Some considerations on DNS and LES in complex geometries

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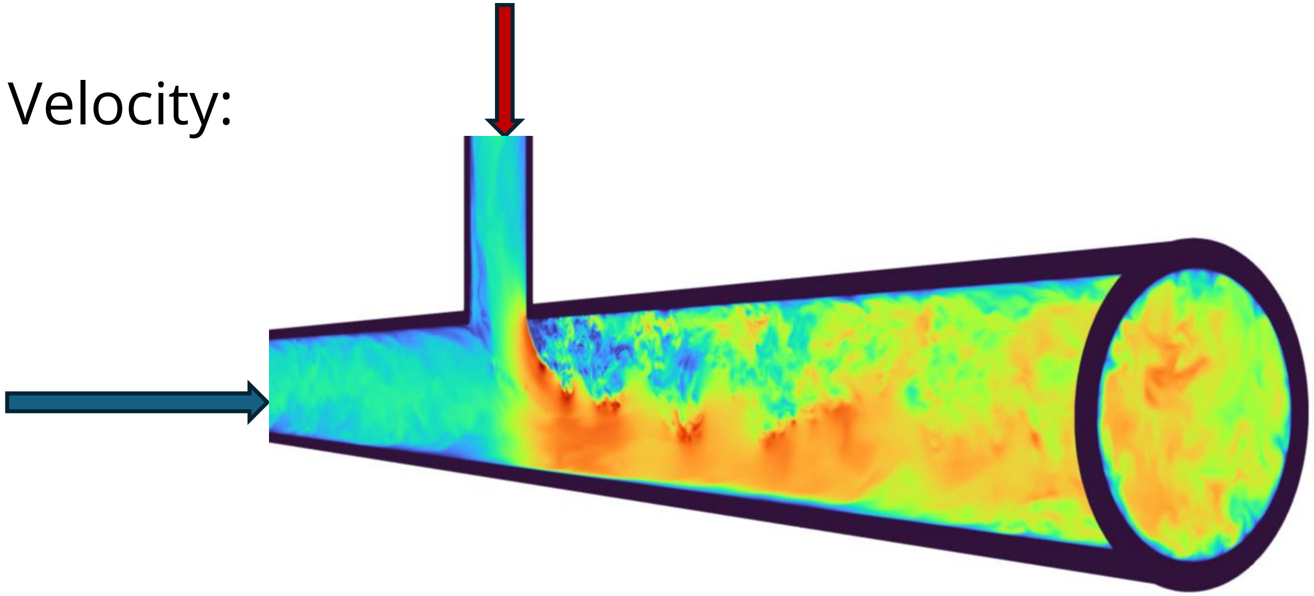
Contents

High-fidelity (HiFi) simulation in complex geometries

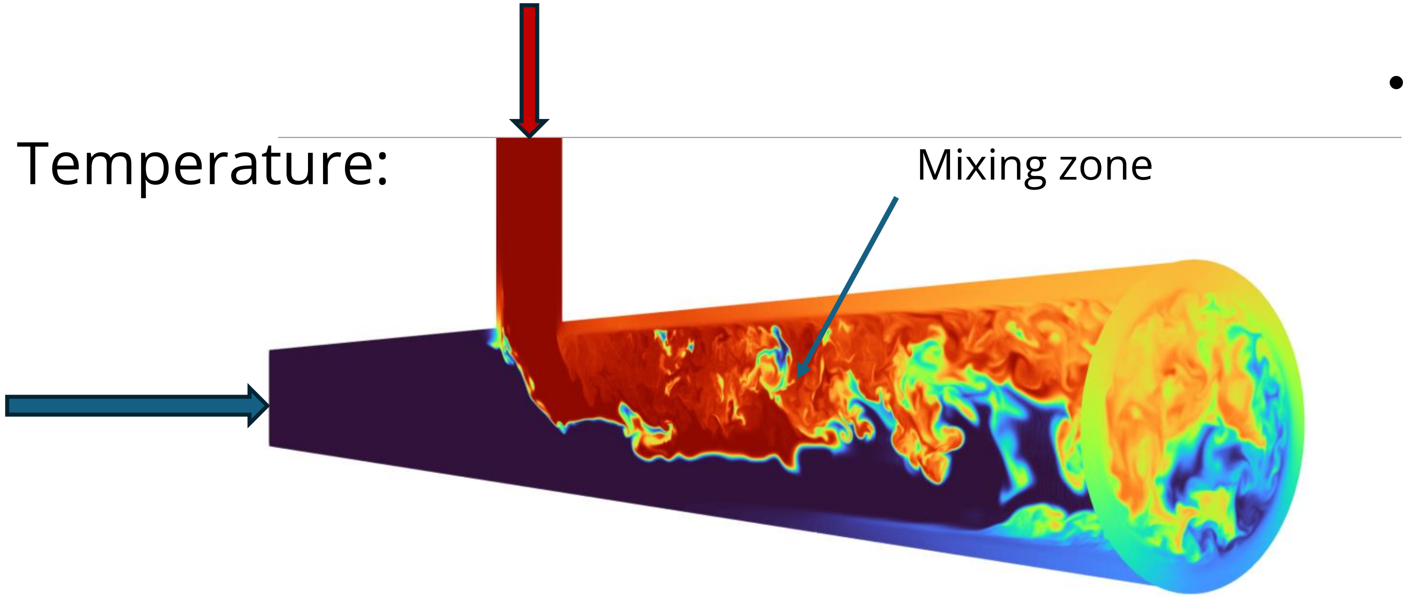
- Single-phase flow HiFi simulations
  - DNS
  - LES
- Two-phase flow HiFi simulations
  - Ambition
  - Numerical challenges
  - Modelling of sub-grid physics
- Concluding remarks

HiFi single-phase simulations - DNS

- Velocity:



- Temperature:

