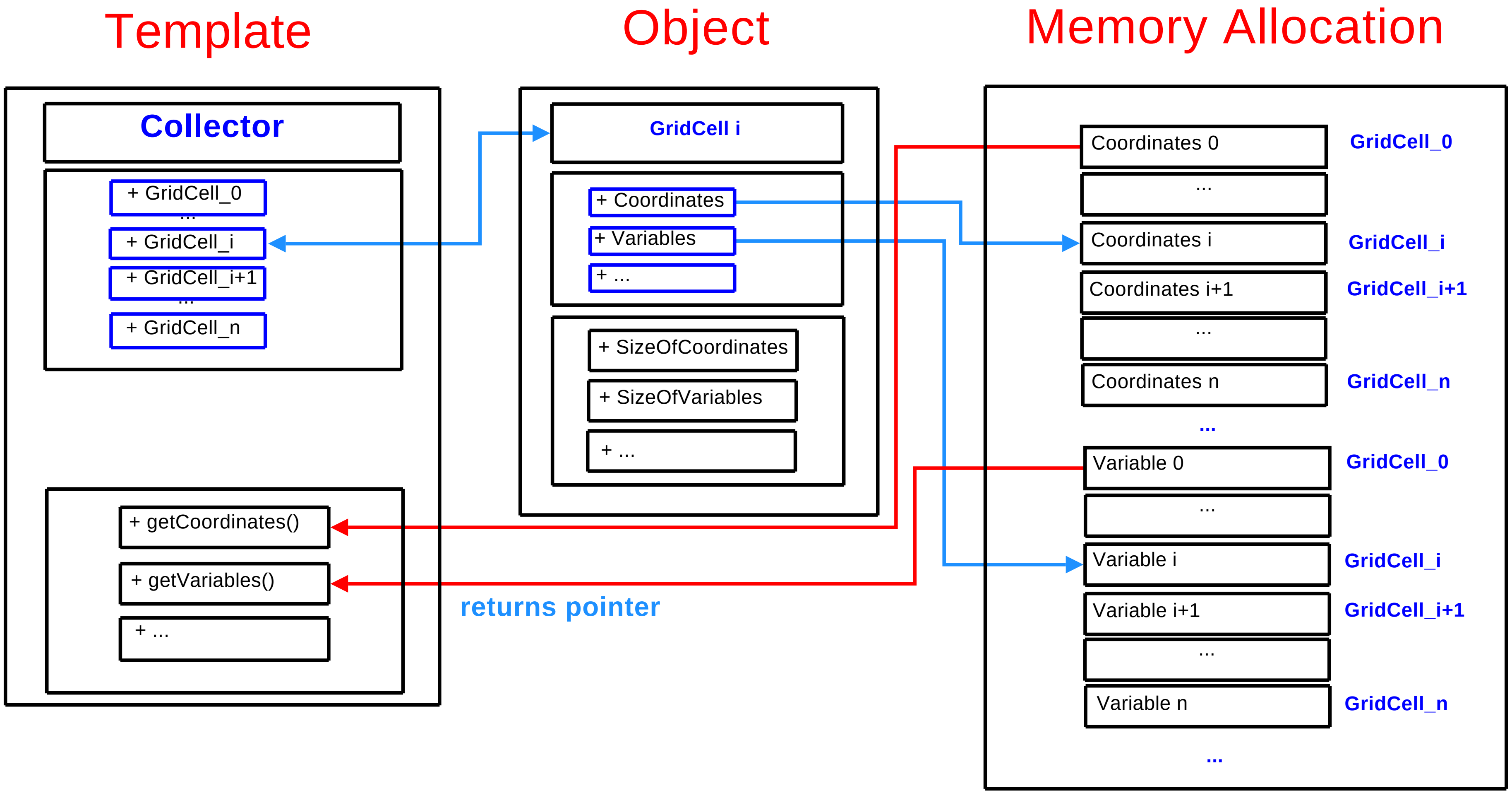


Hilbert Curves



Graph Partitioning (Metis)

Combine object orientation with linear array addressing by using templates for large data objects:



