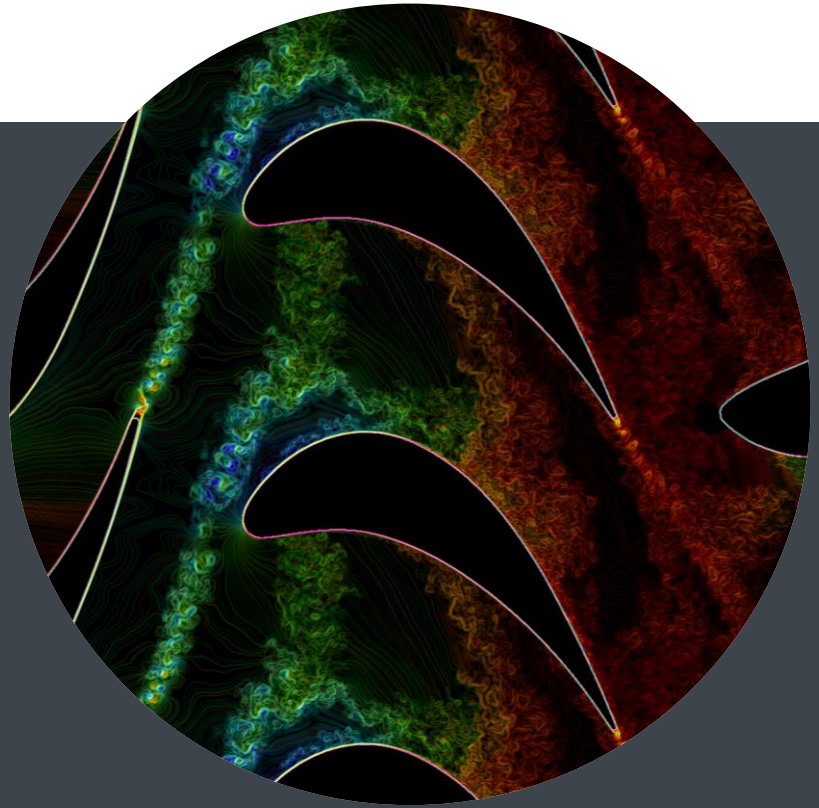
University of Stuttgart
Institute of Aerodynamics and Gas Dynamics

