CUDA-accelerated Computational Fluid Dynamics

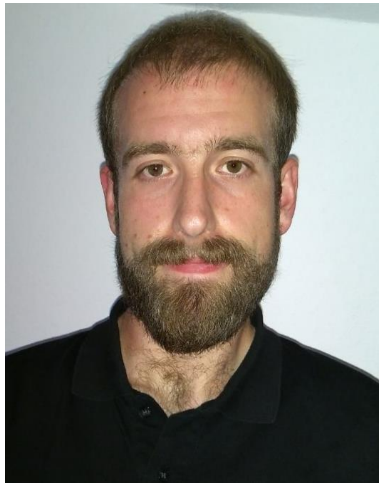
Christian F. Janßen and the elbe team

Hamburg University of Technology

Speakers today

Christian F. Janßen

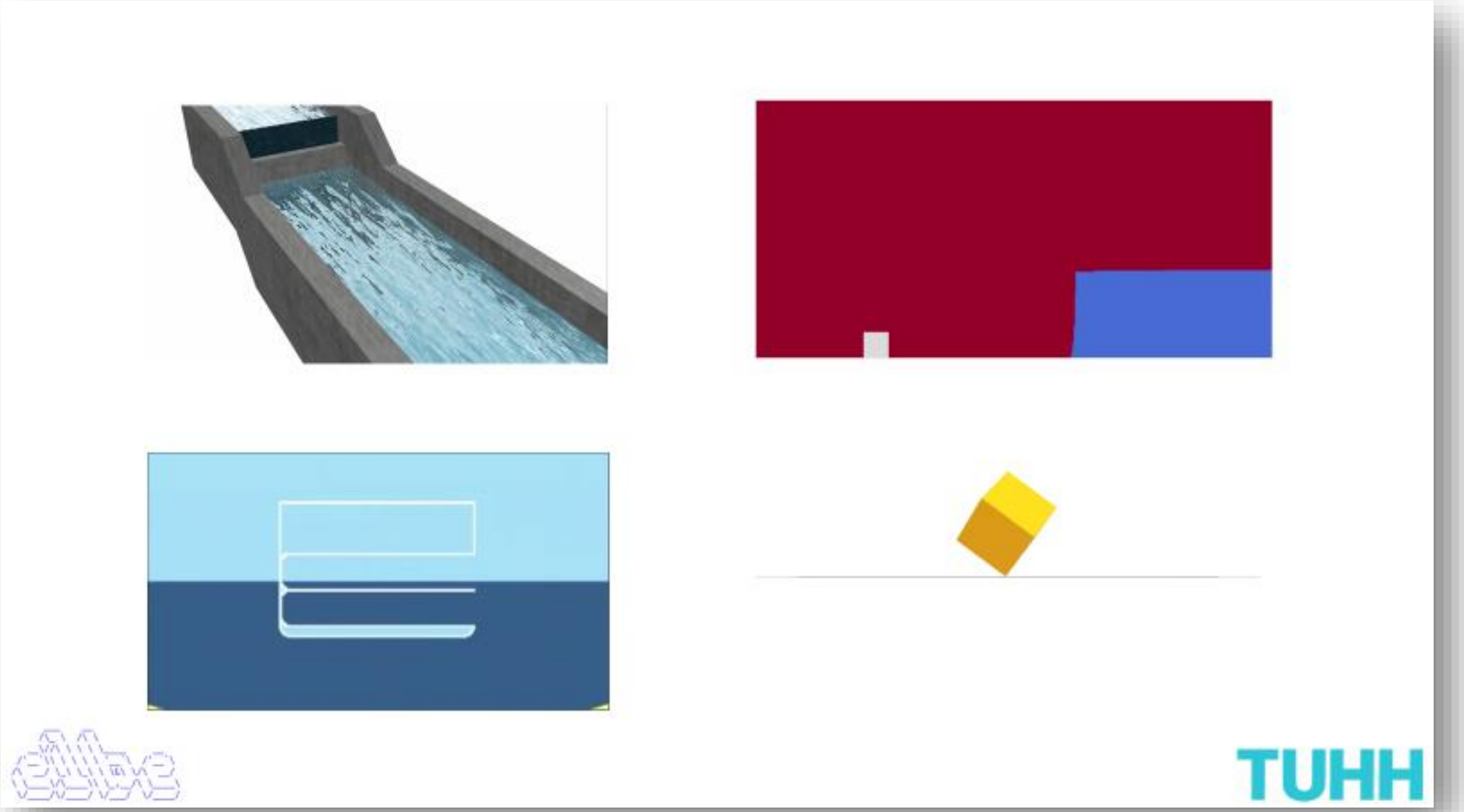
Dennis Mierke



Martin Gehrke

Henrik Asmuth

Animation



GPU Hardware

NVIDIA GTX TITAN X, 3072 cores, 12 GB memory

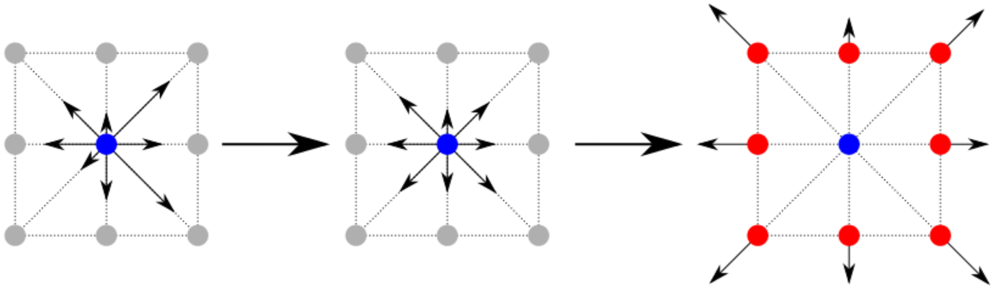
NVIDIA Tesla K80, 4992 cores, 24 GB memory

The *efficient lattice boltzmann environment* elbe

- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - GPU-accelerated pre- and post-processing
- Up to 120 million lattice nodes and 1,000 million node updates per second per GPU board
- Supported by NVIDIA since 2011: Academic Partnership Program, CUDA Research Center

Collision

$$\bar{f}_i(t,\mathbf{x}) = f_i(t,\mathbf{x}) + \Omega_i$$



Propagation

$$f_i(t+\Delta t,\mathbf{x}+\mathbf{e}_i\Delta t) = \bar{f}_i(t,\mathbf{x})$$

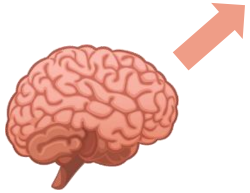
J. Tölke, *J. Comput. Visual Sci.* **13**(29), 2010, first online 24 July 2008.
J. Tölke and M. Krafczyk, *Int. J. Comp. Fluid Dynamics* **22**(7):443-456, 2008.

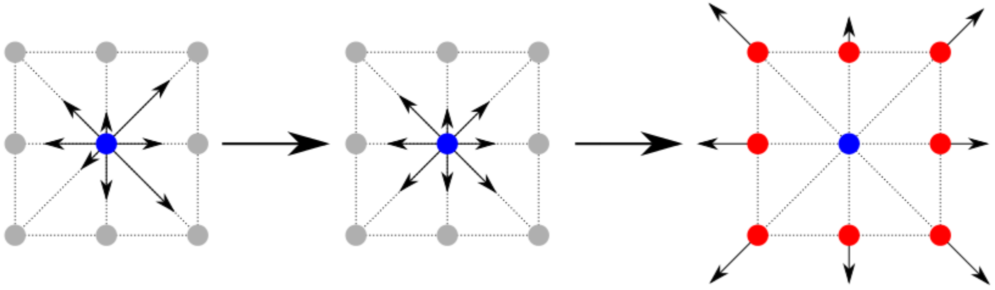
The *efficient lattice boltzmann environment* elbe

- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - GPU-accelerated pre- and post-processing
- Up to 120 million lattice nodes and 1,000 million node updates per second per GPU board
- Supported by NVIDIA since 2011: Academic Partnership Program, CUDA Research Center

Collision

$$\bar{f}_i(t, \mathbf{x}) = f_i(t, \mathbf{x}) + \Omega_i$$





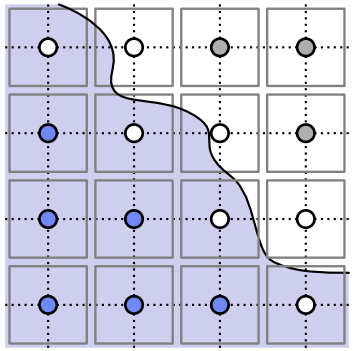
Propagation

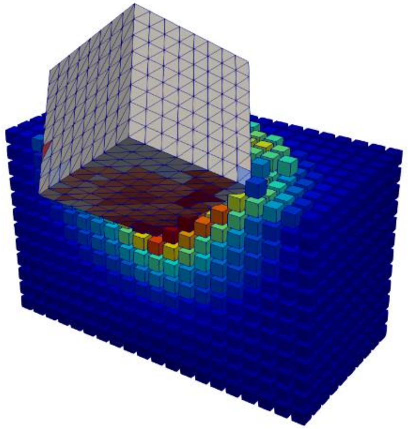
$$f_i(t + \Delta t, \mathbf{x} + \mathbf{e}_i \Delta t) = \bar{f}_i(t, \mathbf{x})$$

M. Geier, A. Pasquali, M. Schönherr, *J. Comp. Phys.* **348**(1):862-888, 2017
M. Geier, A. Pasquali, M. Schönherr, *J. Comp. Phys.* **348**(1):889-898, 2017

The *efficient lattice boltzmann environment* elbe

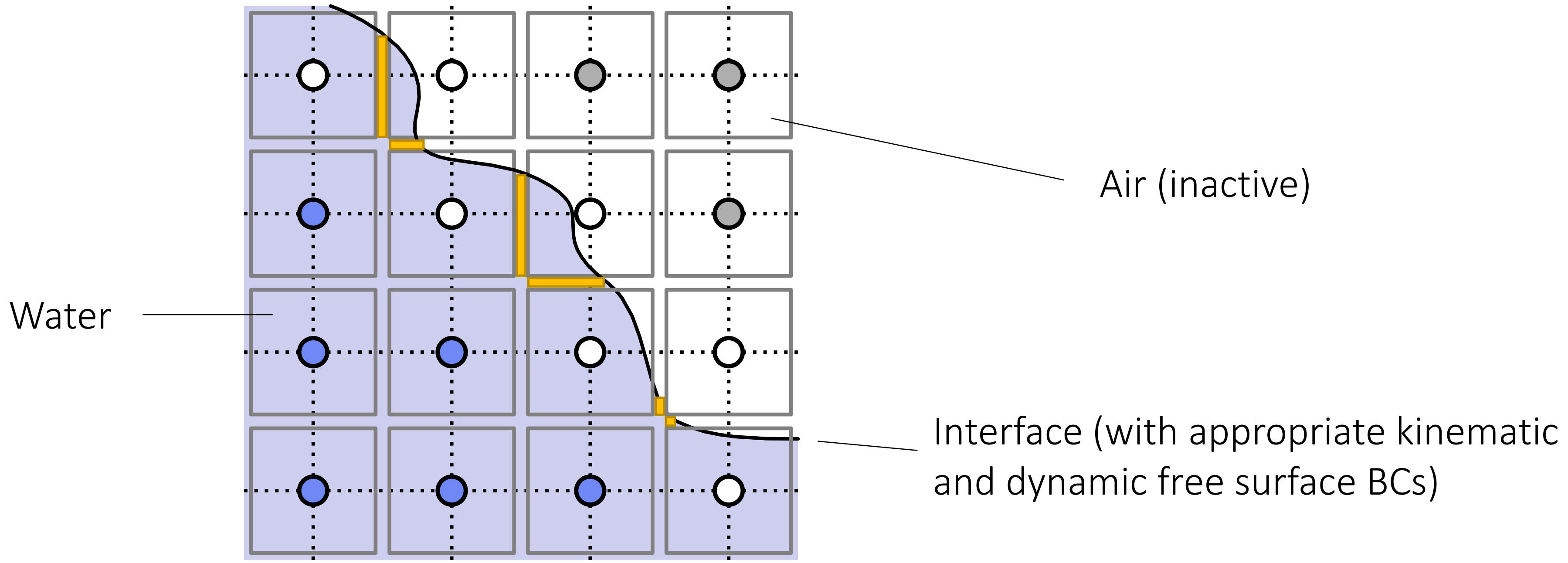
- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - GPU-accelerated pre- and post-processing
- Up to 120 million lattice nodes and 1,000 million node updates per second per GPU board
- Supported by NVIDIA since 2011: Academic Partnership Program, CUDA Research Center