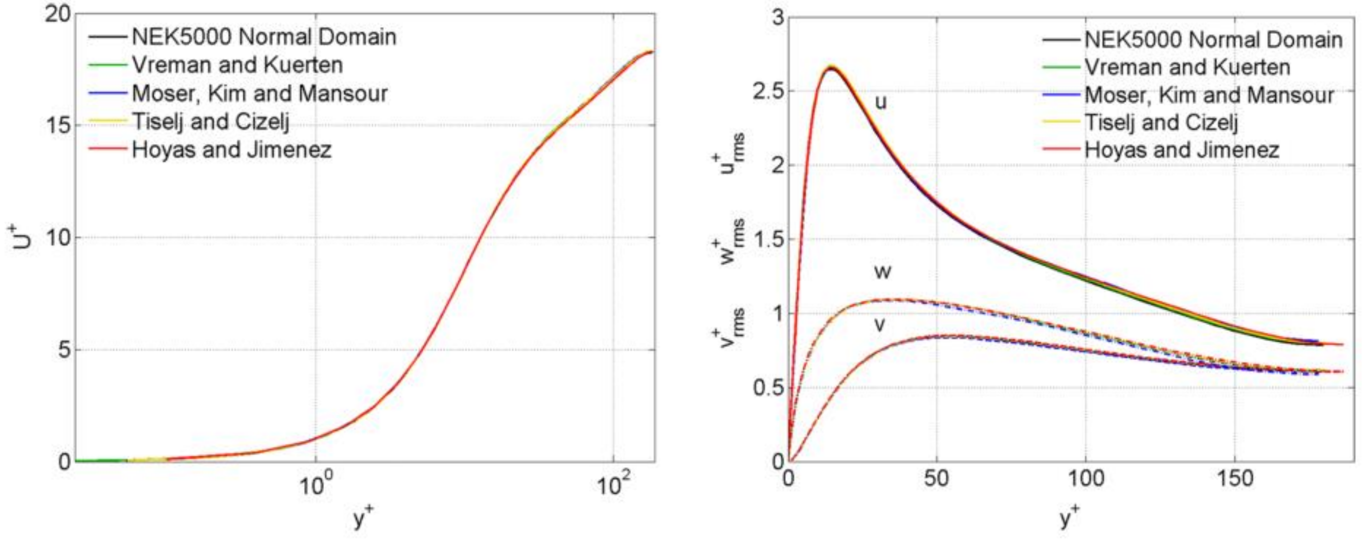


A DNS example:

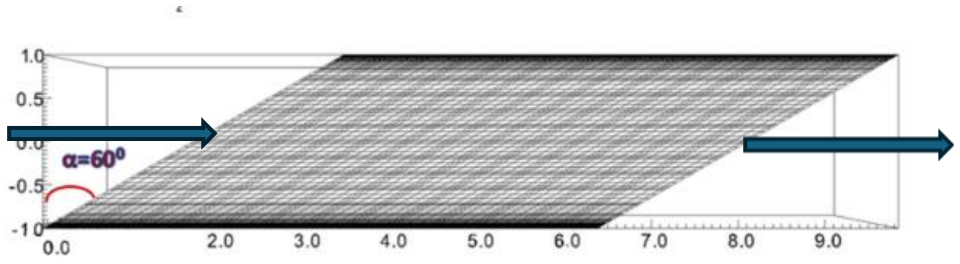
- Thermal-fatigue issue
- NEK-RS spectral element method
  - Lagrange interpolants on a Gauss-Lobatto-Legendre points distribution
- Purpose: knowledge and reference data for turbulence model development & validation

HiFi single-phase simulations - DNS

- NEK-5000 / NEK-RS spectral element method
  - High-order accuracy in complex geometries[1]
    - DNS of turbulent channel flow



Mean and RMS velocities



Front view

[1]Shams and Komen *FTAC*, 2018

HiFi single-phase simulations - DNS

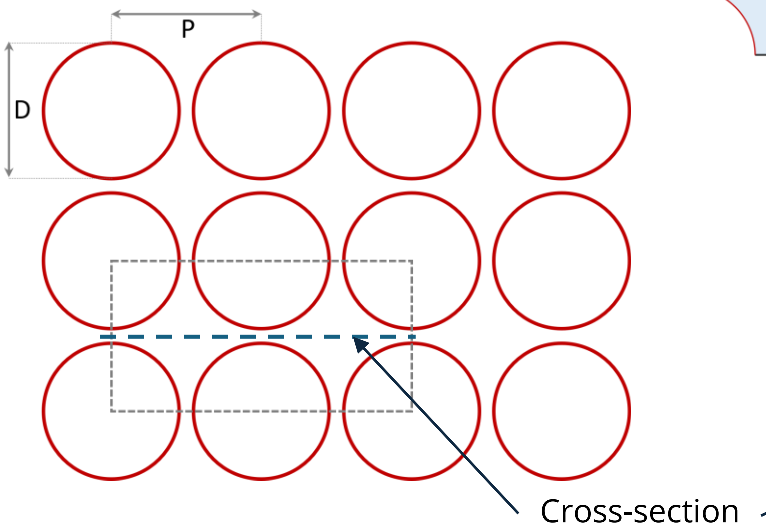
- NEK-RS / NEK5000 spectral element method
  - Accurate, yes! Efficient?
  - Costs vs accuracy assessments:
    - [1]Kooij et al, *Computers & Fluids*, 2018
      - Rayleigh–Bénard (RB) convection in cubic and cylindrical containers
    - [2]Capuano et al, *Eur. J. Mech. B Fluids*, 2023
      - Turbulent flow over a sphere
  - Conclusion: NEK5000 less efficient[1] than or similarly efficient[2] as Cartesian / cylindrical grid finite difference / volume solvers using FFTs.

23-1-2026

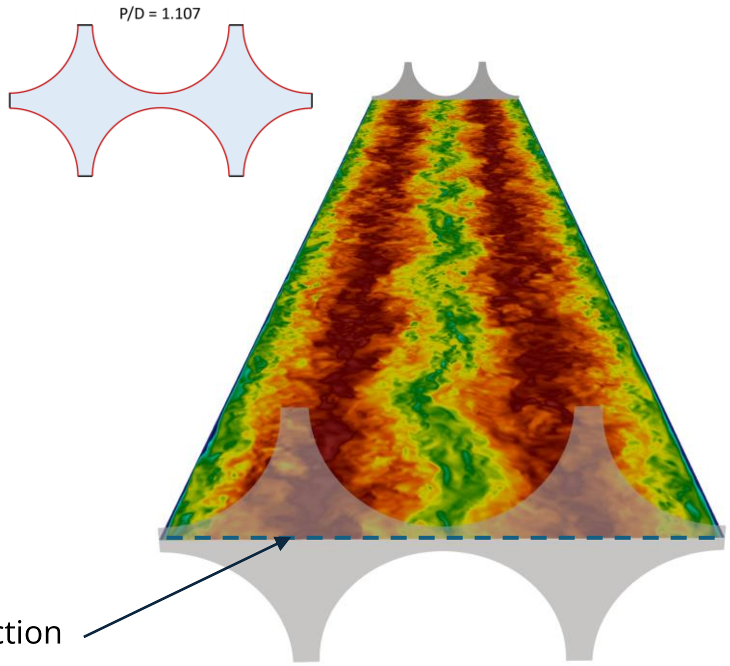
HiFi single-phase simulations - DNS

- NEK-RS / NEK5000 spectral element method
  - Efficiency: depends on Re number and geometry[2]
    - IBM needs refinement in multiple coordinate directions for clustering grid points in boundary layer → Cost increases fast with Re number