NRG

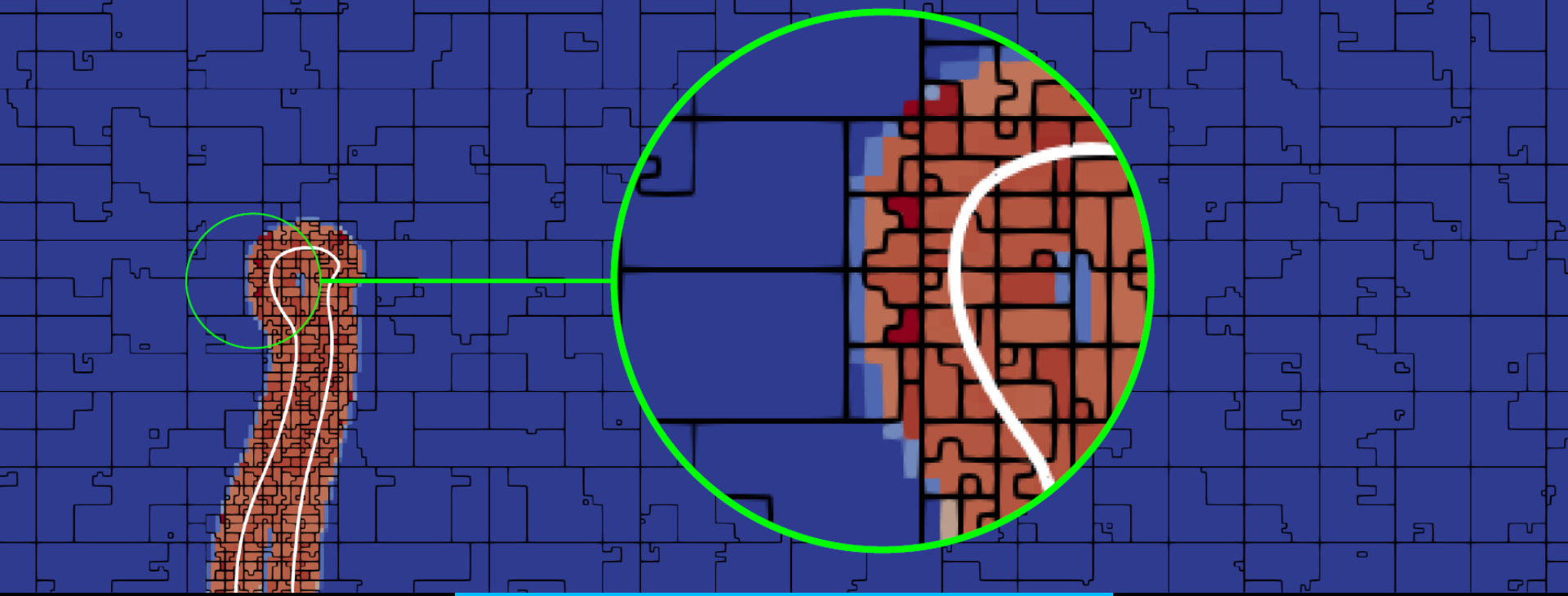


Discretization Consistent LES Closure Strategies

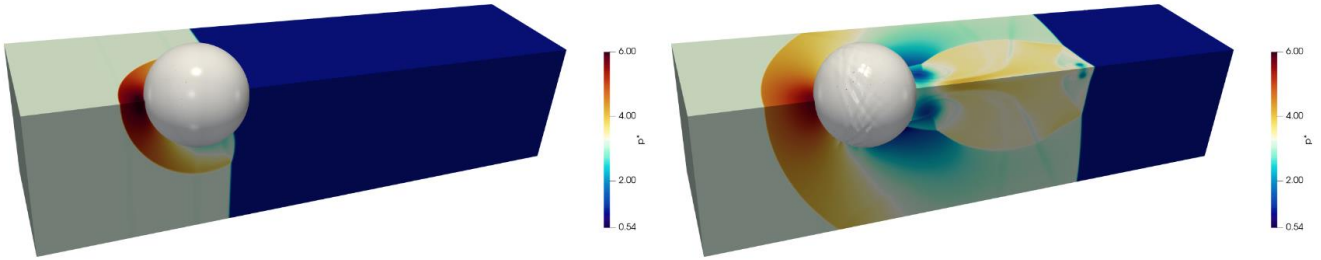
Andrea Beck
Institute of Aerodynamics and Gas Dynamics (IAG) &
Stuttgart Center for Simulation Science (SC SimTech)

All simulations shown here are conducted with FLEXI by members of the Numerics Research Group. I would like to thank all my present and former Ph.D. students, M.Sc. students, PostDocs and all the other colleagues I have had the pleasure of working with.