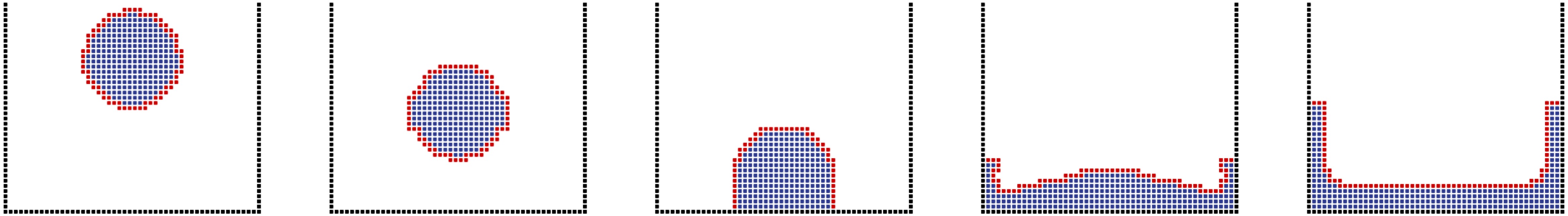
M. Geier, A. Pasquali, M. Schönherr, *J. Comp. Phys.* **348**(1):862-888, 2017
M. Geier, A. Pasquali, M. Schönherr, *J. Comp. Phys.* **348**(1):889-898, 2017

Challenge I: Free surface model



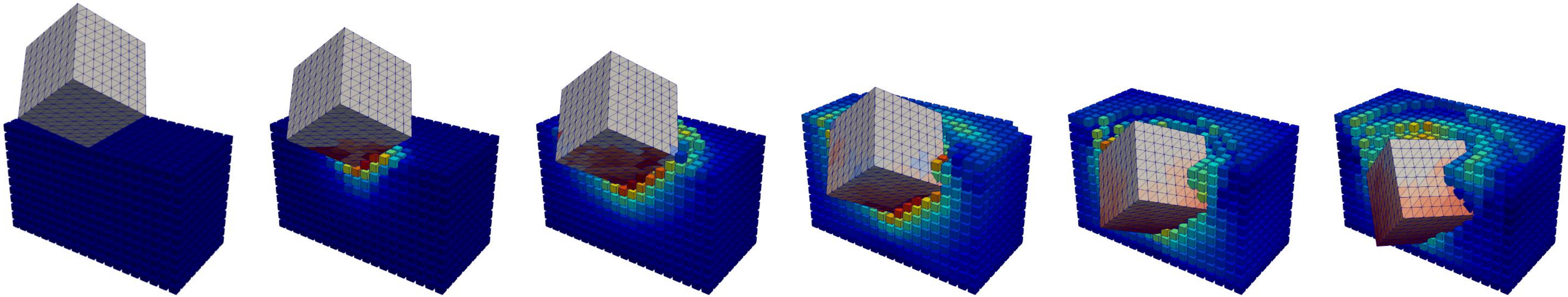
Using CUDA unbound - CUB

- cub::DeviceSelect::{If,Flagged}()
  - Concentrate GPU-power: dynamically identify the interface nodes that need further processing, e.g., the fill level update and the free surface pressure boundary condition

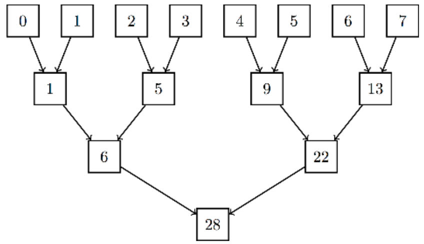


- cub::{Counting,Transform}InputIterator()
  - Manipulates alignment and offset of the InputIterator, e.g., for indirect addressing purposes
  - Can be used in combination with most other CUB functions

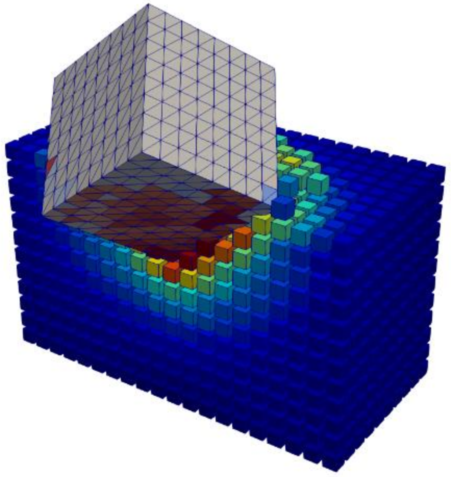
Challenge II: Fluid-Structure Interaction



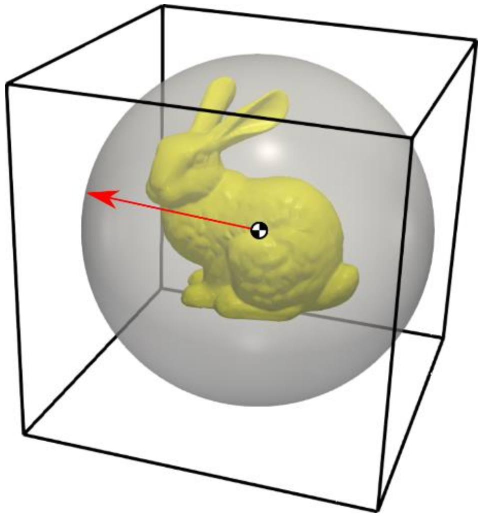
cub::DeviceReduce::Reduce()



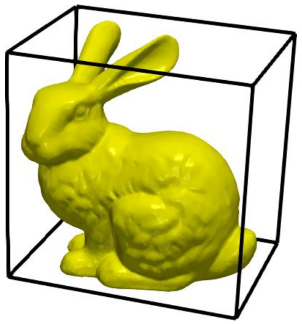
- **Sum()**-Functor:
  - Fluid load summation over every triangle of each obstacle geometry
  - Fluid mass summation over every fluid node
  - Summation of statistics at every time step
    - spatially averaged values (e.g., flow velocity)
    - pressure loss at in/outlet



- **MaxSquare()**-Functor:
  - Measure bounding sphere radius of triangulated geometries



- **Min/Max()**-Functor:
  - Generate AABB of triangulated geometries

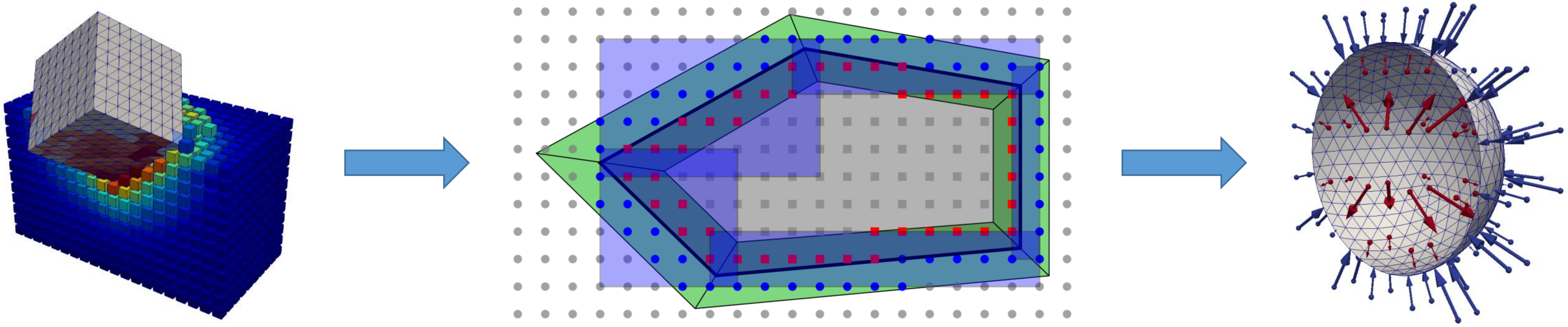


Source Stanford Bunny: http://graphics.stanford.edu/data/3Dscanrep/

TUHH

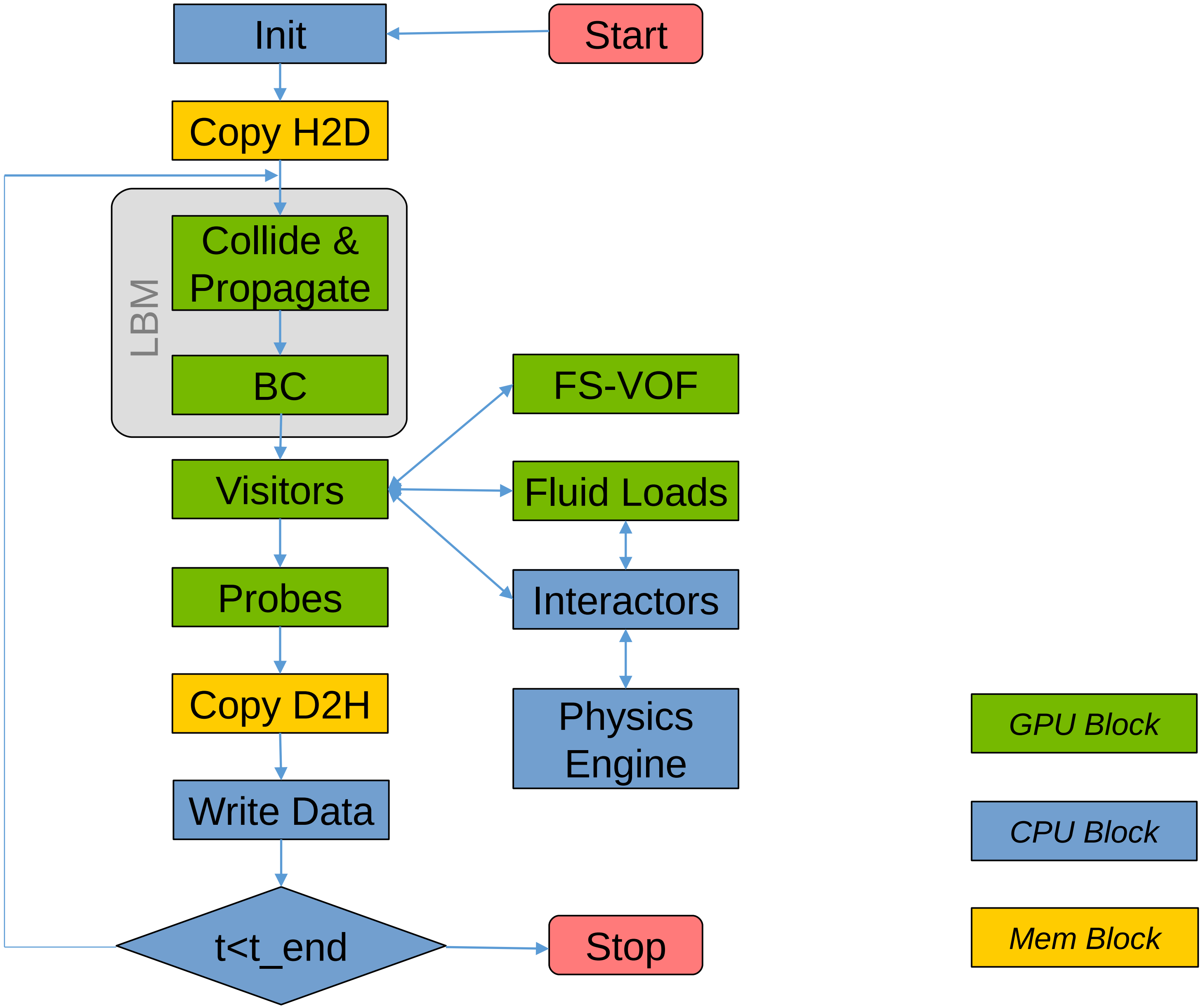
GPU-accelerated grid generation

- Coupling to a collision-resolving physics engine, that calculates the object positions
- Development of an efficient, thread-parallel grid update algorithm
- Efficient calculation and storage of geometry information for higher-order boundary conditions