Parallel Mesh generation

Requirements

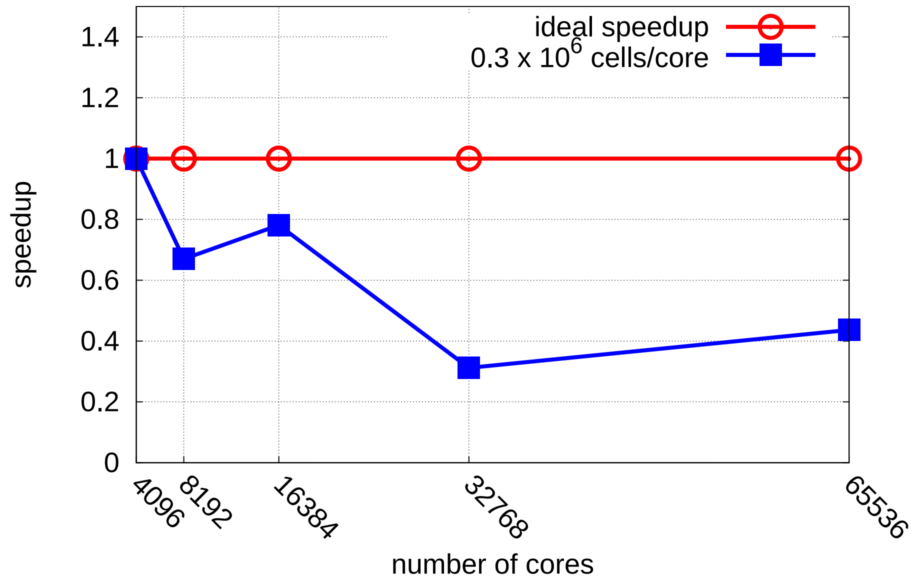
- Generation of arbitrarily large meshes
- Save mesh and solution data in single files with parallel IO
- Restart of the solution process should be possible with different processor numbers

Solution strategy

- exploit hierarchy of the Cartesian mesh, i.e. generate a coarse uniform base level of the mesh
- discard cells outside the domain
- domain decompositioning by Hilbert curves
- refine mesh on indivdual subdomains
- write mesh (and solution data) with parallel netcdf
- each subdomain writes consecutive data, cells remain sorted along the Hilbert curve
- solver can read cells of subdomains efficiently for various core numbers