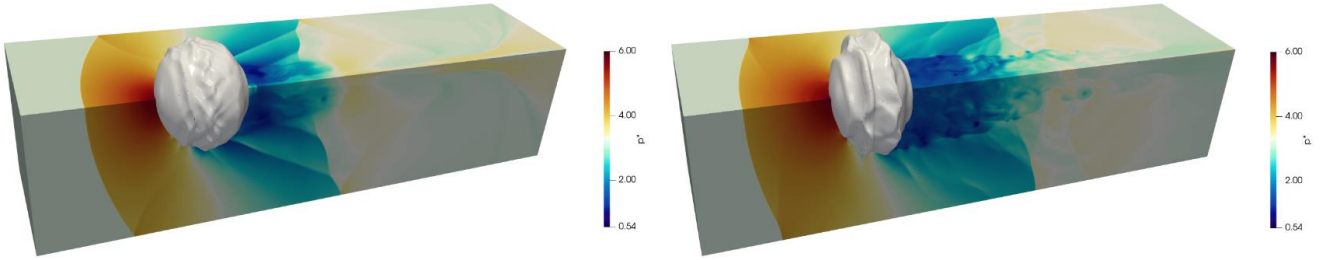
NRG



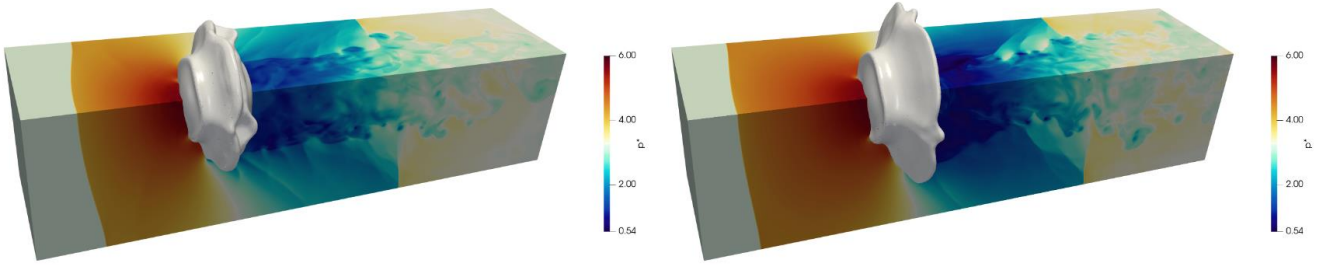
Multi-X problems



(a) $t^* = 0.8$ (b) $t^* = 2.4$



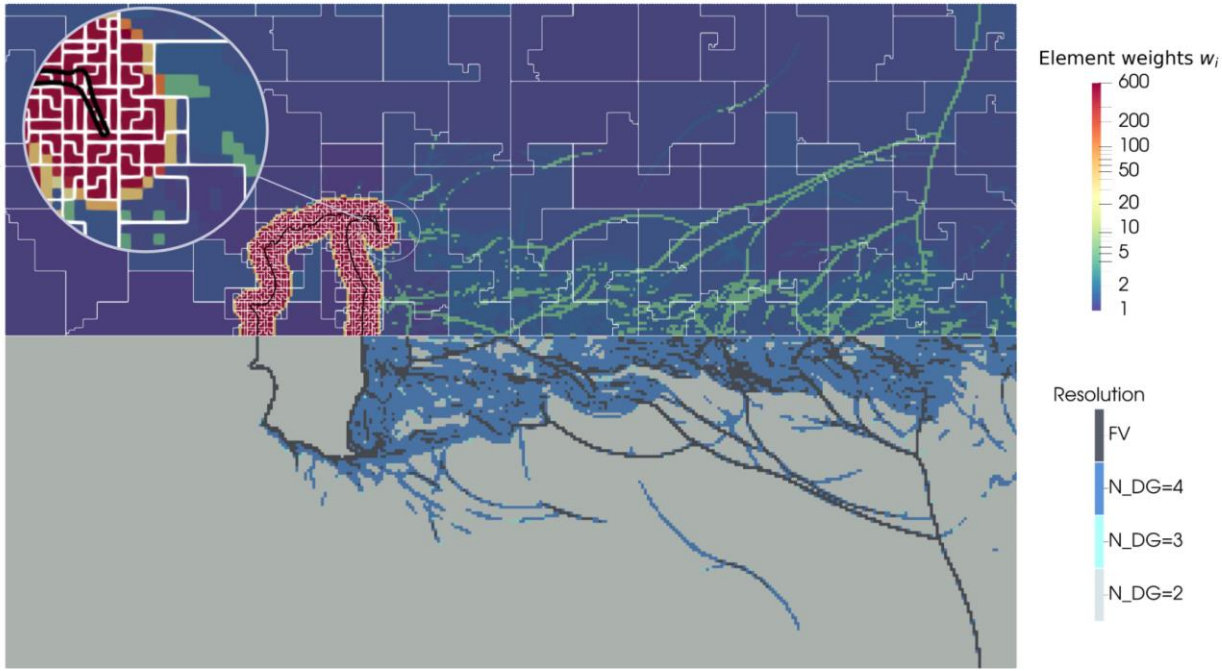
(c) $t^* = 4.7$ (d) $t^* = 7.0$



(e) $t^* = 9.4$ (f) $t^* = 11.8$

Multiphase, Multiscale, Multimethod: Shock Droplet Interaction

- Sharp-Interface simulation of 3D water droplet – shock interaction at Ma = 2.4 and We = 100
- About 140 DOF / droplet diameter
- hp-adaptive DGSEM / FV scheme with DLB
- 7200 CPUh on HAWK



Mossier et al., An Efficient hp-Adaptive Strategy for a Level-Set Ghost Fluid Method, arxiv, 2023
Jöns et al., Riemann solvers for phase transition in a compressible sharp-interface method, JCP, 2023
Mossier et al., A p-Adaptive Discontinuous Galerkin Method with hp-Shock Capturing. Journal of Scientific Computing, 2022

Multiphase, Multiscale, Multimethod: Icing on Airfoils



EIROS project via http://www.eirosproject.com/project/case-study-applications/



Stefano Fornasier via http://tesi.cab.unipd.it/50432/1/STEFANO_FORNASIER_1147354_assignsubmission_file_Fornasier_Stefano_1056548.pdf



Chicago Tribune

Tuesday, November 1, 1994

Chicago-bound plane crashes; 68 are killed

By Flynn McRoberts and George Papajohn
Tribune Staff Writers

The blustery weather that raked Chicago and Northwest Indiana on Monday will be examined closely as federal safety investigators try Tuesday to determine what caused an American Eagle turboprop to plummet from the sky, killing all 68 people aboard.

Flight 4184, a twin-engine Super ATR-72, was bound from Indianapolis to O'Hare International Airport at about 4 p.m. Monday when it plunged into a farm field about 25 miles southeast of Gary near Interstate Highway 65 and Indiana Highway 110 near Roselawn, Ind.

Twenty-one of the passengers were bound for Chicago and the other 43 passengers were connecting to other flights at O'Hare, airline officials said.

The tragedy followed by less than two months the 132 deaths in the crash of a USAir jet bound from Chicago to Pittsburgh, an accident that remains under investigation.

"It looked like there was no wing on the left-hand side" of the American Eagle plane, said Larry Midkiff, a 39-year-old construction worker who was driving home to Roselawn when he saw the plane in a steep descent. "I'm not sure because it might have been the angle of the aircraft."

Midkiff said he saw smoke streaming from the plane.

"It was coming down real steep, real hard, nose down," he said. "It wasn't coming down like it was trying to make an emergency landing. . . . It kind of dipped down behind some trees. Then it made a big puff of black smoke."

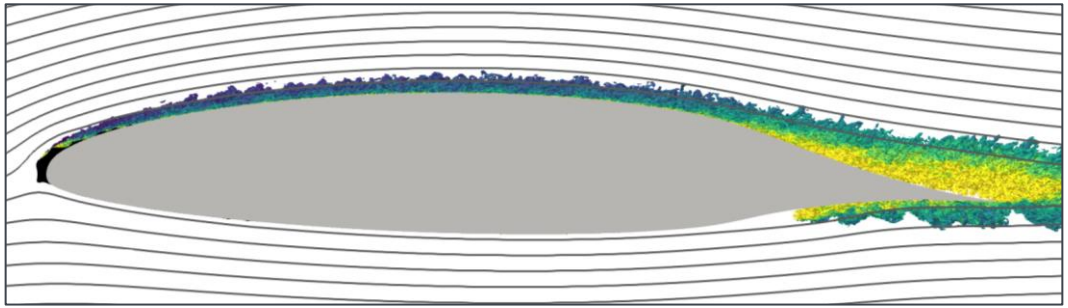
Farmer Norman Prohosky was tinkering with a grain

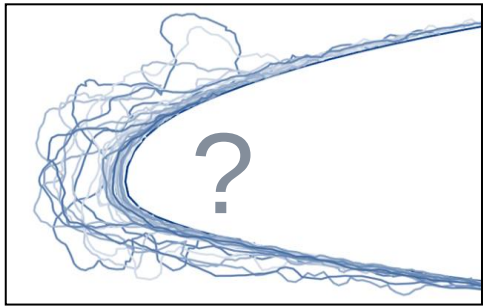
Disaster in stormy Indiana skies

■ American Eagle airline has a good safety record. Page 21.