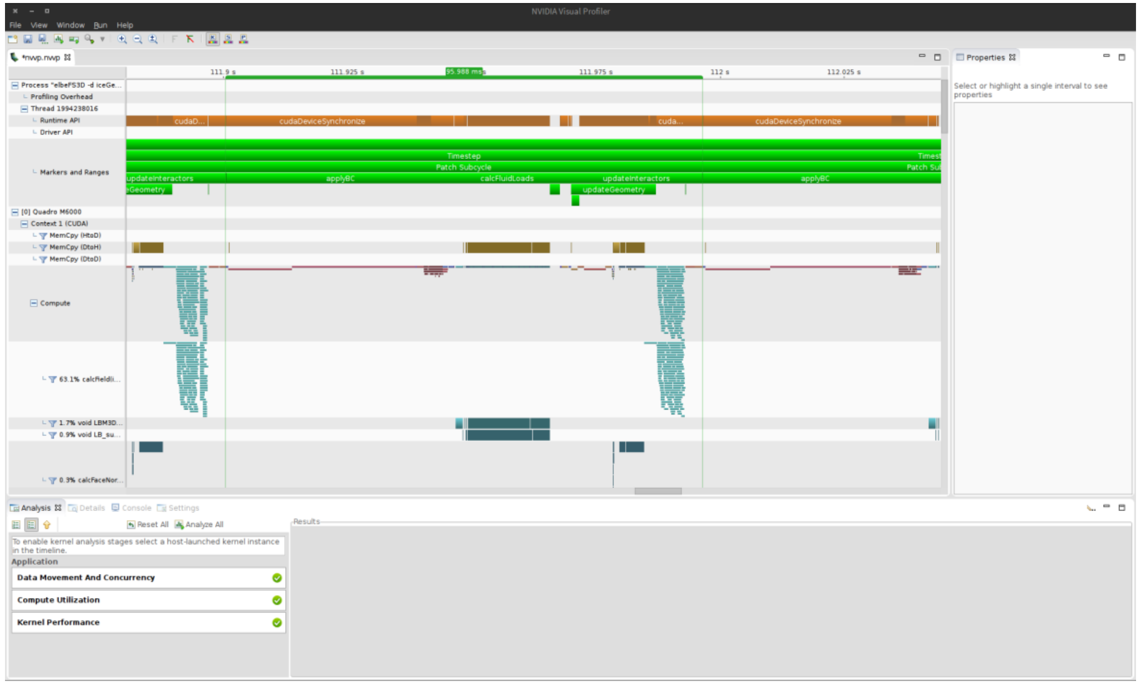
C.F. Janßen, N. Koliha and T. Rung, *Comm. Comp. Phys.* 17(5):1246-1270, 2015; DOI: 10.4208/cicp.2014.m414
D. Mierke, C.F. Janßen and T. Rung, *Comp. Math. W. Appl.*; DOI: 10.1016/j.camwa.2018.04.022

Basic simulation procedure



Profiling tools

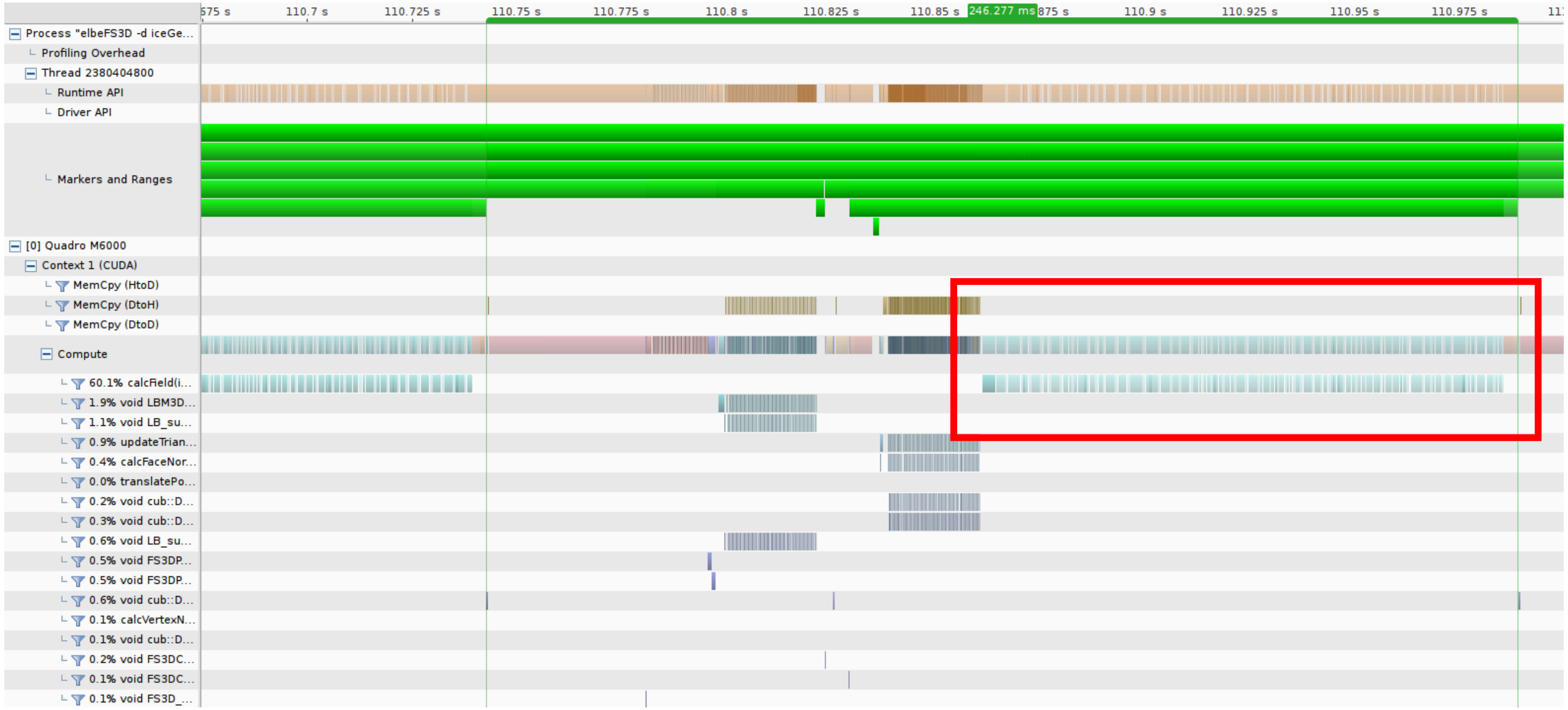
- nvprov: command-line profiling on clusters
- nvvp: visual profiling on workstations
  - Use markers for easier orientation (nvtxRange{PushA,Pop}())
- Detect bottlenecks, performance leaks and unused/vacant GPU resources



Example: Streams

- Concurrent streams to fully utilize the GPU with “small” kernels
  - E.g., one stream for each solid body (boundary condition, geometry update, …)
  - Parallel mapping, transformations, field manipulations, ...

Original version

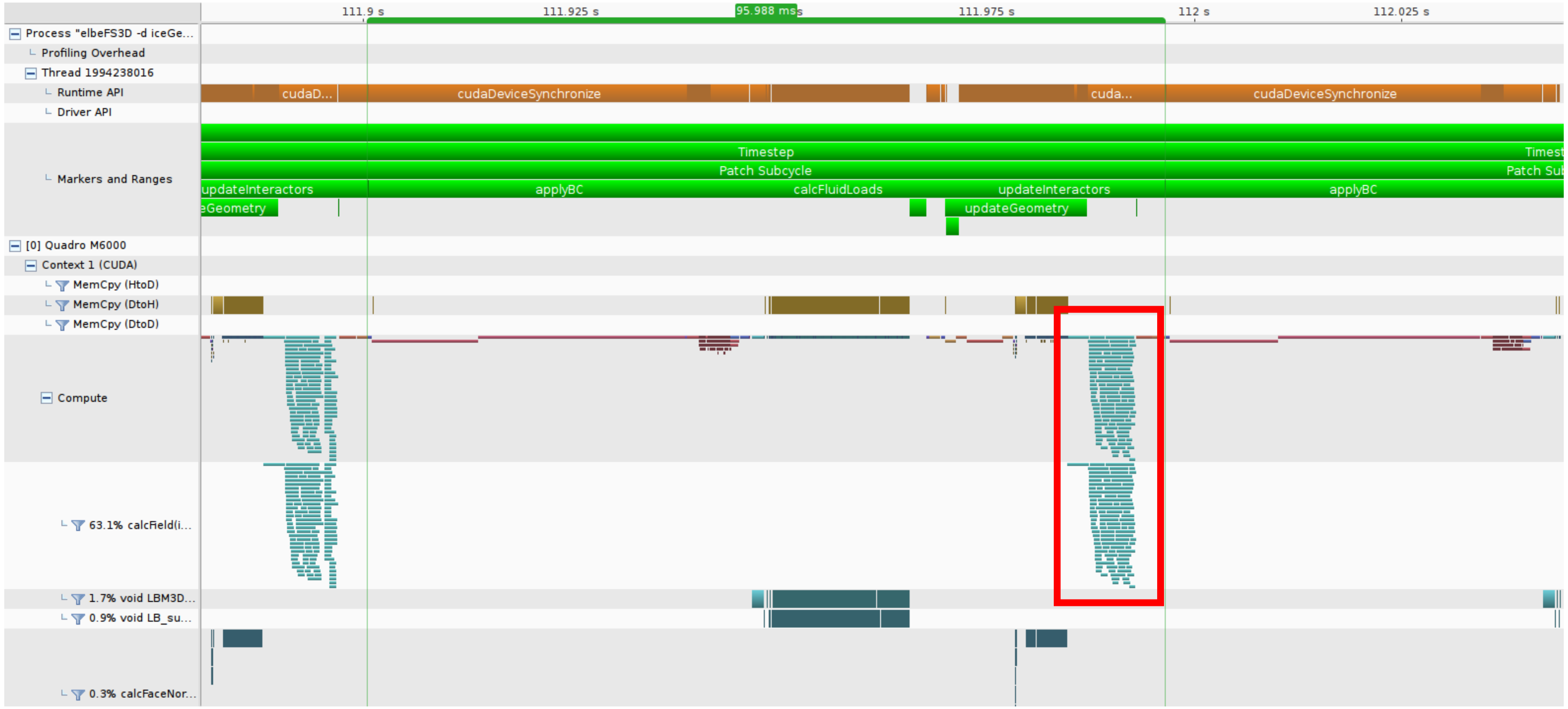


TUHH

Example: Streams

- Concurrent streams to fully utilize the GPU with “small” kernels
  - E.g., one stream for each solid body (boundary condition, geometry update, …)
  - Parallel mapping, transformations, field manipulations, …