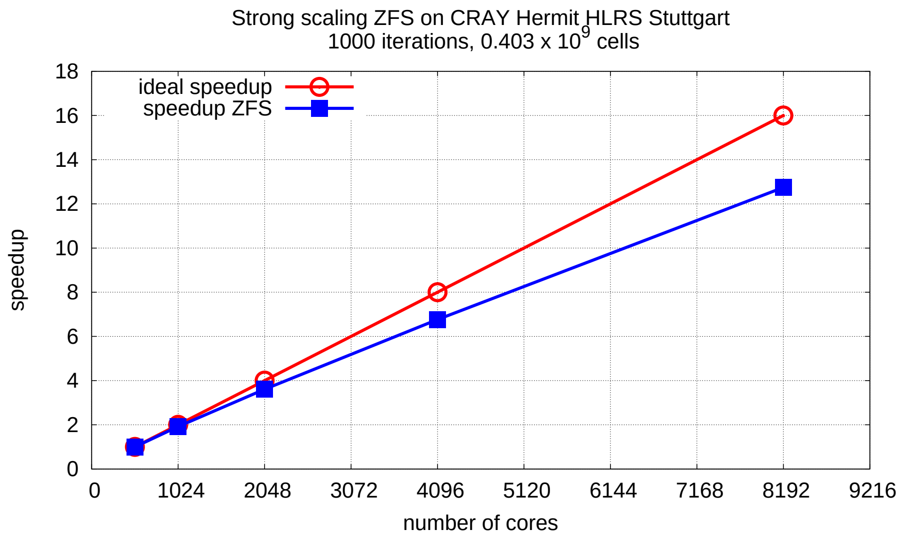
Parallel Mesh generation

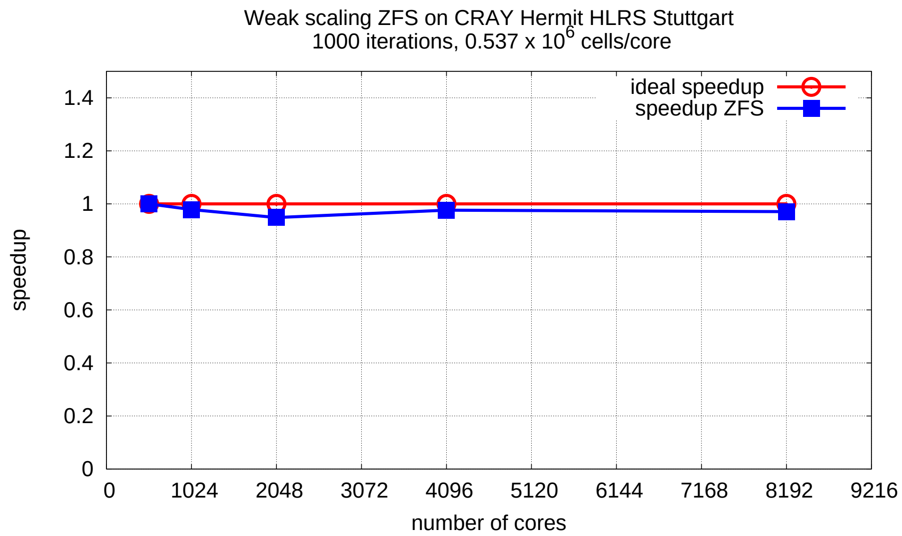
cores	*# of cells*	*time[s]*	*speedup*
4096	1.23×10^9	9.82	1.0
8192	2.45×10^9	14.65	0.67
16384	4.91×10^9	12.57	0.78
32768	9.82×10^9	31.47	0.31
65536	17.64×10^9	22.48	0.44