■ List of major U.S. fatal airplane crashes since 1963. Page 21.

Chicago Tribune via https://www.newspapers.com/clip/14788830/american-eagle-flight-4184-crashes-in-in/

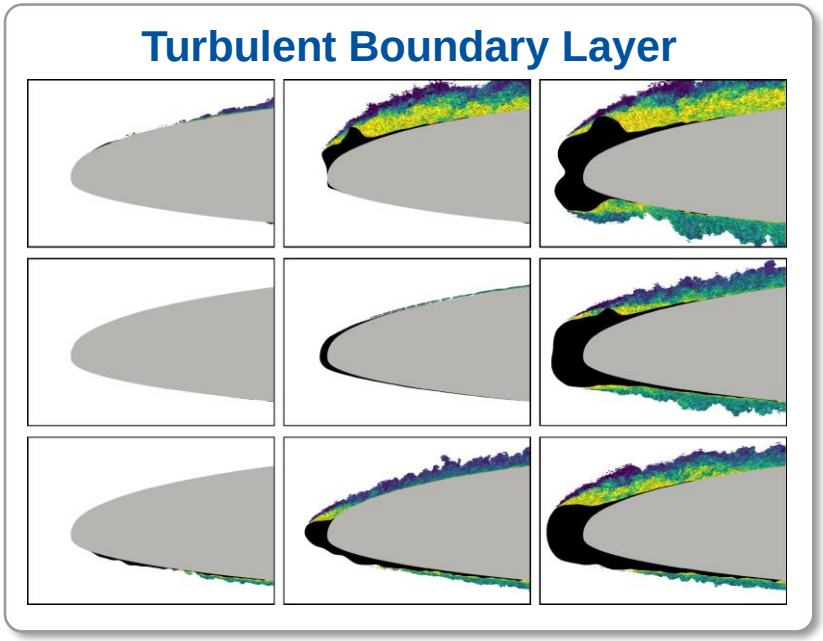


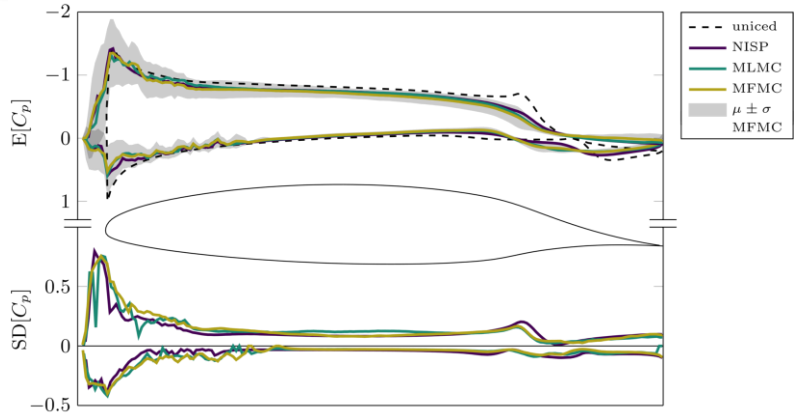


NRG

Multiphase, Multiscale, Multimethod

- Uncertainty Quantification Analysis of Icing on Airfoil Performance
- Parameterization of iced shapes via POD / PCA
- Automated grid generation for wall-resolved LES on hexa-only grids
- Non-intrusive Spectral Projection, MLMC and MFMC of 3D LES computations
- PoUnce-Framework for HPC scheduling and management of UQ workflow