Optimized version



TUHH

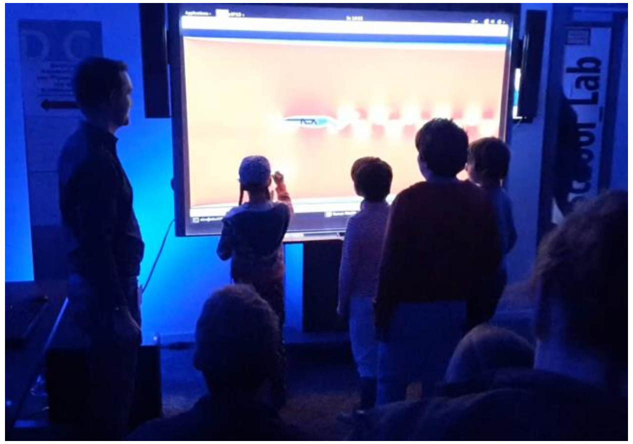
Application: A numerical ice tank

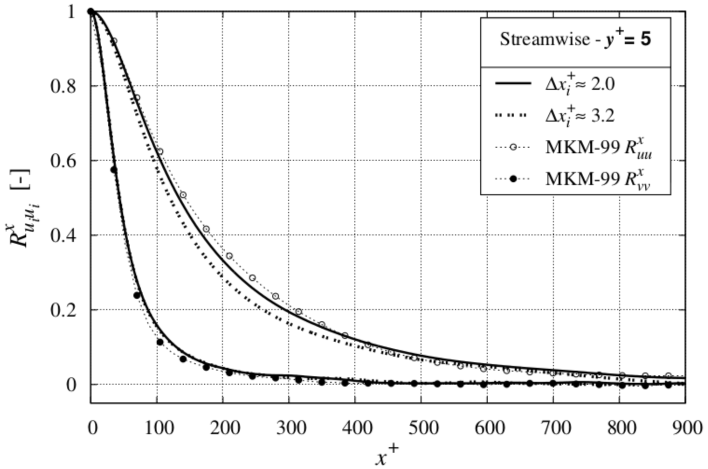
- Project goal: Minimize propeller-ice interactions to improve the propulsion-efficiency of ice-going vessels
- Below, a full scale simulation with 60 ice floes is shown. The simulation contains 50M grid nodes, 300K surface triangles and took less than 6h on one GTX Titan X GPU

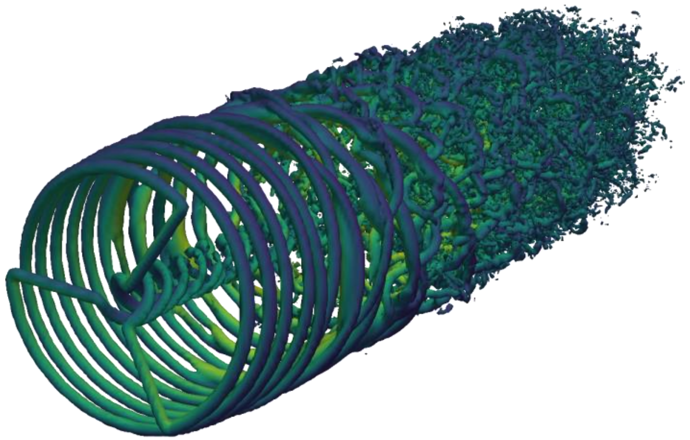
On the development of an efficient numerical ice tank for the simulation of fluid-ship-rigid-ice interactions on graphics processing units. C.F. Janßen, D. Mierke and T. Rung, *Computers & Fluids* **155**:22-32, September 2017

Animation

elbe in higher education and research



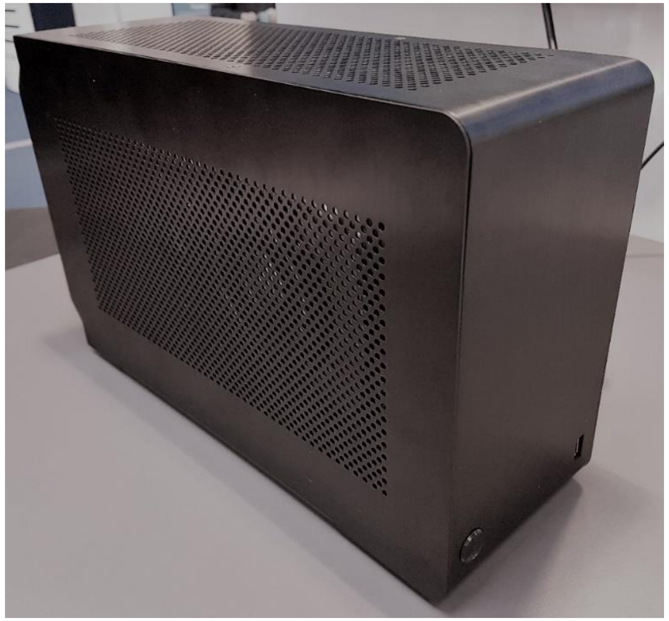




TUHH

The *efficient lattice boltzmann environment* elbe

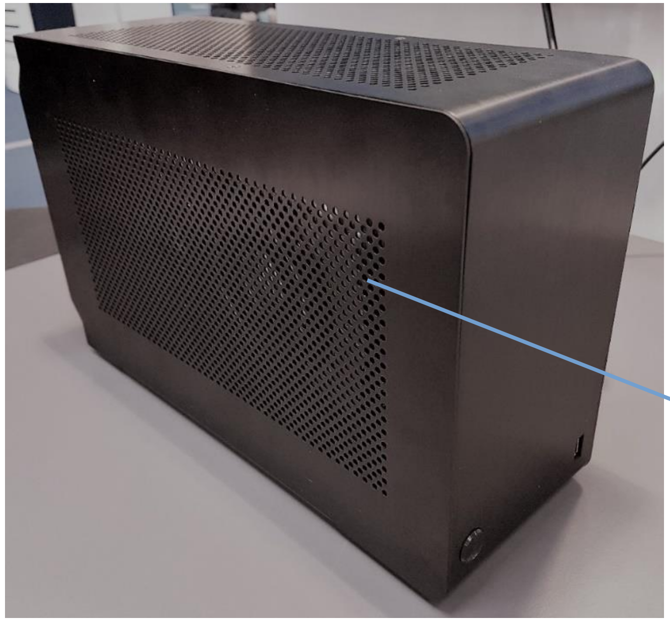
- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - GPU-accelerated pre- and post-processing

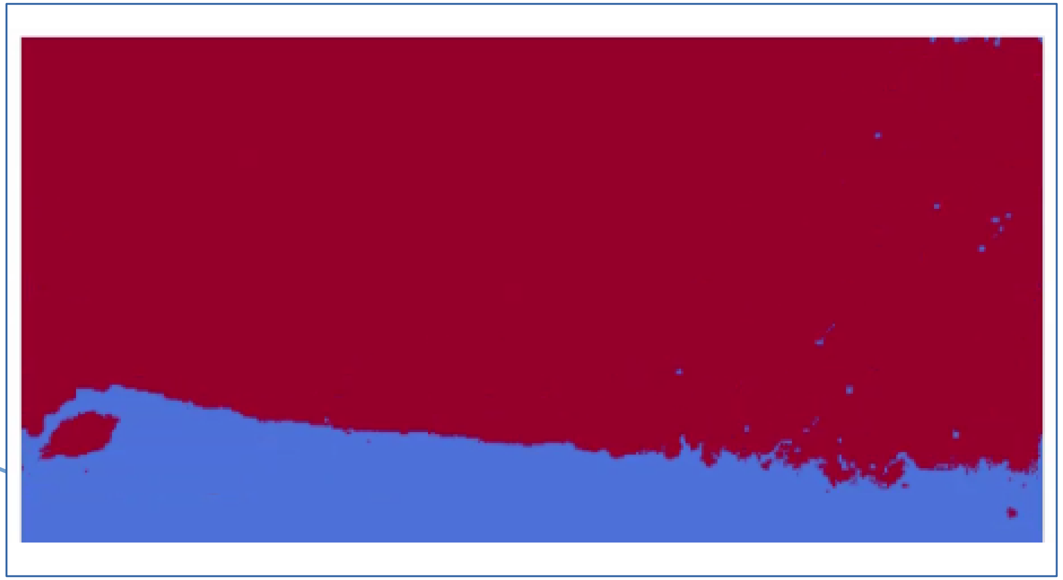


Towards online visualization and interactive monitoring of real-time CFD simulations on commodity hardware
N. Koliha, C.F. Janßen and T. Rung, *Computation* **3**(3):444-478, 2015; DOI: 10.3390/computation3030444

The *efficient lattice boltzmann environment* elbe

- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - <u>GPU-accelerated pre- and post-processing</u>

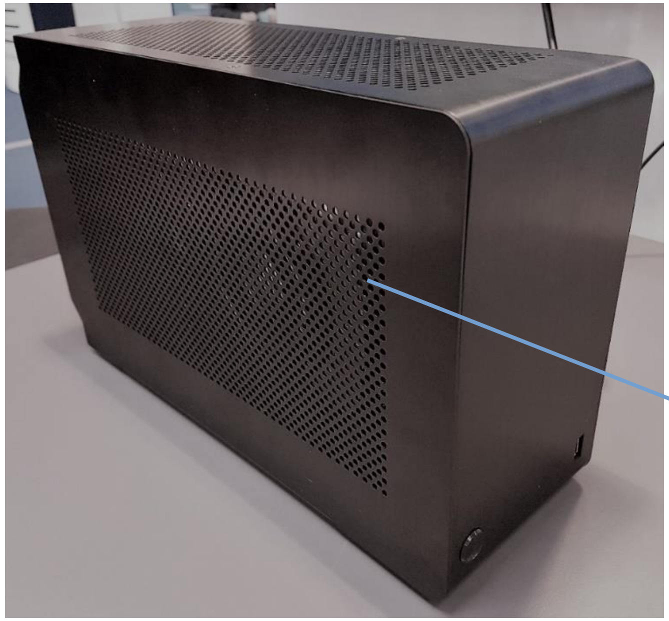


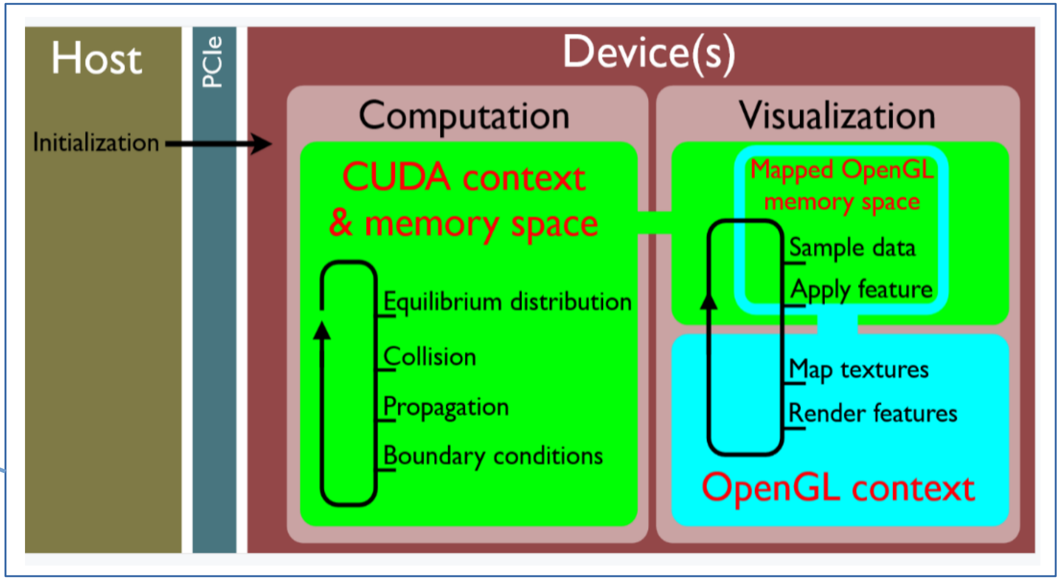


Towards online visualization and interactive monitoring of real-time CFD simulations on commodity hardware
N. Koliha, C.F. Janßen and T. Rung, *Computation* **3**(3):444-478, 2015; DOI: 10.3390/computation3030444