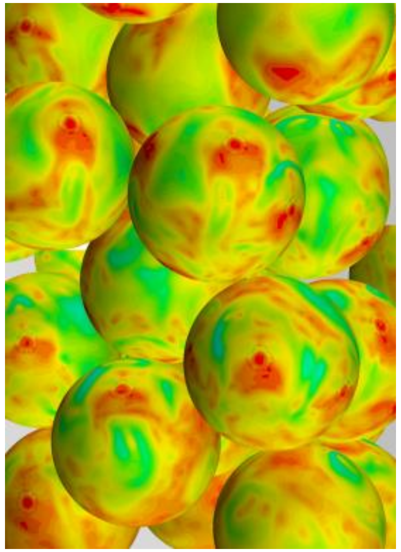
[2]Capuano et al, *Eur. J. Mech. B Fluids*, 2023



Subchannel fuel rod bundle



Instantaneous flow field

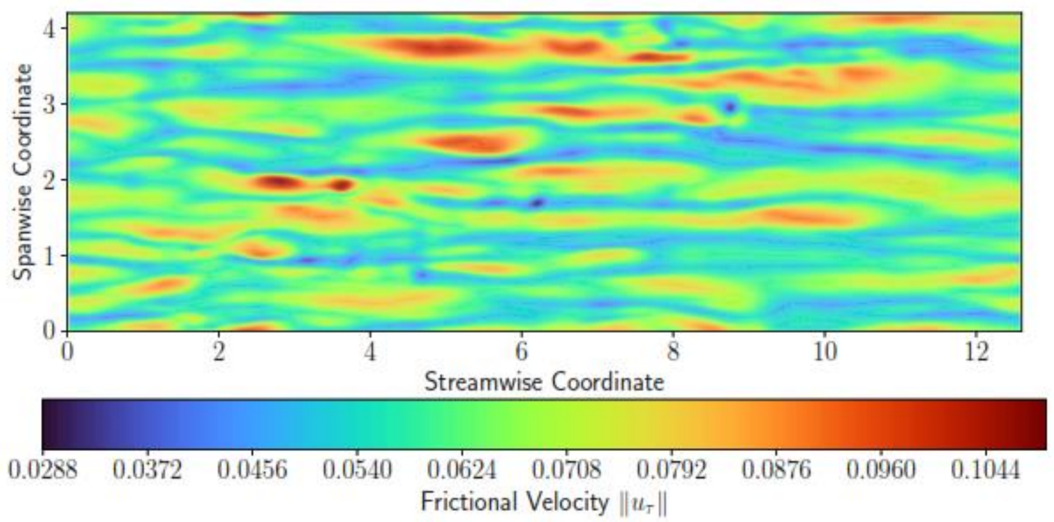


Pebble bed

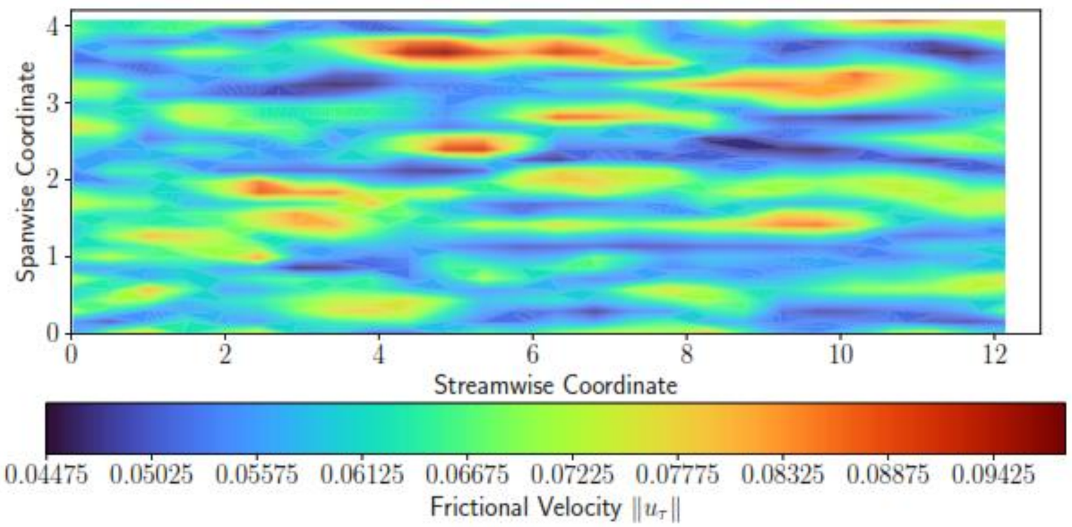
- Comparison higher-order moments

HiFi single-phase simulations - LES

- LES: effect of implicit top-hat filter
  - DNS turbulent channel flow data → top-hat filtering to match UDNS grid resolution, with the same wall normal resolution in DNS and UDNS resolution*



Friction velocity, DNS resolution



Filtered friction velocity, UDNS resolution

Top-hat filter → projection flow topology at lower Reynolds

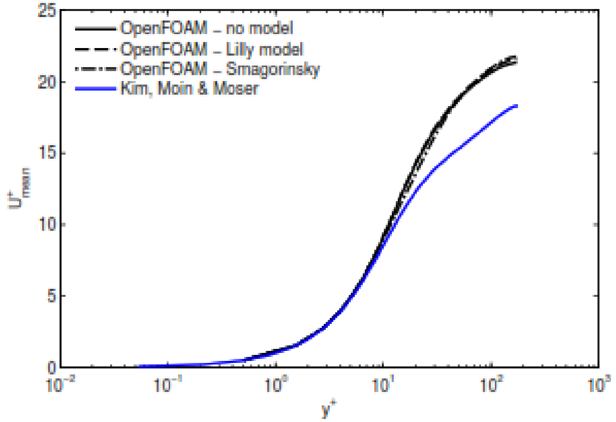
* Mathur and Sajuhudeen

HiFi single-phase simulations - LES

- LES: effect of implicit top-hat filter
  - DNS turbulent channel flow data → top-hat filtering to match UDNS grid resolution, with the same wall normal resolution in DNS and UDNS resolution

Case	Re_τ scaling				Re_{bulk} scaling			
	u_τ	U_{bulk}	Re_τ	Re_{bulk}	u_τ	U_{bulk}	Re_τ	Re_{bulk}
Vreman	1.000	15.70	180.0	5650	1.000	15.70	180.0	5650
OpenFOAM *30-Grid*	1.007	15.68	181.3	5643	0.998	15.66	179.6	5638
OpenFOAM *60-Grid*	1.007	17.24	181.3	6205	0.924	15.66	166.3	5637
OpenFOAM *90-Grid*	1.000	18.68	179.9	6723	0.839	15.66	150.9	5637

Frictional and bulk Reynolds number for Vreman DNS data and 3 OpenFOAM UDNS simulations*