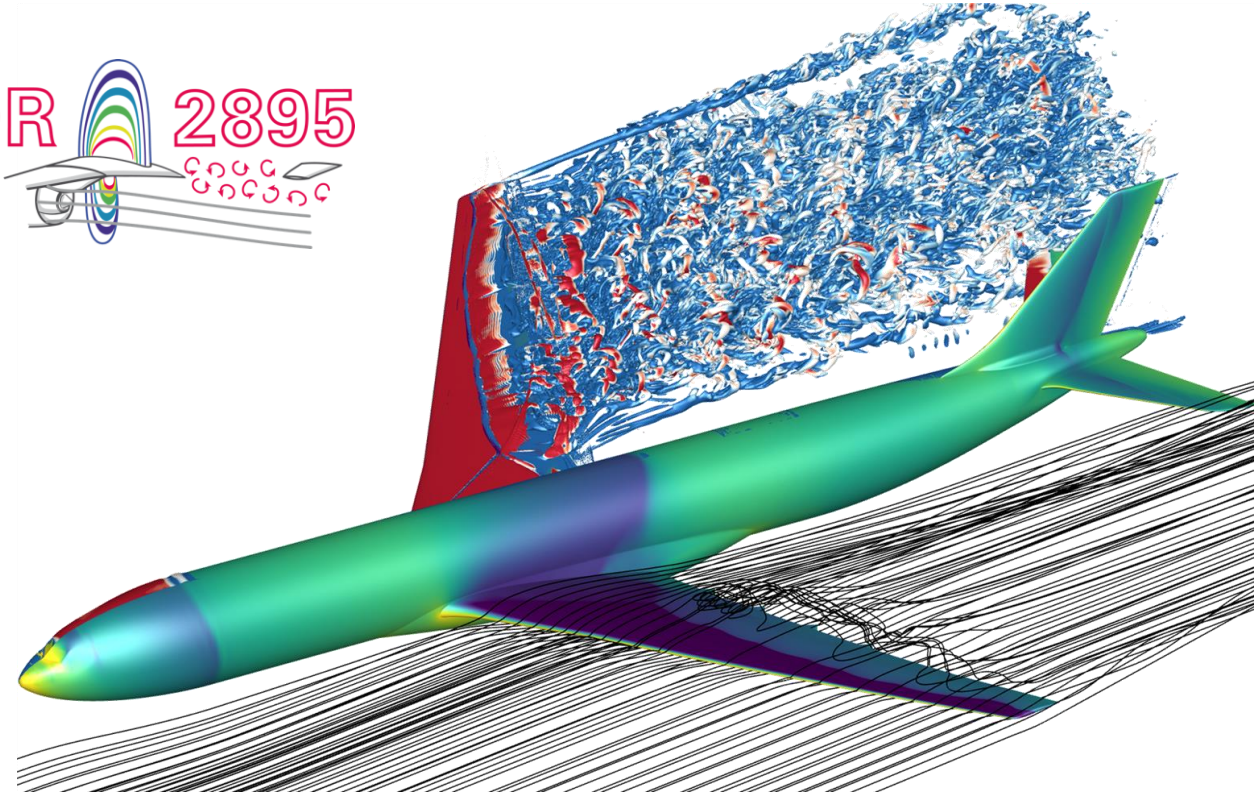


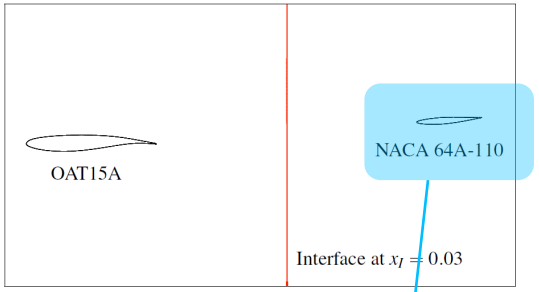


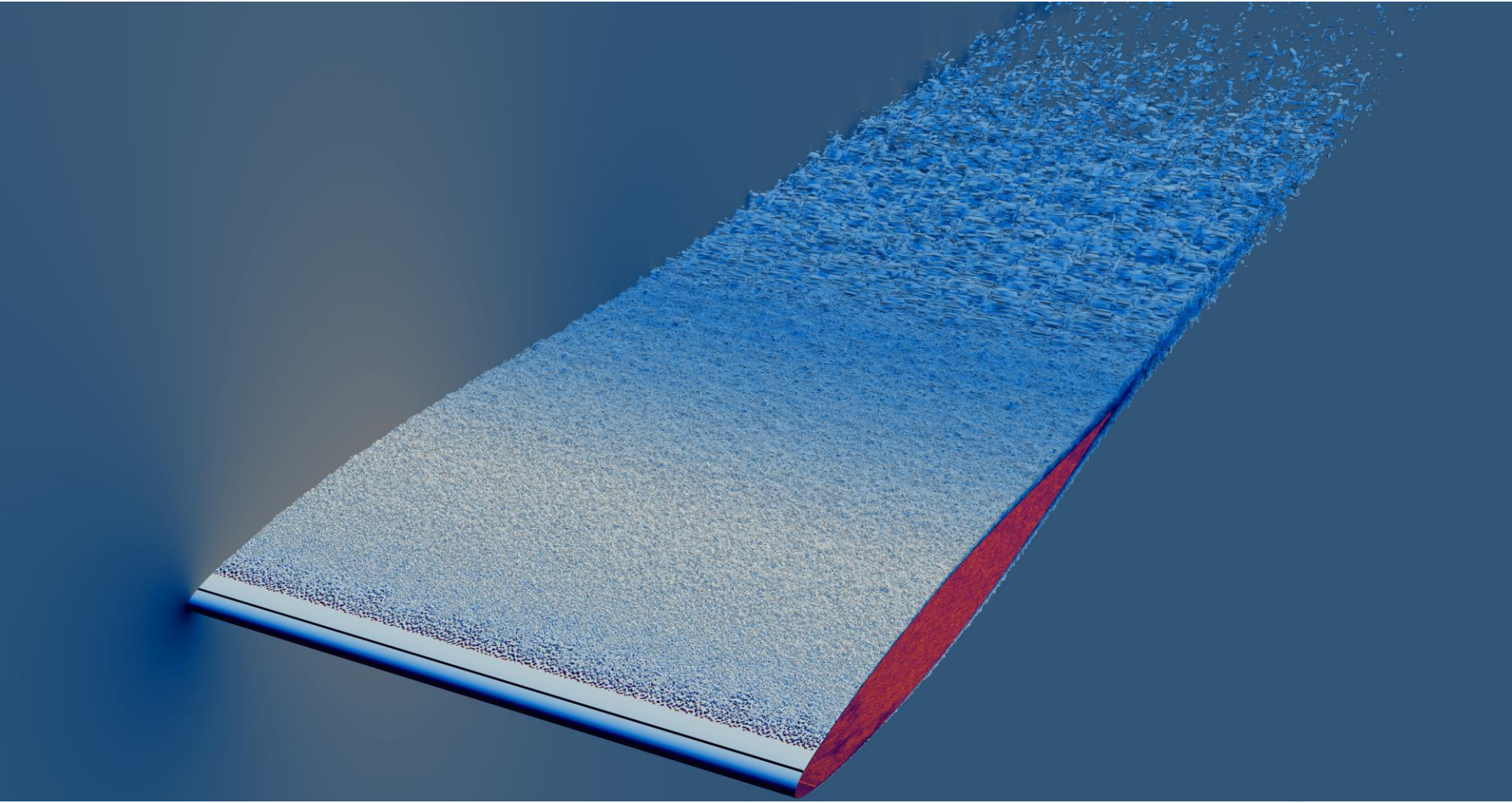
Baden-Württemberg Stiftung

Friedrich und Elisabeth BOYSEN Stiftung für Forschung und Innovation

Multiphase, Multiscale, Multimethod: Wake / HTP interaction under buffet

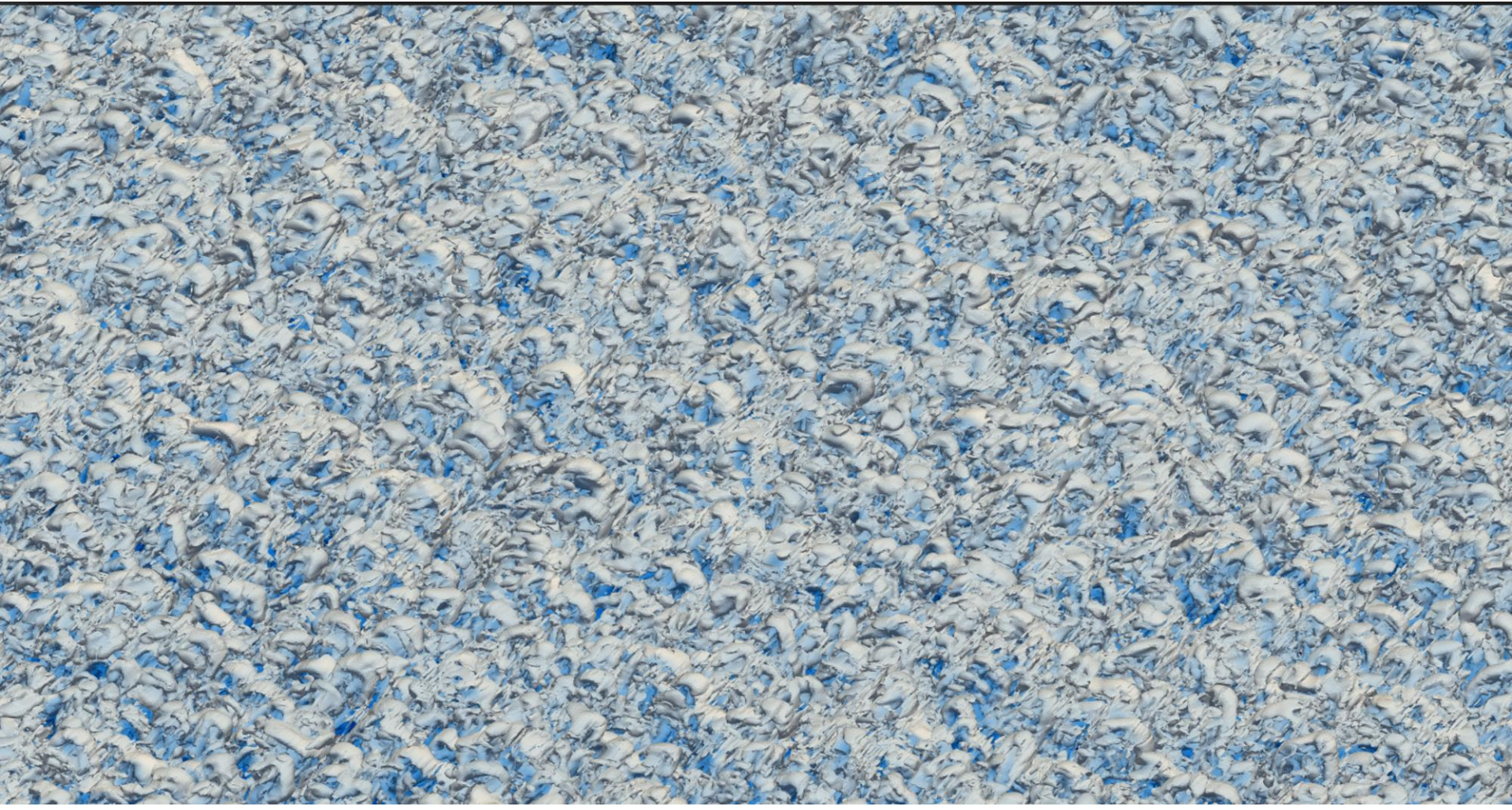



OAT15A
NACA 64A-110
Interface at $x_I = 0.03$



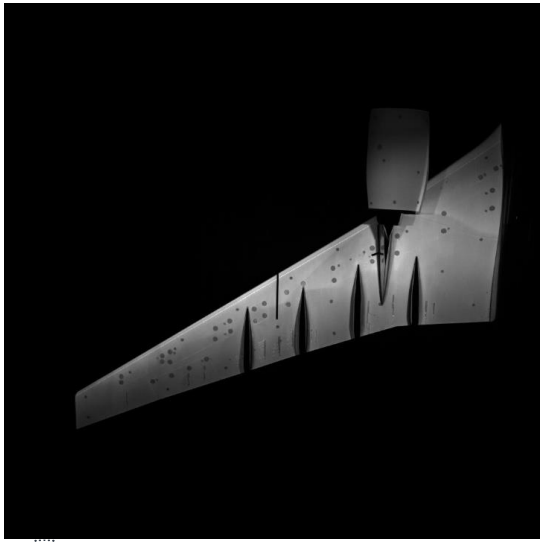


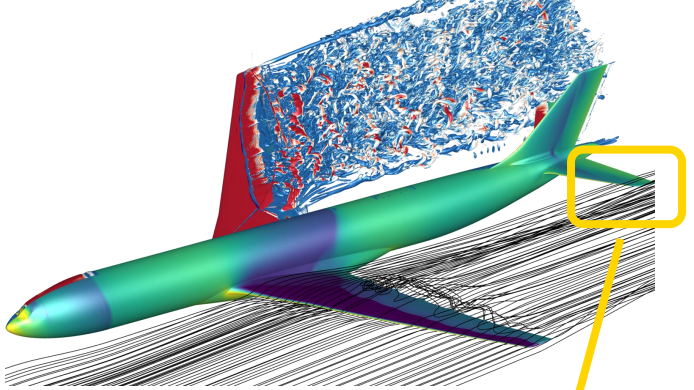


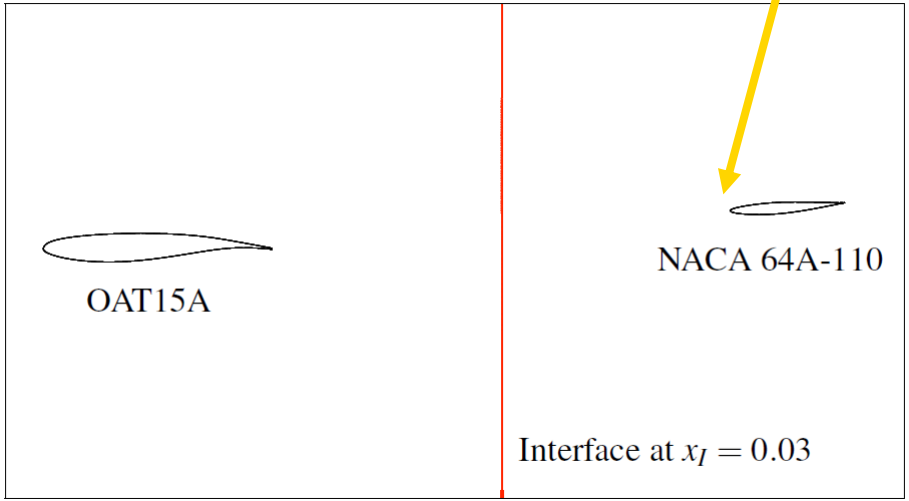