The *efficient lattice boltzmann environment* elbe

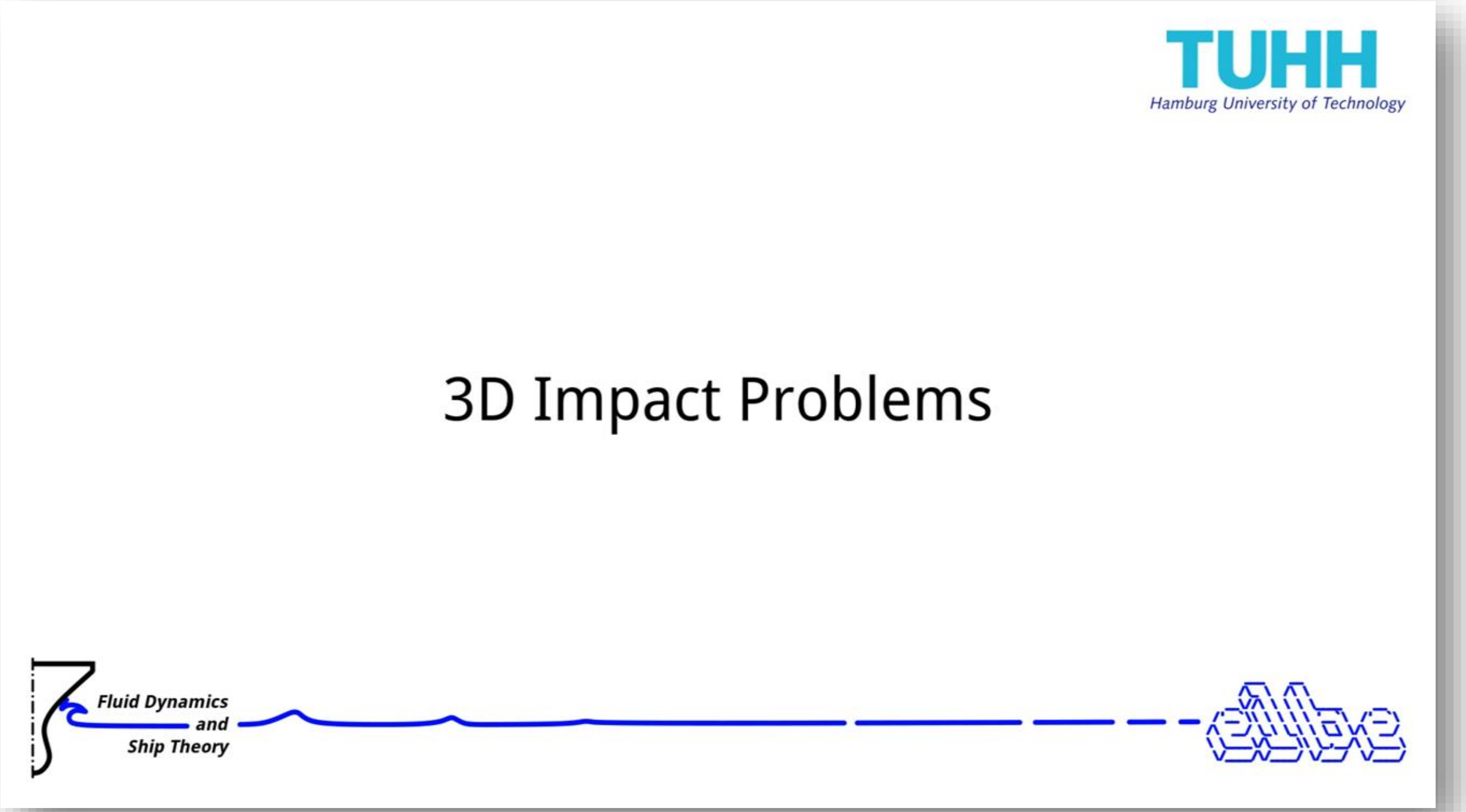
- Key ingredients:
  - 1D, 2D and 3D Lattice Boltzmann models, LES turbulence modeling
  - VOF interface capturing, bidirectional fluid-structure interaction, overset grids
  - GPU-accelerated pre- and post-processing





Towards online visualization and interactive monitoring of real-time CFD simulations on commodity hardware
N. Koliha, C.F. Janßen and T. Rung, *Computation* **3**(3):444-478, 2015; DOI: 10.3390/computation3030444

Animation


TUHH
Hamburg University of Technology
3D Impact Problems
Fluid Dynamics
and
Ship Theory

Education

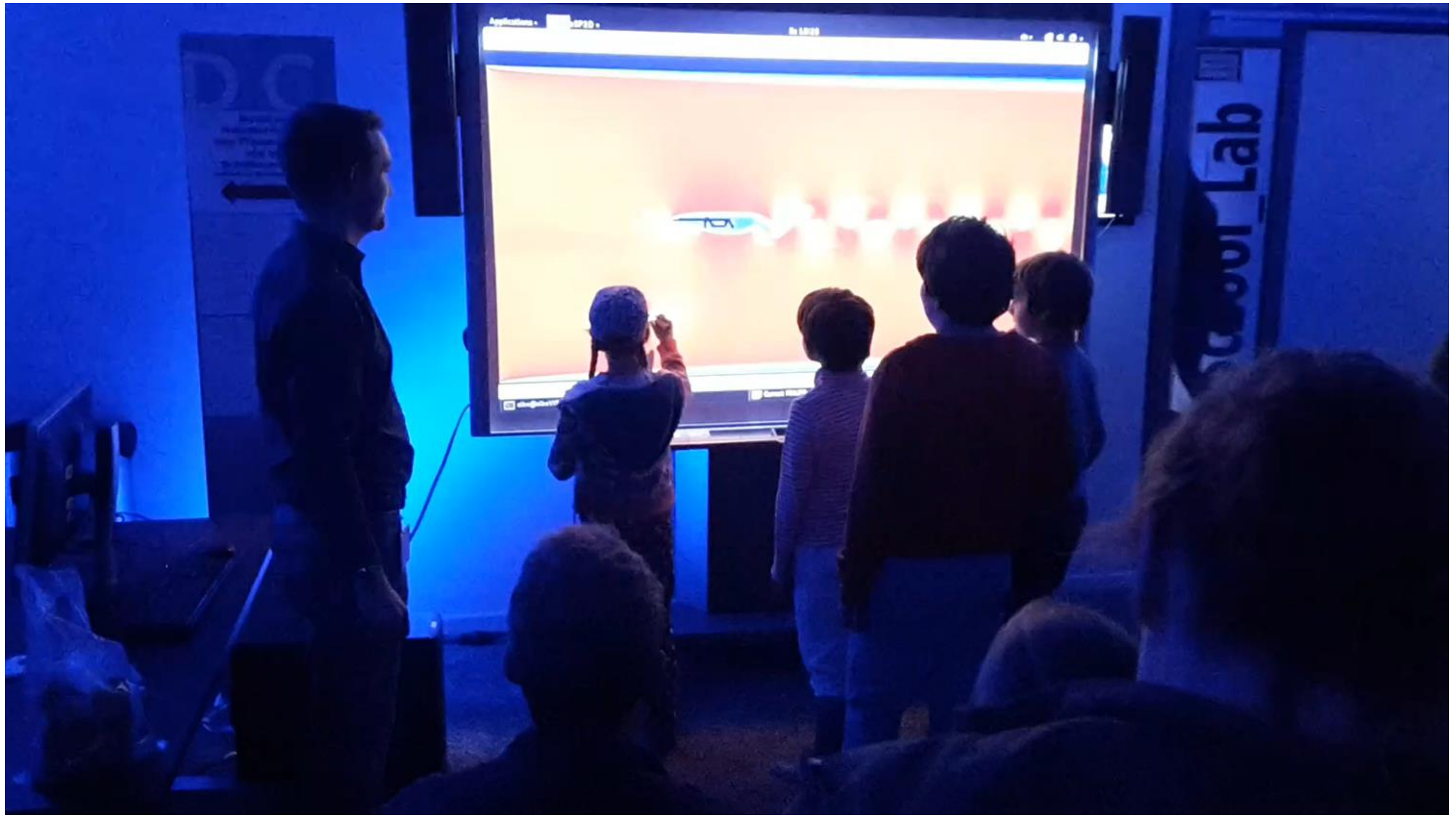
Activity	Topic of the Task		
	Scientific Results	**Scientific Methods**	**Scientific Processes**
Consumption	Students consume research results.	Students consume research methods.	Students receive explanations of scientific processes.
Examples:	*Attend lectures or presentations at science nights on recent CFD results.* *Watch animated results of numerical simulations on YouTube.*	*Listen to a presentation on numerical methods.* *Attend a lecture on fluid mechanics with a live demo.*	*Listen to a presentation on the history of ELBE.* *Participate in an excursion to a model basin to compare experimental results with numerical results.*
Application	Students discuss or transfer research results.	Students discuss or practice existing methods.	Students discuss or develop research processes.
Examples:	*Read literature to write a wiki article on turbulent mixing.* *Learn from an ELBE simulation of wing profiles in a wind tunnel to improve personal sailing skills.*	*Determine if the grid resolution that meets the computational constraints is sufficient to answer a question.* *Replicate a predefined ELBE test scenario in order to practice running the code.*	*Decide for/against higher grid resolution (vs. duration of calculation) for a numerical simulation.* *Figure out a research design to answer questions on nonlinear flow physics using ELBE.*
Research	Students systematically study the literature on a scientific topic	Students apply existing methods to a research question.	Students apply the full scientific research cycle.
Examples:	*Find a suitable parametrization for an array of wind turbines for a simulation in ELBE.* *Find the state of the art knowledge on parametrizations of turbulent mixing to consider modifications to the ELBE code.*	*Figure out a way to determine the influence of the shape of a blade on the efficiency of mixing of a gas into a liquid using ELBE simulations.* *Suggest a parametrization from literature to parametrize the shape of pools and tanks subject to violent sloshing.*	*Address own research questions using ELBE.* *Extend ELBE with novel algorithms to be able to address the new problem.*

Using an interactive Lattice Boltzmann solver in fluid mechanics instruction
M.S. Glessmer and C.F. Janßen, *Computation 2017* **5**(3), July 2017; DOI: 10.3390/computation5030035