(a) *90-Grid* - mean velocity

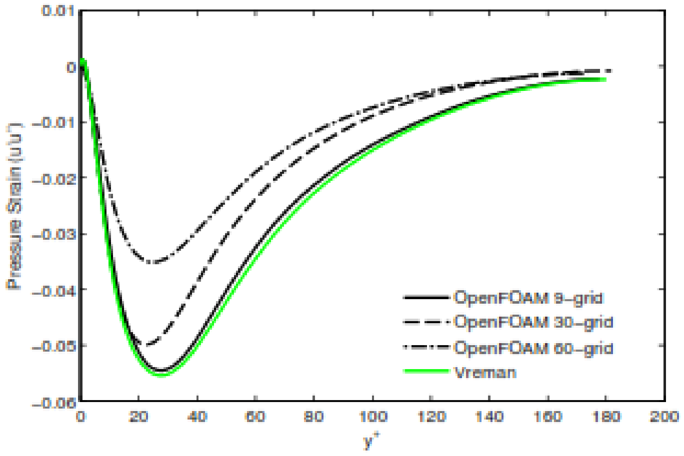
  - Top-hat filtering → projection at lower Reynolds flow topology
  - LES SGS viscosity (algebraic models) → additional projection
  - Issue: engineers are not interested in a filtered reality

*Komen, *Tue PhD thesis*, 2025

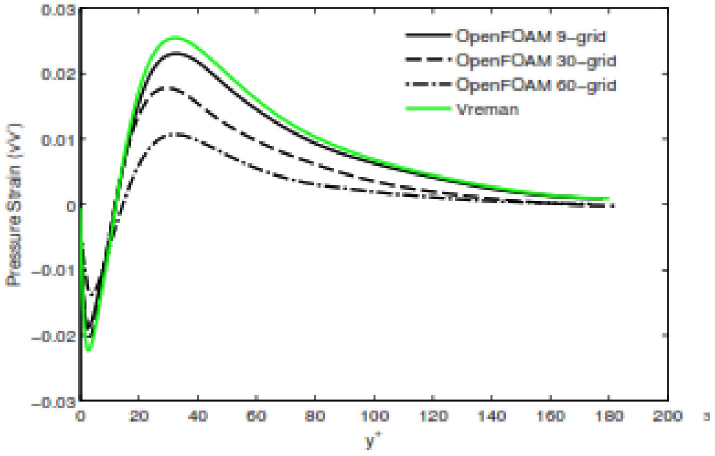
HiFi single-phase simulations - LES

- LES: issue with algebraic models for wall resolved LES
  - Case: DNS and UDNS of turbulent channel flow[1]
    - Systematic coarsening of the UDNS grid resolution gives:
      - progressive underprediction of pressure strain rate terms →
      - progressive underprediction of redistribution of kinetic energy →
      - progressive overprediction of u'u', and underpredictions of v'v' and w'w'

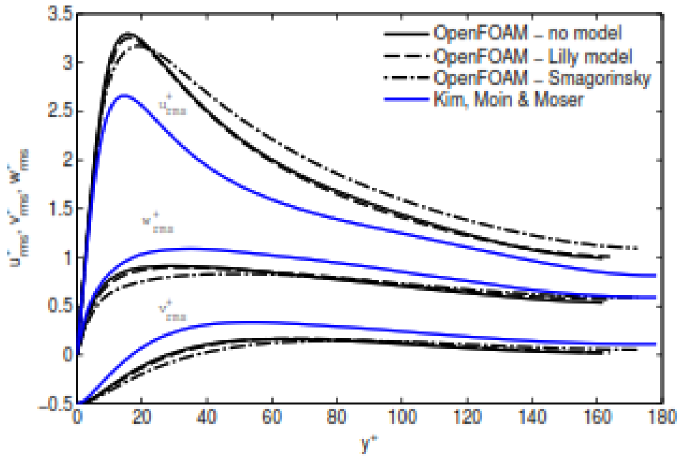
[1]Komen et al, *JCP*, 2017



(b) Pressure strain rate of $\overline{u'u'}^+$



(d) Pressure strain rate of $\overline{v'v'}^+$



(d) *60-Grid* - RMS velocities

High-Fidelity single-phase simulations

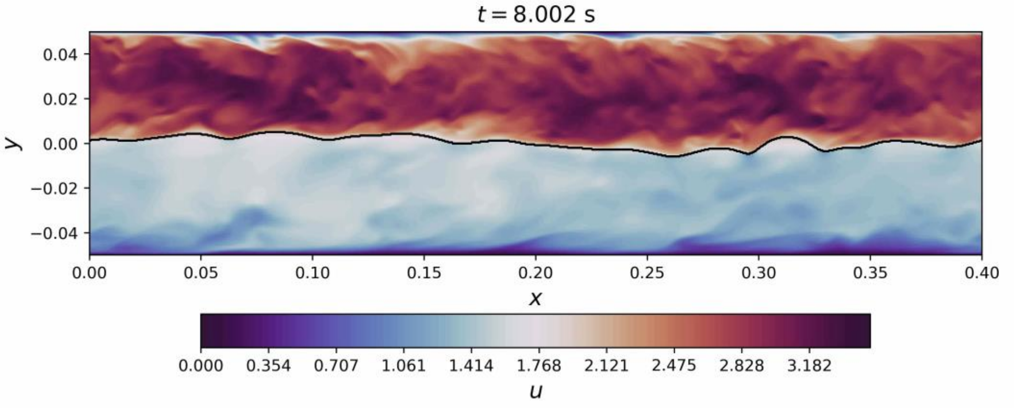
- LES: issue with algebraic models for wall resolved LES
  - Case: DNS and UDNS of turbulent channel flow[1]
    - Issue: algebraic LES models cannot compensate for this deficiency in redistribution of turbulent kinetic energy!
    - Instead, they needs grid resolutions approaching DNS grid resolutions
      - for which LES model contribution becomes negligible
    - Isotropy assumption of the SGS stresses does not hold in wall resolved simulations → (probably) anisotropic models needed
    - How to predict the correct friction velocity?