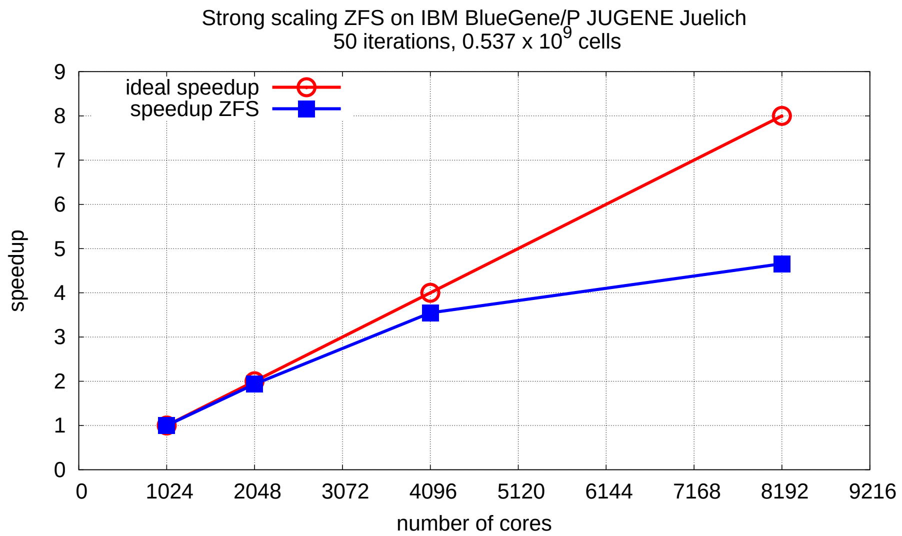


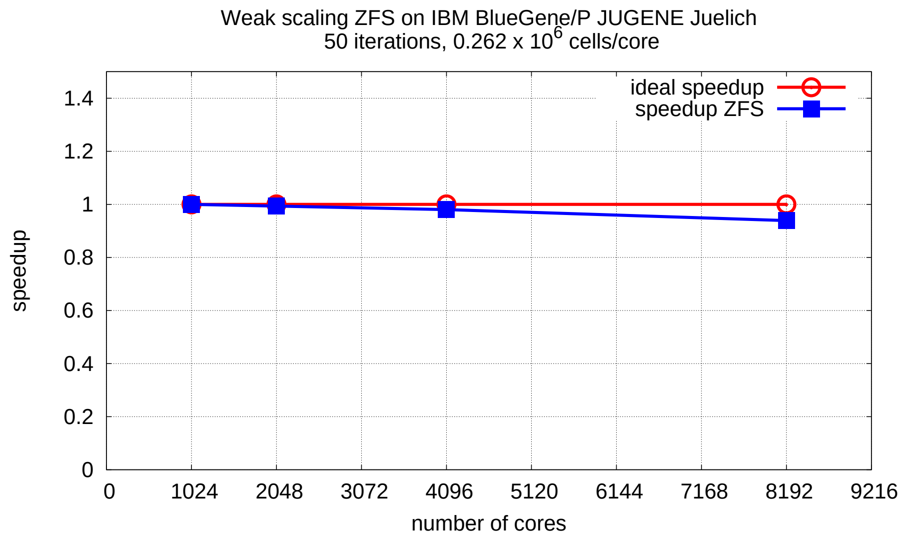
Weak scaling test for the grid generation
local mesh size: 0.3×10^6 cells per core