Education – Consumption level

„Students consume research results“

„Students discuss or transfer research results“



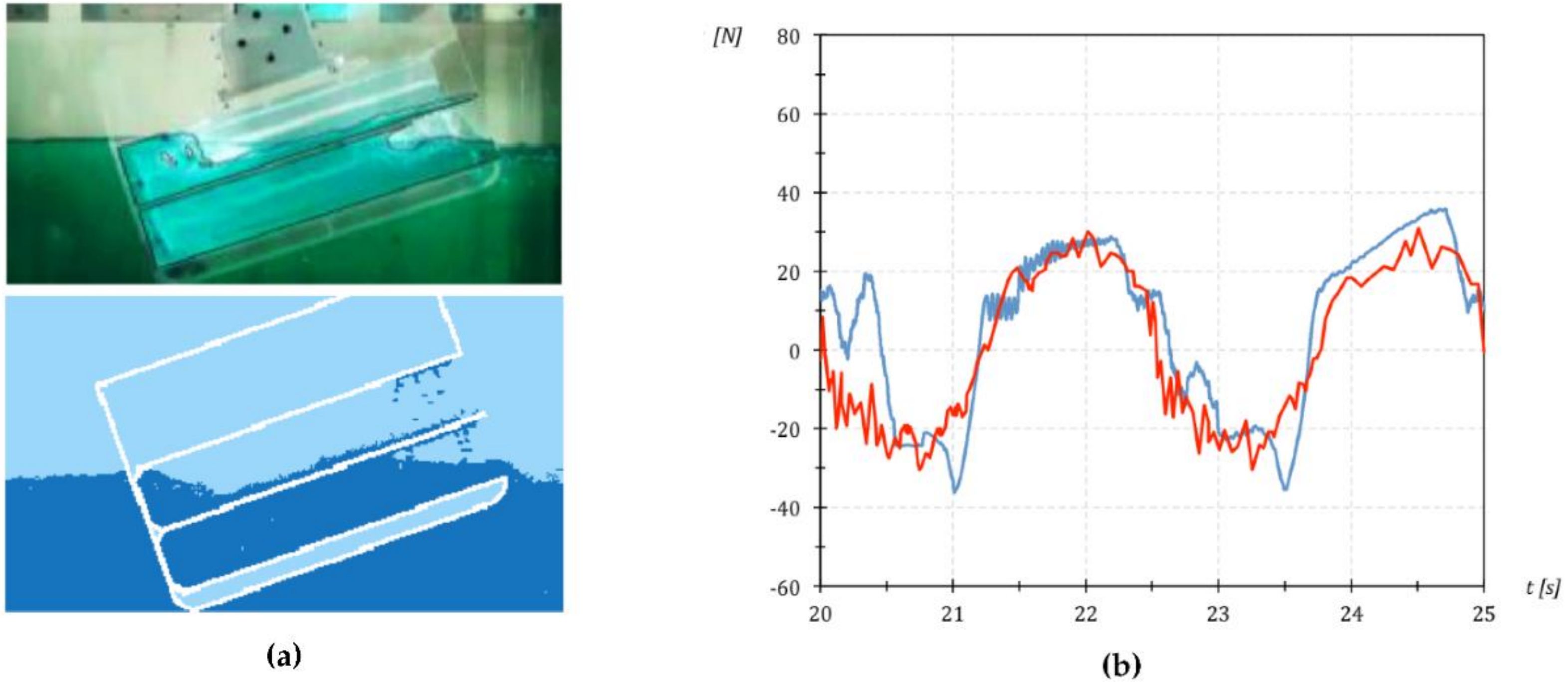
Using an interactive Lattice Boltzmann solver in fluid mechanics instruction
M.S. Glessmer and C.F. Janßen, *Computation 2017* **5**(3), July 2017; DOI: 10.3390/computation5030035

TUHH

Education – Application level

„Students discuss or practice existing methods“

„Students discuss or develop research processes“



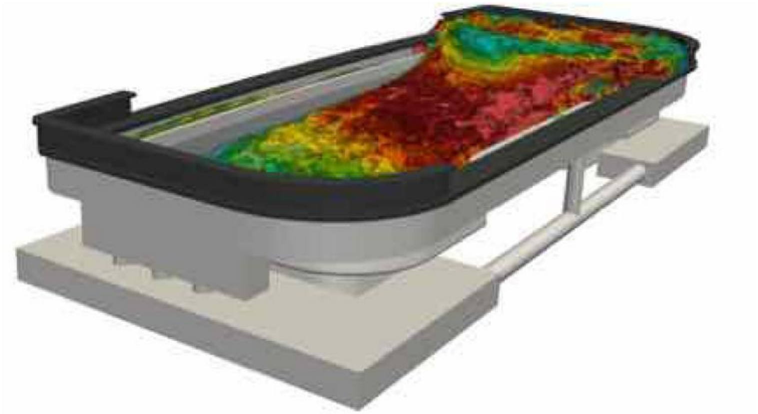
Problem-based learning task in the lecture *Application of CFD in Naval Architecture*, 2014.

Using an interactive Lattice Boltzmann solver in fluid mechanics instruction
M.S. Glessmer and C.F. Janßen, *Computation 2017* **5**(3), July 2017; DOI: 10.3390/computation5030035

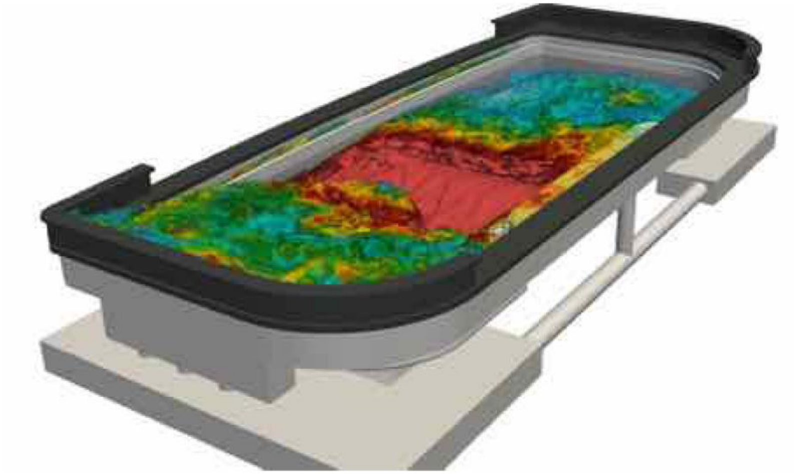
Education – Research level

„Students apply existing methods to a research question“

„Students apply the full scientific research cycle“



(a)

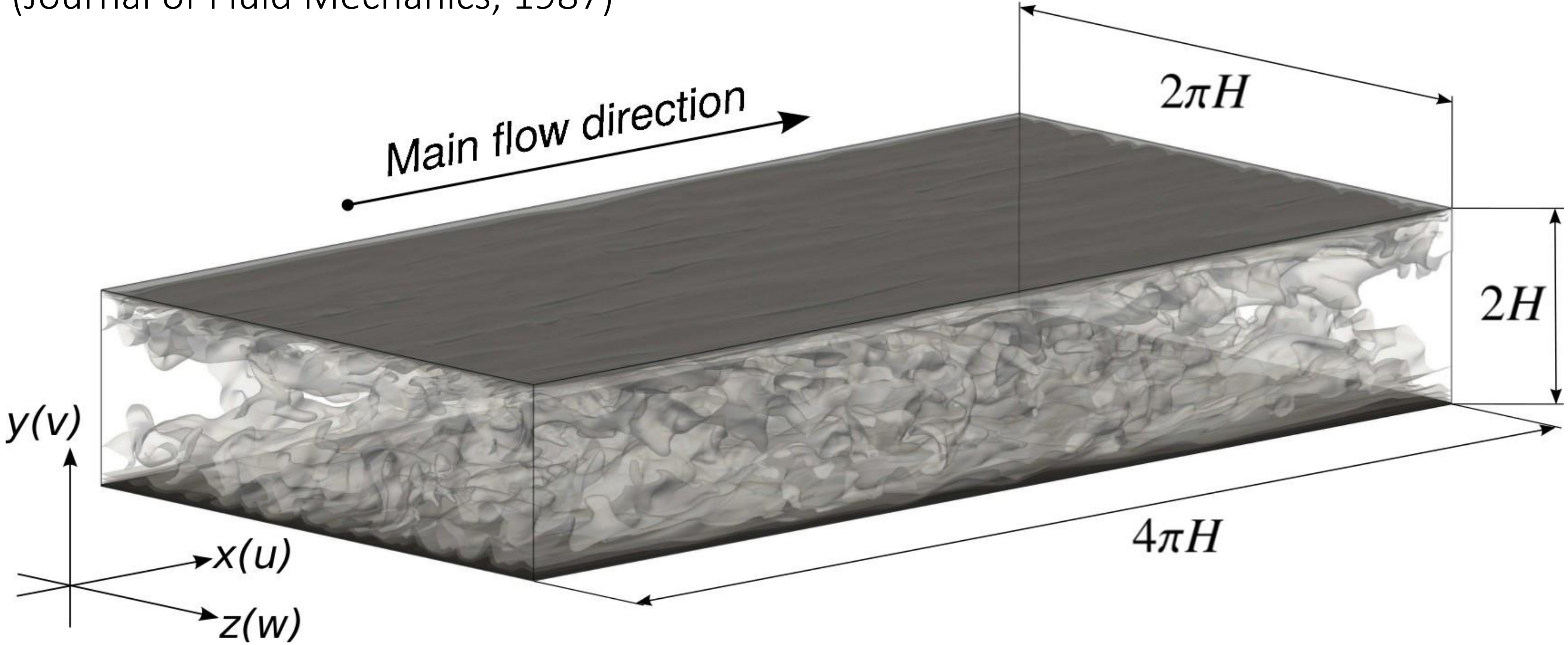


(b)

A. Budde, *Pool sloshing aboard mega yachts*, Master thesis, October 2016.

Turbulent channel flow (DNS)

- Comparison of elbe results for $Re_\tau = 180$ to reference data from Kim, Moin and Moser (Journal of Fluid Mechanics, 1987)

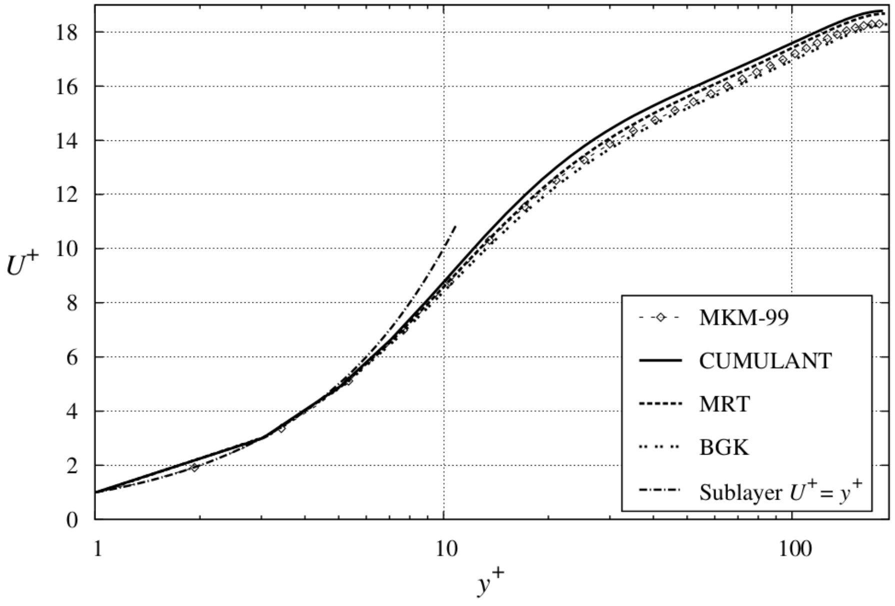


Scrutinizing lattice Boltzmann methods for direct numerical simulations of turbulent channel flows.
M. Gehrke, C.F. Janßen, T. Rung, *Computers and Fluids* **156**:247–263, 2017; DOI: 10.1016/j.compfluid.2017.07.005

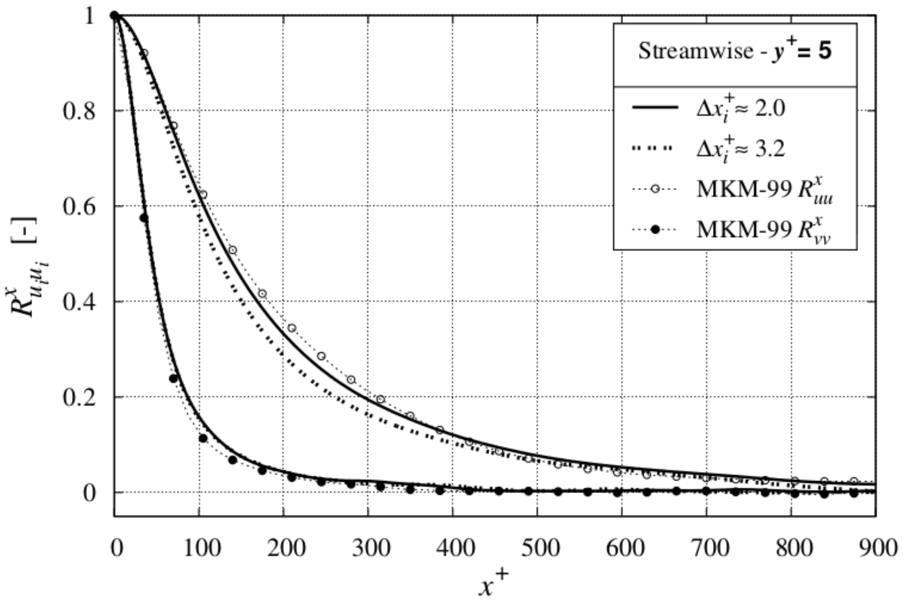
Turbulent channel flow (DNS)