[1]Komen et al, *JCP*, 2017

HiFi two-phase simulations - DNS

UDNS, Gas Re_τ = 450, liquid $Re_{\tau,}$ = 250,

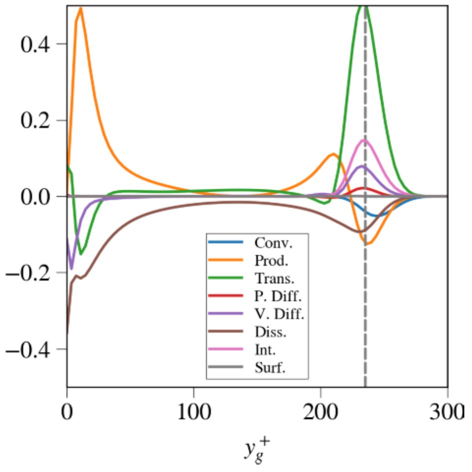
- velocity:



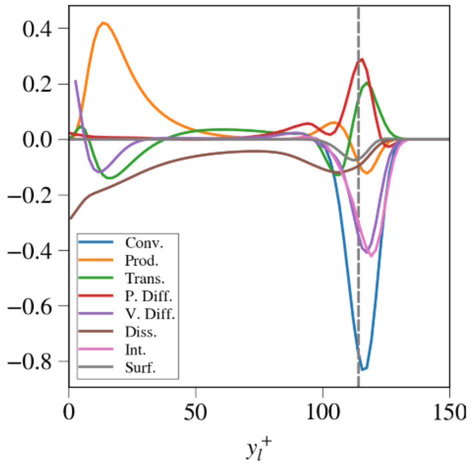
DNS, Gas Re_τ = 240, liquid $Re_{\tau,}$ = 120,

- TKE budgets:

Gas phase



Liquid phase

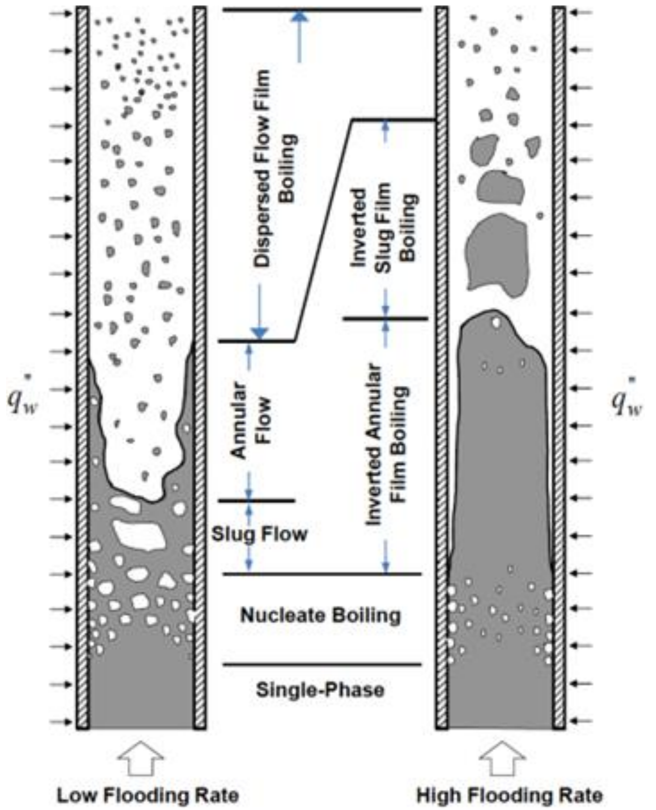


A DNS example:

- Stratified two-phase flow simulation
- 2nd-order accurate finite volume method
- PLIC VOF
- Purpose: knowledge and reference data for turbulence model development & validation
  - Near interface turbulence damping in RANS models

HiFi two-phase simulations - Ambition

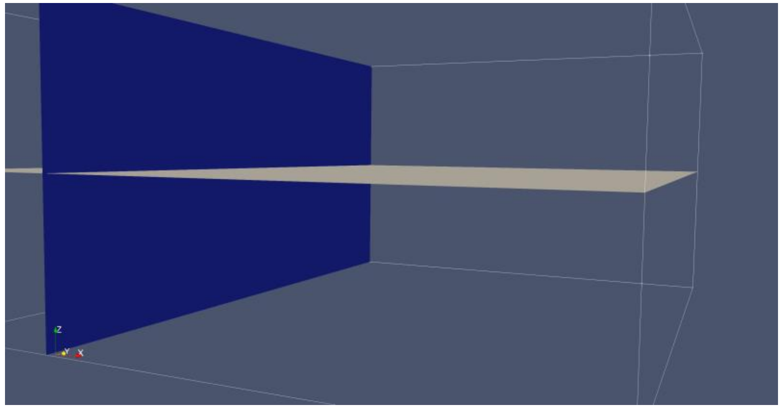
- Ambition must be to do
  - More complicated geometries
    - Subchannels, fuel assembly, spacers, mixing vanes,
  - More physics (coalescence, break-up, interfacial heat & mass transfer)
  - More realistic conditions



- To achieve this, we need
  - Better and more efficient numerical methods:
    1. 'Common' approach: structured grid, 2^{nd}-order
    2. 'Refined' approach: unstructured grid, higher-order
  - Better / more accurate sub-grid models

HiFi two-phase simulations – 'Common' approach

- Interface is second order at best → preference for high resolution over high order
  - *Does this rationale hold also for high-order discretization?*
- Structured staggered meshes:
  - VOF: geometric reconstruction relatively simple
  - Fast Poisson solvers:
    - FFTs (Schumann[1])
    - Constant coefficient pressure equation (Dodd & Ferrante[2])
    - *Large density ratios remains a challenge*
  - IBMs for complex geometries → *increases overhead and inaccuracies*
- Open-source examples: Basilisk, Briscola, CaNS (phase field, GPU)



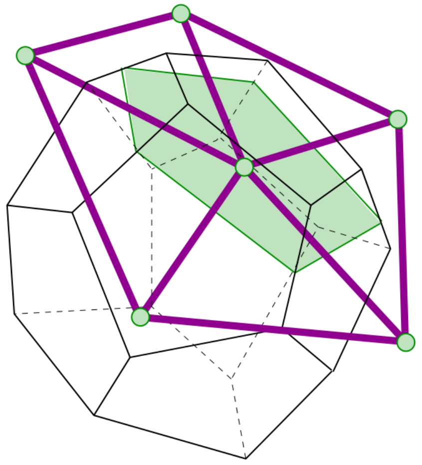
B. J. Boersma.
DLES13, Udine, Italy, 2022

131 mio cells

[1]Schumann, U., & Sweet, R. A. Journal of Computational Physics, 1998
[2]Dodd, M. S., & Ferrante, A. Journal of Computational Physics, 2014

HiFi two-phase simulations – 'Refined' approach

- Complex geometries → Unstructured (collocated) grids
- Development of unstructured geometric VOF
  - Polyhedron truncation
    - Open-source toolboxes gVOF, VOFTools[1]
  - Unsplit advection[2]
    - More general, more complicated, not necessarily conservative
- Higher-order
  - e.g., implementation of LS in Nek5000/NekRS,



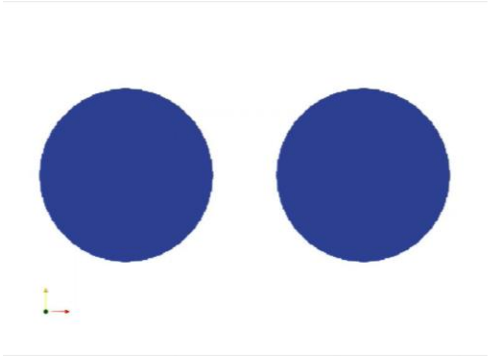
Truncation of an arbitrary polyhedron, Lopez & Hernández[1]

López, J., & Hernández, J.. *Computer Physics Communications*, *2022*
Marić, T., Kothe, D. B., & Bothe, D. *Journal of Computational Physics*, *2020*.