Weak and Strong Scaling Tests for ZFS
Lattice Boltzmann Method



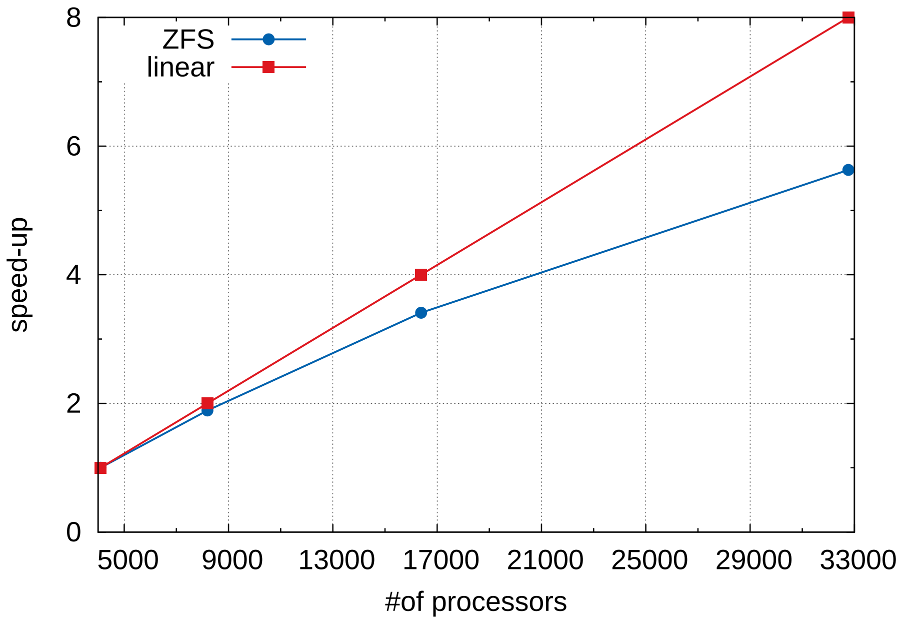




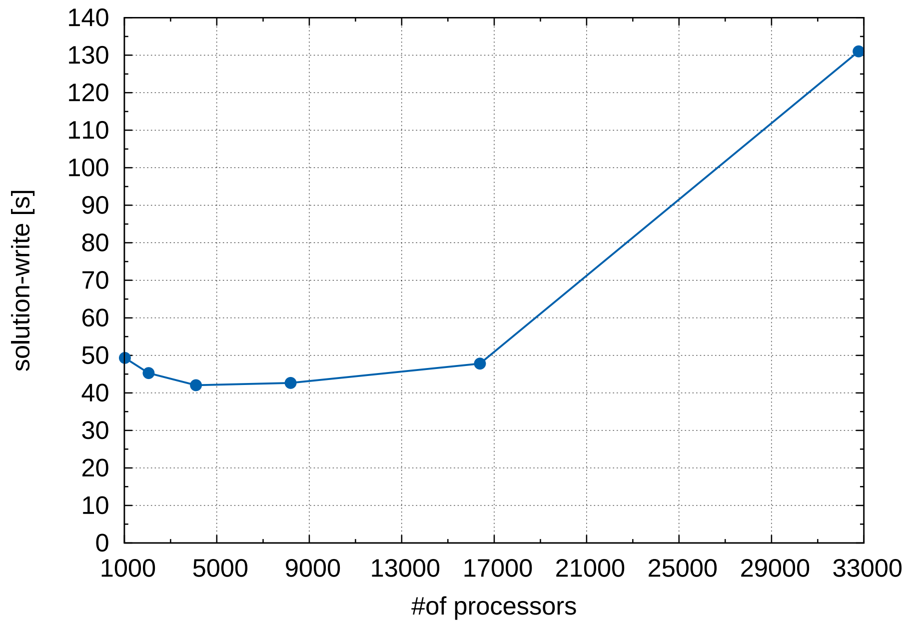


Scaling Tests for ZFS
Finite-Volume Method

strong scaling test @ Cray XE6



Time required for data I/O



- $1.2 \cdot 10^9$ cells
- 4-5 Terabyte memory
- 2-3 Gigabyte/1 million cells
- lower limit of approx. 200000 cells / computing core

- $1.2 \cdot 10^9$ cells
- approx. 100 Gigabyte written by parallel NetCDF in one file
- 1000 time samples require 100 Terabyte
- 32000 cores need 36 hours to write 1000 samples

Postprocessing of Data

- Postprocessing, e.g. for statistical data is integrated within ZFS
- Advanced data analysis by dynamic mode decompositioning is currently being parallelized for large data sets
- Parallel visualization by ParaView
  - Plugin which reads the data by parallel NetCDF
  - Use D3 filter for generation of Halo cells
- Problem: postprocessing of huge data volume, i.e. O(100) Terabyte

Conclusions

- A solution method based on Cartesian meshes has been presented
- Applications in various fields prove the method to be flexible and efficient also for cases with moving surfaces
- Work still to be done: increase the parallel efficiency for non-trivial problems, adaptivve mesh refinement and particle tracking

Some lessons learned

- All components of the simulation chain must be parallel (trivial)
- Parallelization of a little more complex algorithms is not trivial
- Parallel visualizaton will require data reduction techniques and still O(100) cores for large simulation runs
- Determination of statistical data and/or advanced postprocessing will be a considerable problem

References

1. R.P.J. Kunnen, C. Siewert, M. Meinke, W. Schröder, K.D. Beheng: *Numerically determined geometric collision kernels in spatially evolving isotropic turbulence relevant for droplets in clouds*, Atmos. Res., 2013
2. L. Schneiders, D. Hartmann, M. Meinke and W. Schröder: *An accurate moving boundary formulation in cut-cell methods*, J. Comp. Phys., 235, 2013.
3. C. Günther, L. Schneiders, M. Meinke, W. Schröder, and D. Hartmann. *A Cartesian cut-cell method for sharp moving boundaries*, AIAA Paper 2011-3387, 2011.
4. D. Hartmann, M. Meinke and W. Schröder, *A strictly conservative Cartesian cut-cell method for compressible viscous flows on adaptive grids,* Comput. Meth. Appl. Mech. Eng. 200, pp. 1038-1052, 2011.
5. D. Hartmann, M. Meinke and W. Schröder: *A Level-Set Based Adaptive-Grid Method for Premixed Combustion*, Combust. Flame, 158, 2011
6. D. Hartmann, M. Meinke and W. Schroder: *A general formulation of boundary conditions on Cartesian cut cells for compressible viscous flow*, AIAA Paper 2009-3878, 2009.
7. D. Hartmann, M. Meinke and W. Schröder: *Differential Equation Based Constrained Reinitialization for Level Set Methods*, J. Comput. Phys., doi:10.1016/j.jcp.2008.03.040, 2008.
8. D. Hartmann, M. Meinke and W. Schröder: *An adaptive multilevel multigrid formulation for Cartesian hierarchical grid methods*, Comput. Fluids, doi:10.1016, 2007.