- DNS discretization with 120M grid nodes, 4M discrete time steps
- Ran on 4 x K40 GPUs with up to 1,400 MNUPS, yielding a time-to-solution of <90h per run

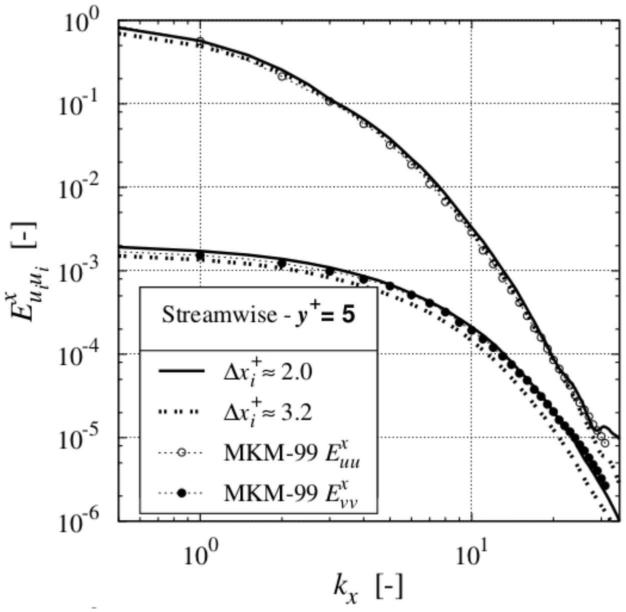
Velocity



Two-point correlations



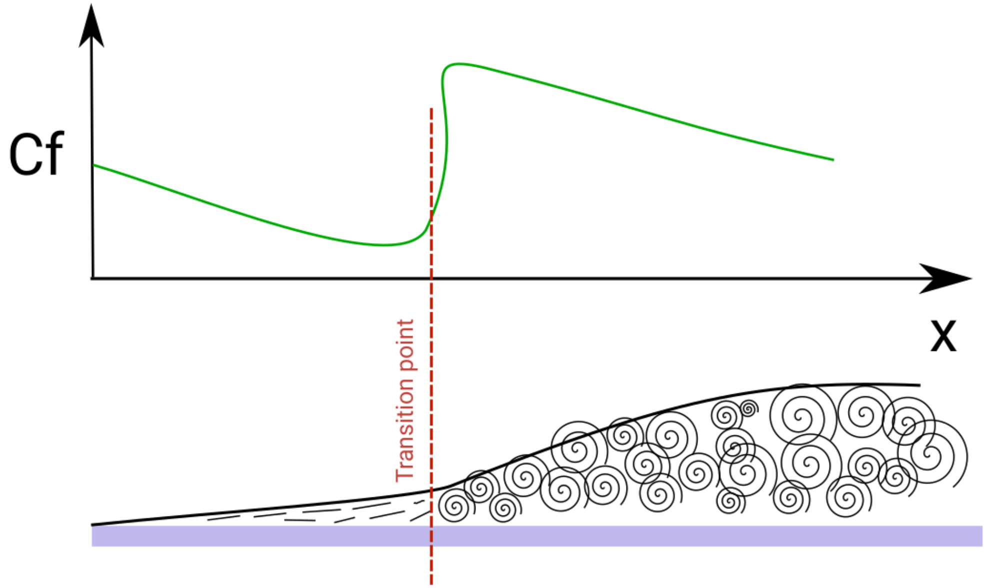
Energy spectra



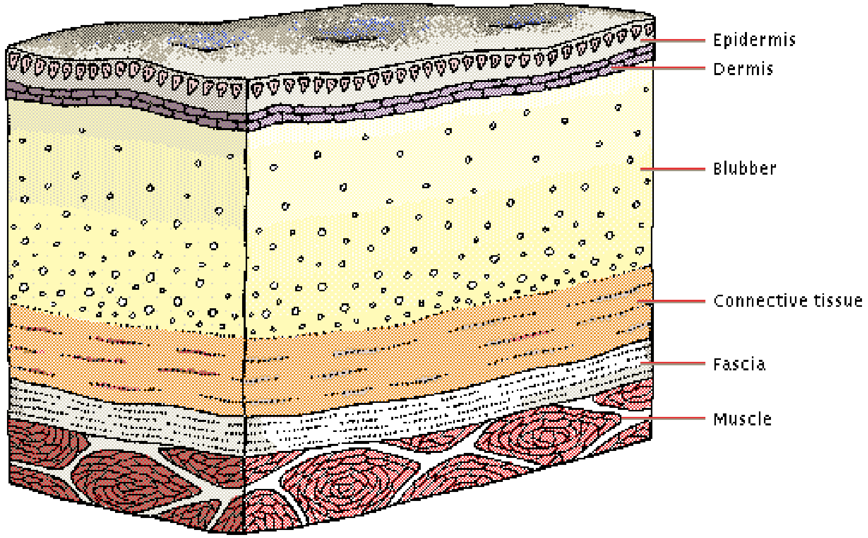
Scrutinizing lattice Boltzmann methods for direct numerical simulations of turbulent channel flows.
M. Gehrke, C.F. Janßen, T. Rung, *Computers and Fluids* **156**:247–263, 2017; DOI: 10.1016/j.compfluid.2017.07.005

Flat-plate boundary layers

- Simulation of natural transition from laminar to fully turbulent flow
- Bio-inspired drag reduction: dolphin skin (viscoelastic blubber layer)
- Idea: delay transition by the use of compliant coatings (on, e.g., ship hulls)



Friction Drag Coefficient

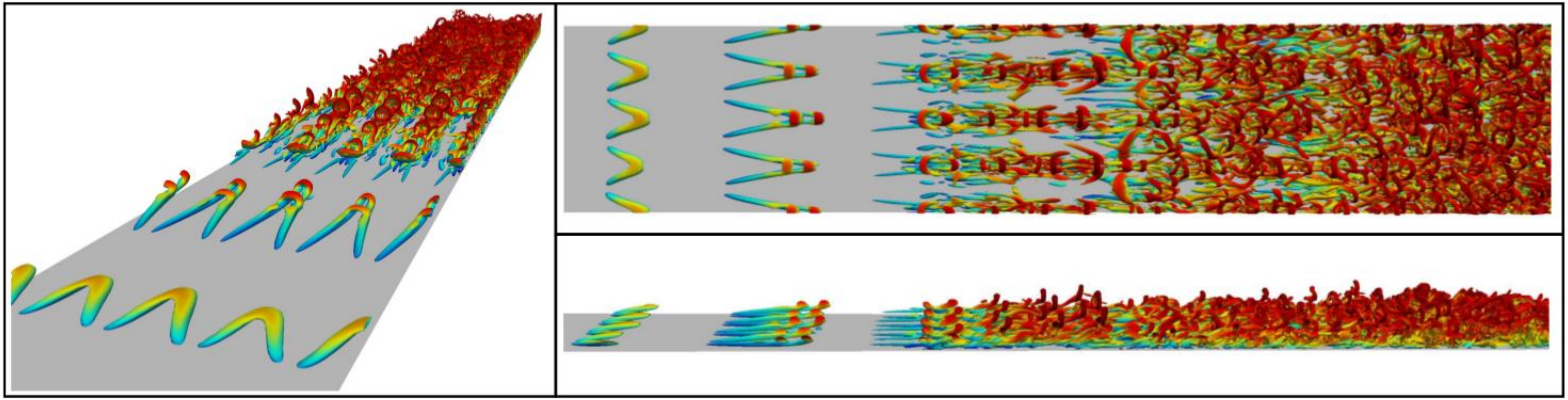


Dolphin skin layers

Source (right): http://aquatic-human-ancestor.org/anatomy/fat.html

Flat-plate boundary layers

- Studying different vortex formation shapes (K-Type transition pattern depicted below)
- 500M grid nodes, 250K discrete time steps, computational time <8h on 4 x K80 boards



Numerical simulation of natural transition with the cumulant lattice Boltzmann method
A. Banari, M. Gehrke, C.F. Janßen, T. Rung, 2019 (in preparation)

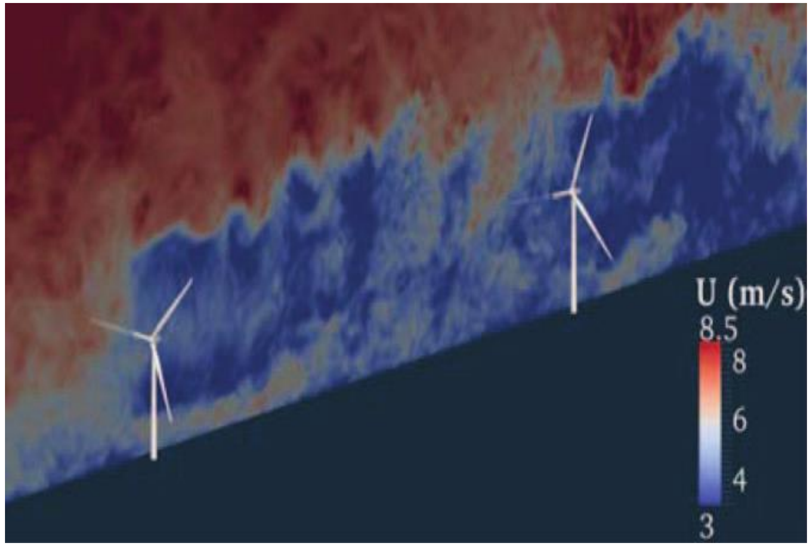
TUHH

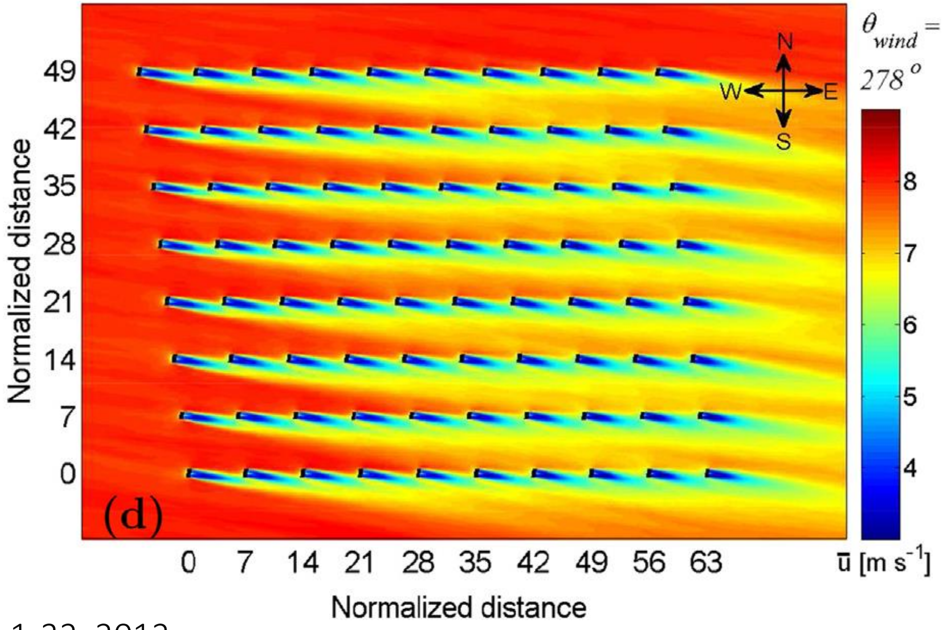
Application: Wake modelling in wind farms

Source: Hasager et al., *Energies* **10**(3), 317, 2017

Why Large-eddy simulations?