HiFi two-phase simulations – sub-grid models

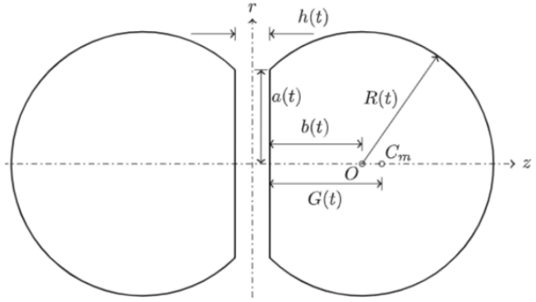
- Needed for:
  - Coalescence: avoid numerical coalescence, film drainage model
  - Break-up
  - Interfacial heat transfer
  - Nucleate boiling: nucleation, micro-layers
- Small-scale trouble: surface tension and viscous effects dominate → (Semi-)analytical solutions?[1]
- This motivates more modeling, not more resolution

[1] G. Tryggvason et al. *Physics of Fluids, 2013.*



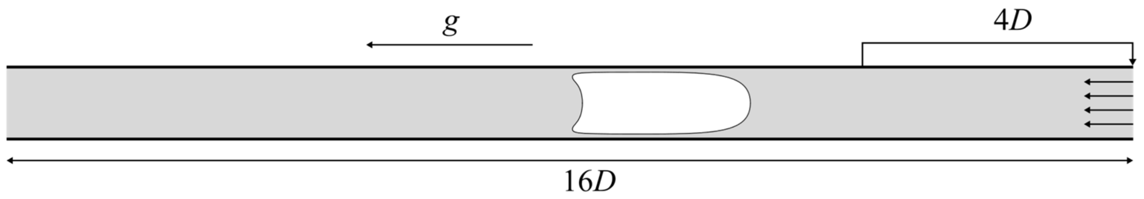
e.g. bubble coalescence:
- scales thin film drainage process O(few tens nm)
- much smaller scale than DNS mesh resolution

→ Semi-analytical sub-models required

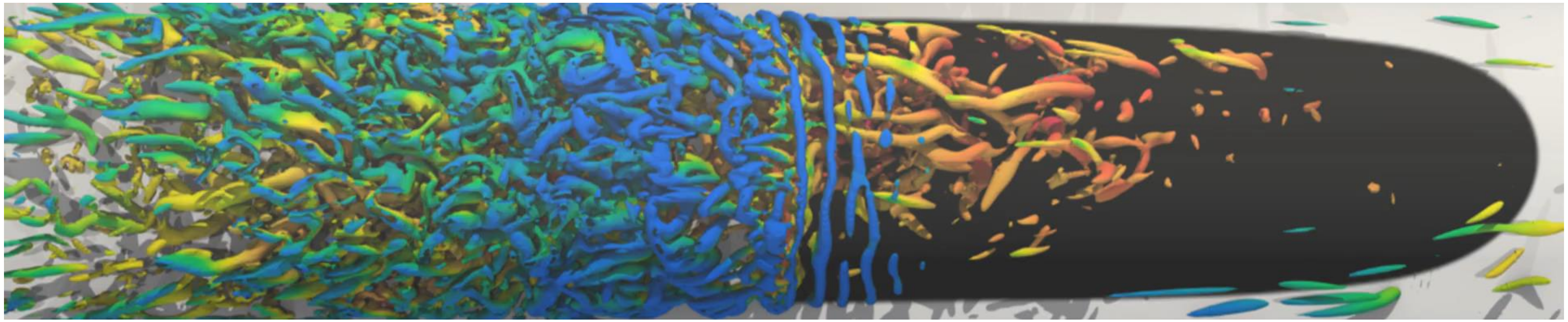


HiFi two-phase simulations – potential

- HiFi two-phase simulations have a large potential
  → more fundamental insight
  - Separate effects
  - At conditions that are experimentally difficult



- Example of co-current Taylor bubble flow simulations with Basilisk



Turbulent Taylor bubble flow with λ_2 iso-surfaces colored by streamwise velocity

Frederix et al. *Nuclear Science and Engineering*, 2023

Concluding remarks

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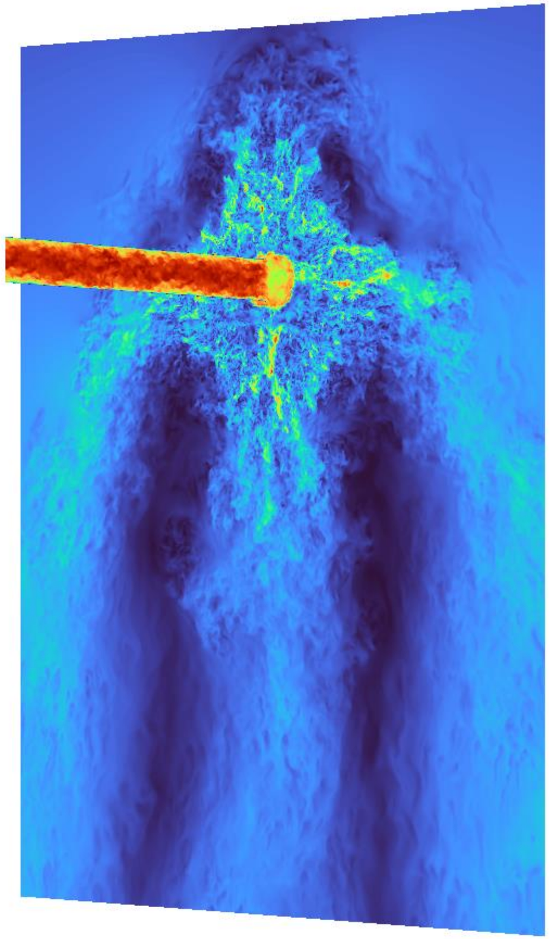
- Single-phase simulations in complex geometries:
  - DNS: possible, e.g. with SEM
  - LES: anisotropic models most needed for wall resolved simulations?
  - LES: implicit filtering → how to predict the correct friction velocity?
- Two-phase HiFi simulations:
- Ambition: 1) complex geometries, 2) more physics, 3) realistic conditions
- To achieve this, we must
  - Improve numerical methods
    - 'Common' approach: structured grid, 2^{nd} -order
    - 'Refined' approach: unstructured grid, higher-order
  - Develop better sub-grid models