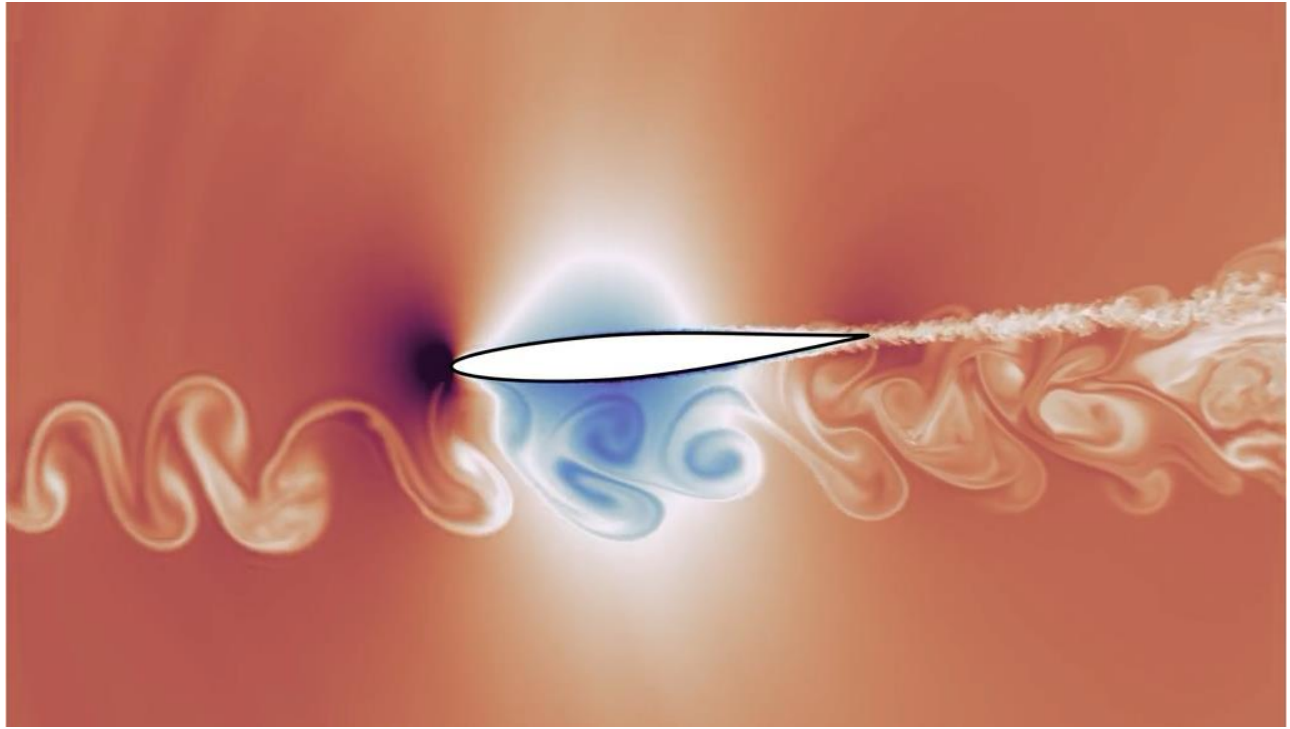


- Measurements at flight Re in the European Transonic Windtunnel









- Approx. 1 Billion DOF, N=7, 70 CTU

$$\int_E J(\vec{\xi}) U_t \phi \, d\vec{\xi} = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} J(\vec{\xi}) \left(\frac{\partial}{\partial t} \sum_{r,s,t=0}^{N} \hat{U}_{rst}(t) \psi^N_{rst}(\vec{\xi}) \right) \psi^N_{ijk}(\vec{\xi}) d\vec{\xi^1} d\vec{\xi^2} d\vec{\xi^3}$$