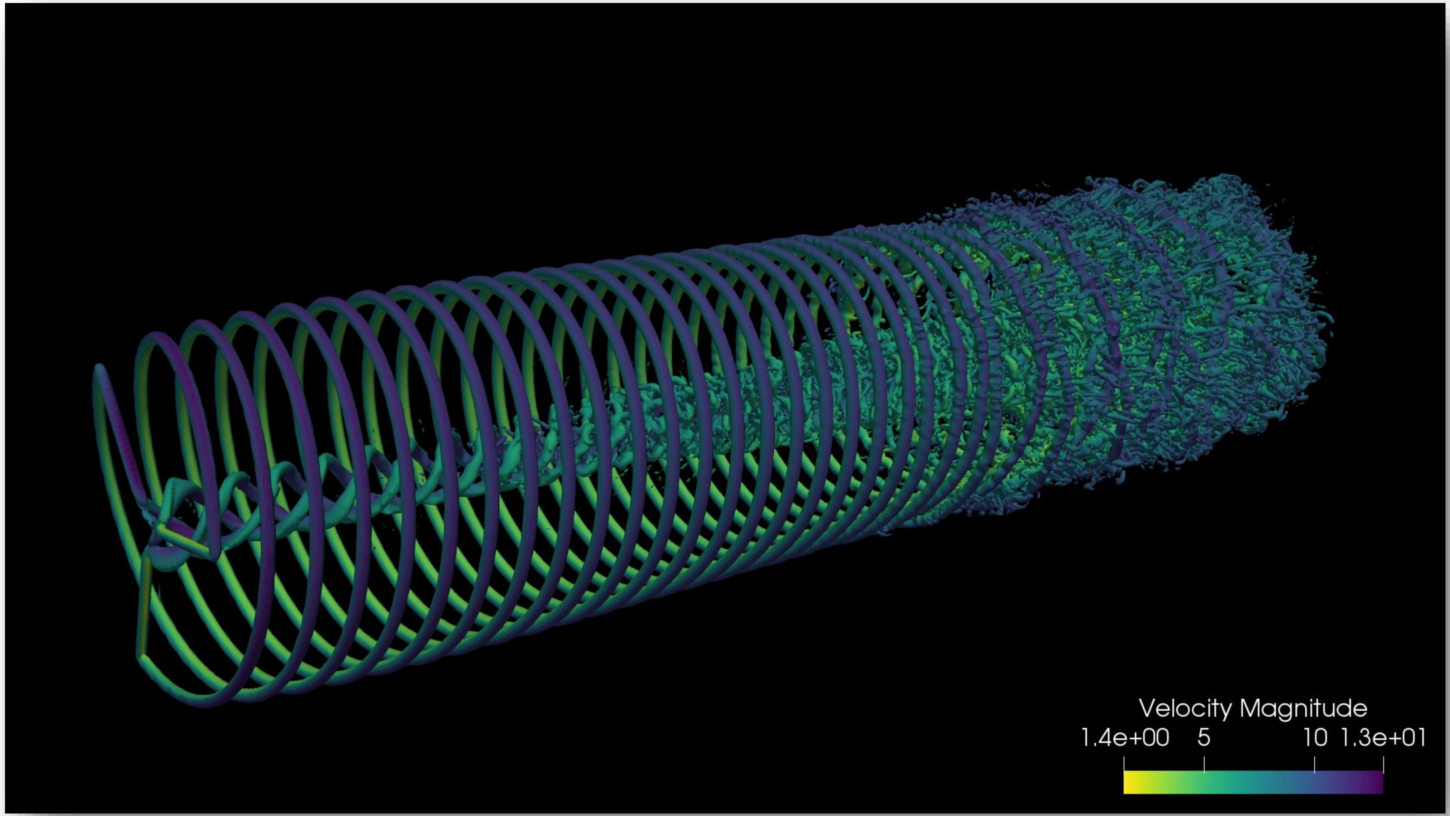
- Transient simulations resolving the large turbulent structures
- Potentially more accurate than steady-state RANS
- Has become the state of the art in academia for wind farm modelling
- Applications: Fundamental investigations, performance and turbine fatigue load analysis, coordinated farm-control





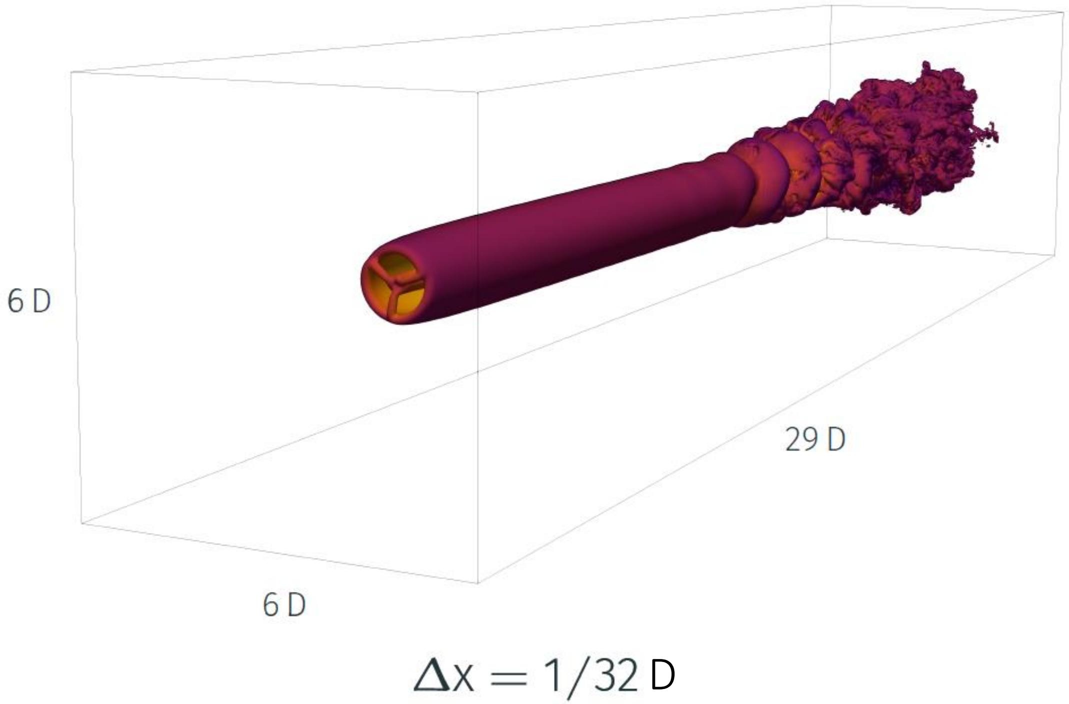
Source (left): Churchfield et al., *Journal of Turbulence* **13**(14):1-32, 2012
Source (right): Wu and Porté-Agel, *Renewable Energy* **75**:945-955, 2015

Animation



Feasibility study

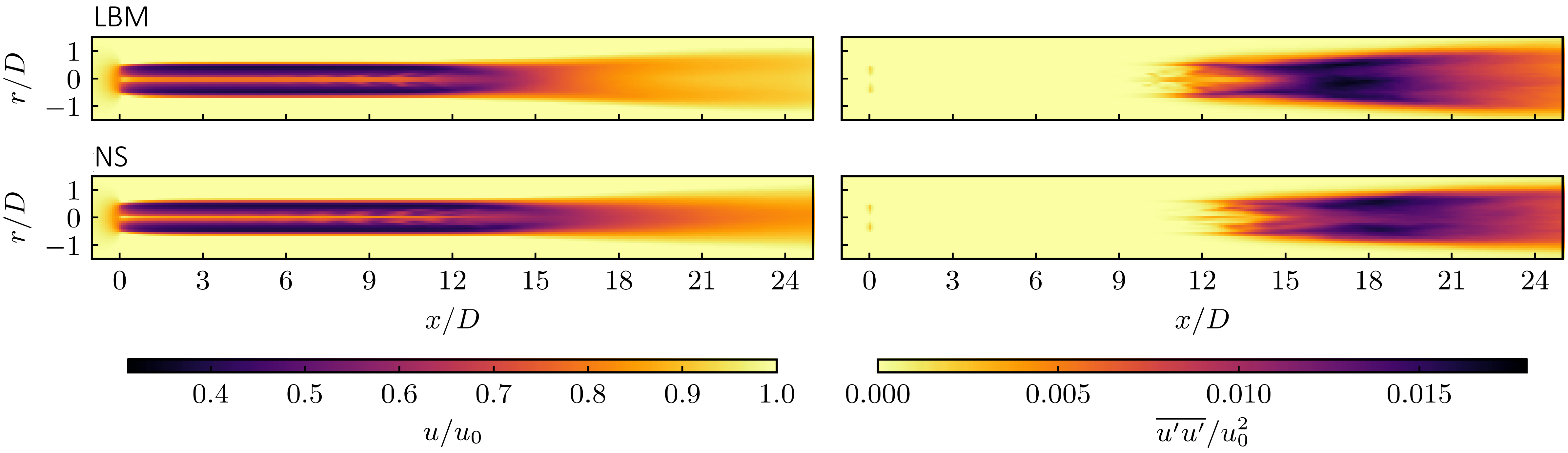
- Actuator Line simulation of a 5MW turbine in uniform laminar inflow
- Parametrized cumulant (PC) LBM
- Smagorinsky turbulence model
- Code-to-code comparison to a finite volume Navier-Stokes approach



Asmuth et al., *Journal of Physics: Conference Series*, in print, 2019.
Asmuth et al., *Wind Energy Science*, in preparation, 2019.

TUHH

Wake characteristics

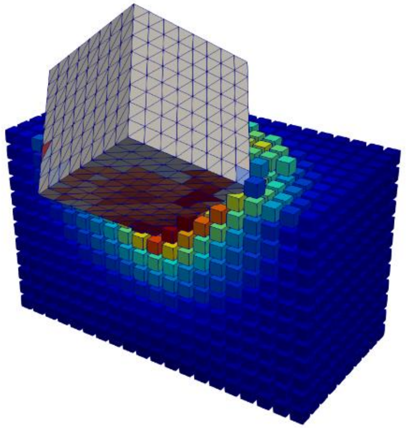


Performance overview

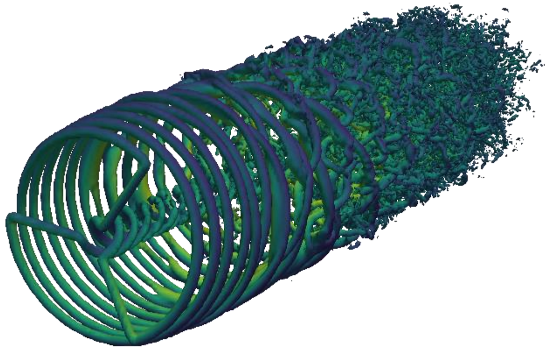
	NS	LBM
Processing Unit	1080 CPU cores (Intel Xeon Gold 6130)	1 GPU (Nvidia RTX 2080 Ti)
Grid nodes	$35 \cdot 10^6$	
Wall time [h]	2h 44m	0h 09m
Process time [CPU-core-h, GPU-h]	**3019.79**	**0.14**
Performance in MNUPS	25	1050
Real time / Comp. time	0.05	0.9

Summary

Together with recent accelerator hardware, innovative Lattice Boltzmann methods can bridge the gap between off-the-shelf desktop hardware and large-scale supercomputers.



Tailor-made numerical methods and optimized pre- and post-processing solutions enable supercomputing on the desktop and simulation-based design.



Efficient new multi-GPU solutions will further strengthen the trend towards real-time solutions of complex flows.

Visit http://www.tuhh.de/elbe