Mathur et al. *IJHMT*, *2024*

BFS

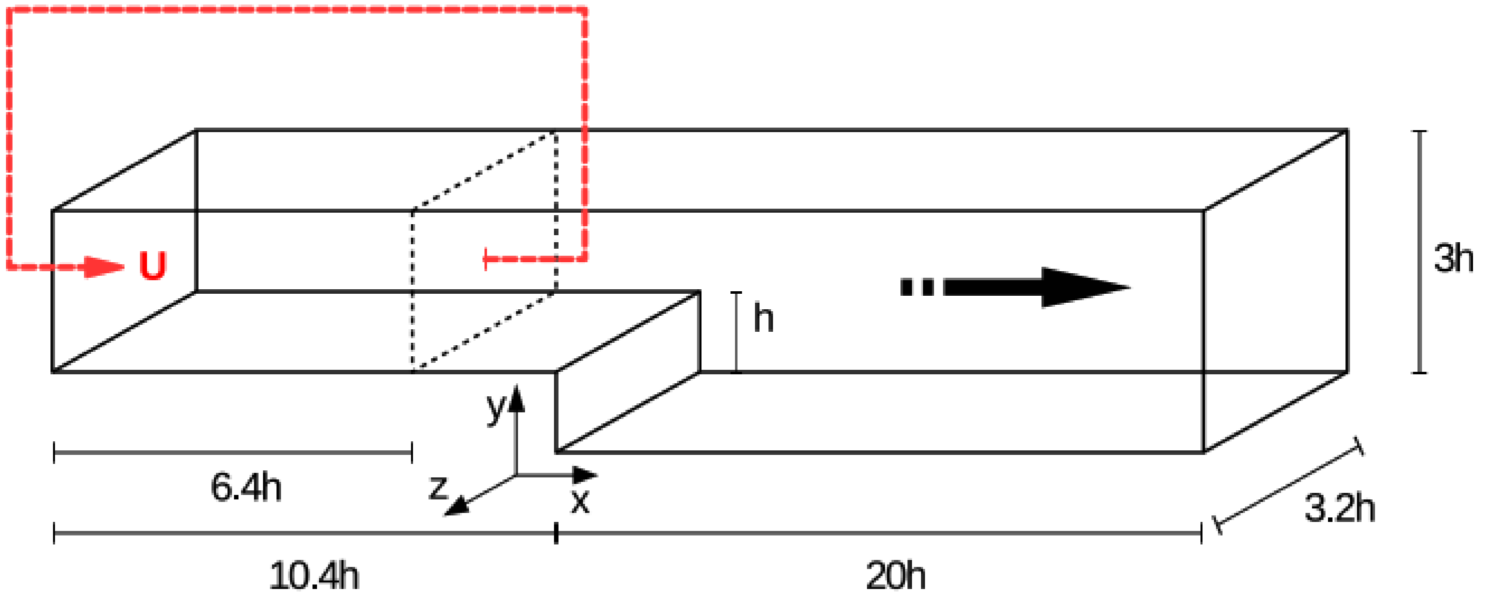


Figure 1: Backward facing step computational domain

BFS

Table 3: Summary of the computational grids used for the present analyses. y^+_{wall} is the non-dimensional distance of the first cell center normal to the wall, whereas Δy^+_{bulk} represents the non-dimensional wall normal cell size in the center of the channel. A stretching ratio of 1.07 is used in the wall normal direction in order to stretch the cells from y^+_{wall} to Δy^+_{bulk}. In the streamwise direction, a stretching ratio of 1.05 is used in in order to refine the cells from Δx^+_{max} to Δx^+_{min} towards step, and subsequently coarsen the cells from Δx^+_{min} to Δx^+_{max} downstream of the step. Δz^+ represent the non-dimensional cell sizes in the spanwise direction. N_{total}, represents the total number of cells. The size of the computational domain are specified in Fig. 1.

Name	Δx^+_{min}	Δx^+_{max}	Δy^+_{min}	Δy^+_{max}	Δz^+	r_{exp}	Re_τ	N_{total}
90-grid	5	90	0.5	30	30	1.05	180	1.144675e06
60-grid	5	60	0.5	20	20	1.05	180	2.122332e06
30-grid	5	30	0.5	10	10	1.05	180	6.849729e06
15-grid	5	15	0.5	7.5	7.5	1.05	180	1.728374e07