$$= \sum_{\alpha,\beta,\gamma=0}^{N} J(\vec{\xi}_{\alpha\beta\gamma}) \left(\frac{\partial}{\partial t} \sum_{r,s,t=0}^{N} \hat{U}_{rst}(t) \underbrace{\ell^N_r(\xi^1_\alpha)}_{=\delta_{r\alpha}} \underbrace{\ell^N_s(\xi^2_\beta)}_{=\delta_{s\beta}} \underbrace{\ell^N_t(\xi^3_\gamma)}_{=\delta_{t\gamma}} \right) \psi^N_{ijk}(\vec{\xi}_{\alpha\beta\gamma}) \omega_\alpha \omega_\beta \omega_\gamma$$

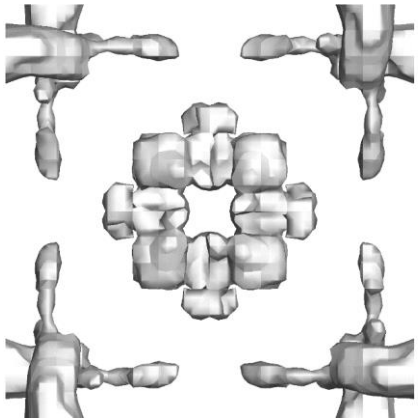
$$= \sum_{\alpha,\beta,\gamma=0}^{N} J(\vec{\xi}_{\alpha\beta\gamma}) \frac{\partial}{\partial