BFS, x/h = 2

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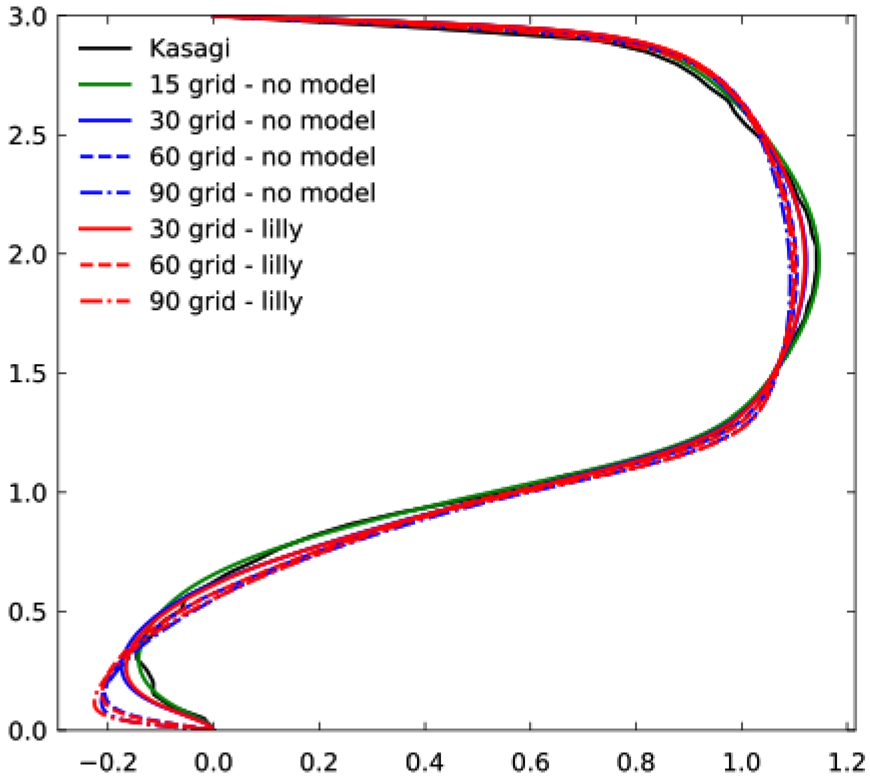
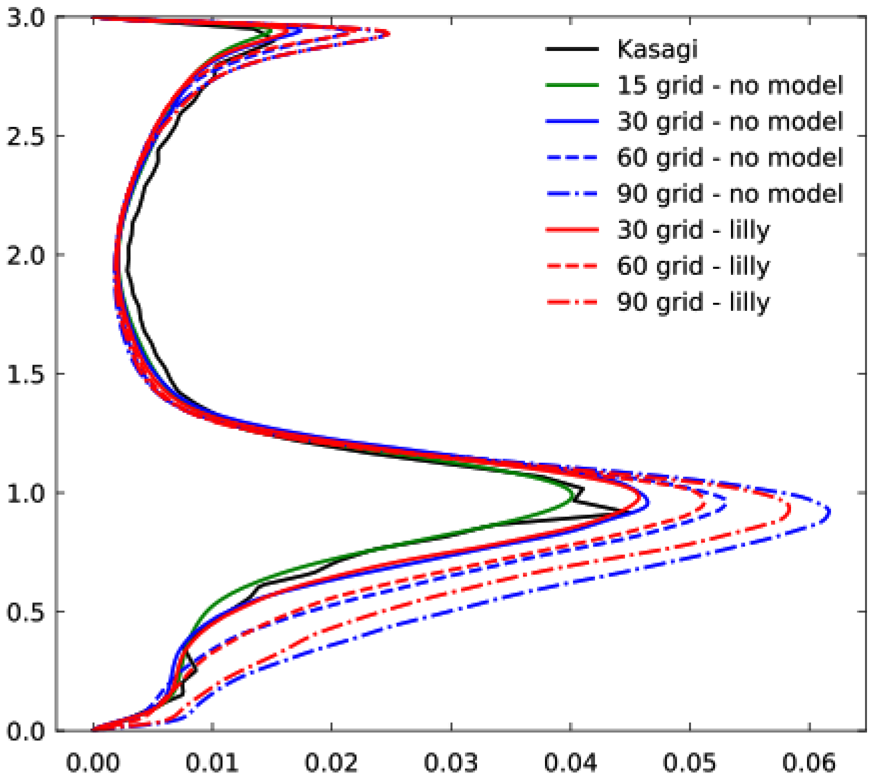
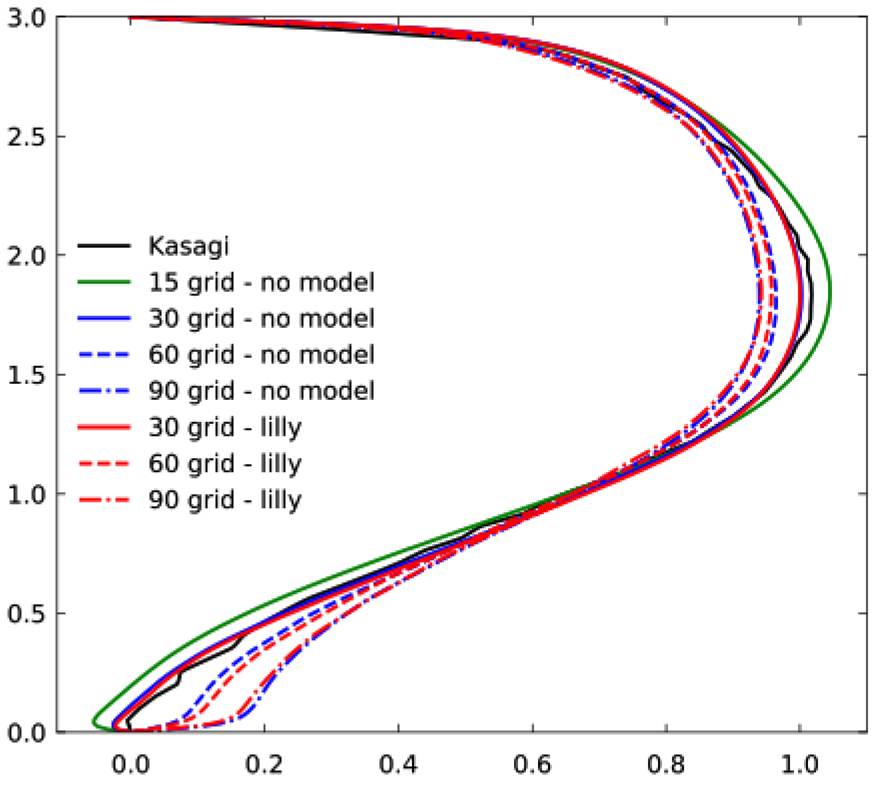


(a) Mean streamwise velocity $\overline{U}/U_{bulk}$

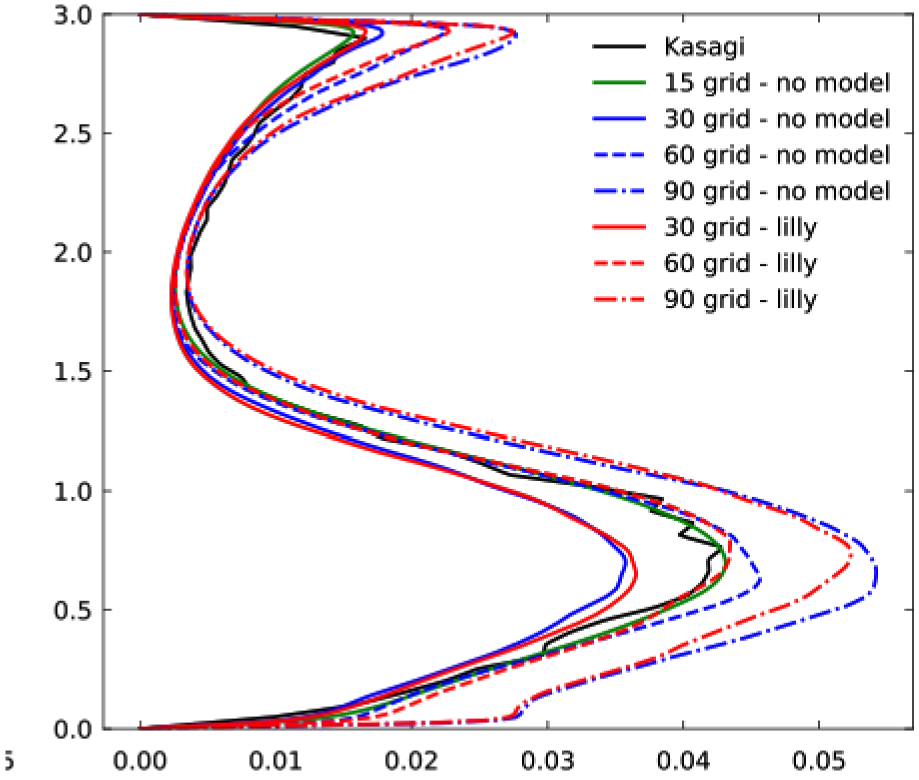


(f) Turbulent kinetic energy $\overline{k}/U_{bulk}^2$

BFS, x/h = 6



(a) Mean streamwise velocity $\overline{U}/U_{bulk}$



(f) Turbulent kinetic energy $\overline{k}/U^2_{bulk}$

BFS