t} \hat{U}_{\alpha\beta\gamma}(t) \underbrace{\ell^N_i(\xi^1_\alpha)}_{=\delta_{i\alpha}} \underbrace{\ell^N_j(\xi^2_\beta)}_{=\delta_{j\beta}} \underbrace{\ell^N_k(\xi^3_\gamma)}_{=\delta_{k\gamma}} \omega_\alpha \omega_\beta \omega_\gamma$$

High Order Schemes

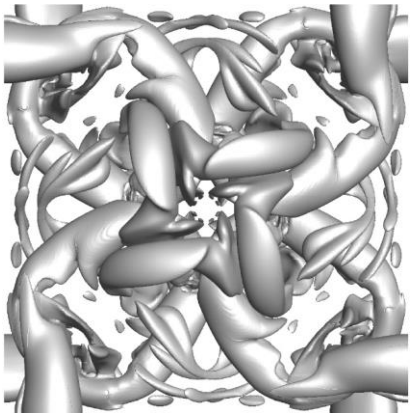
Schemes for multiscale problems

- For a smooth solution and a consistent scheme of order N, we have an error bound

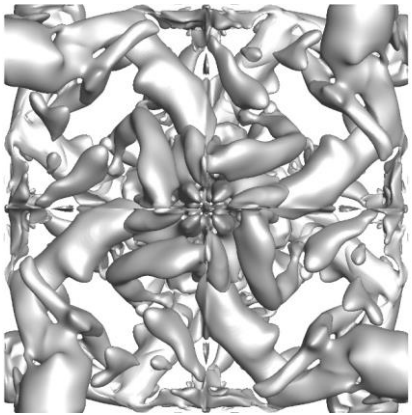
$$\|u - u_h\|_{h,\Omega} \leq Ch^{N+1}$$



N=1, 64 DOF

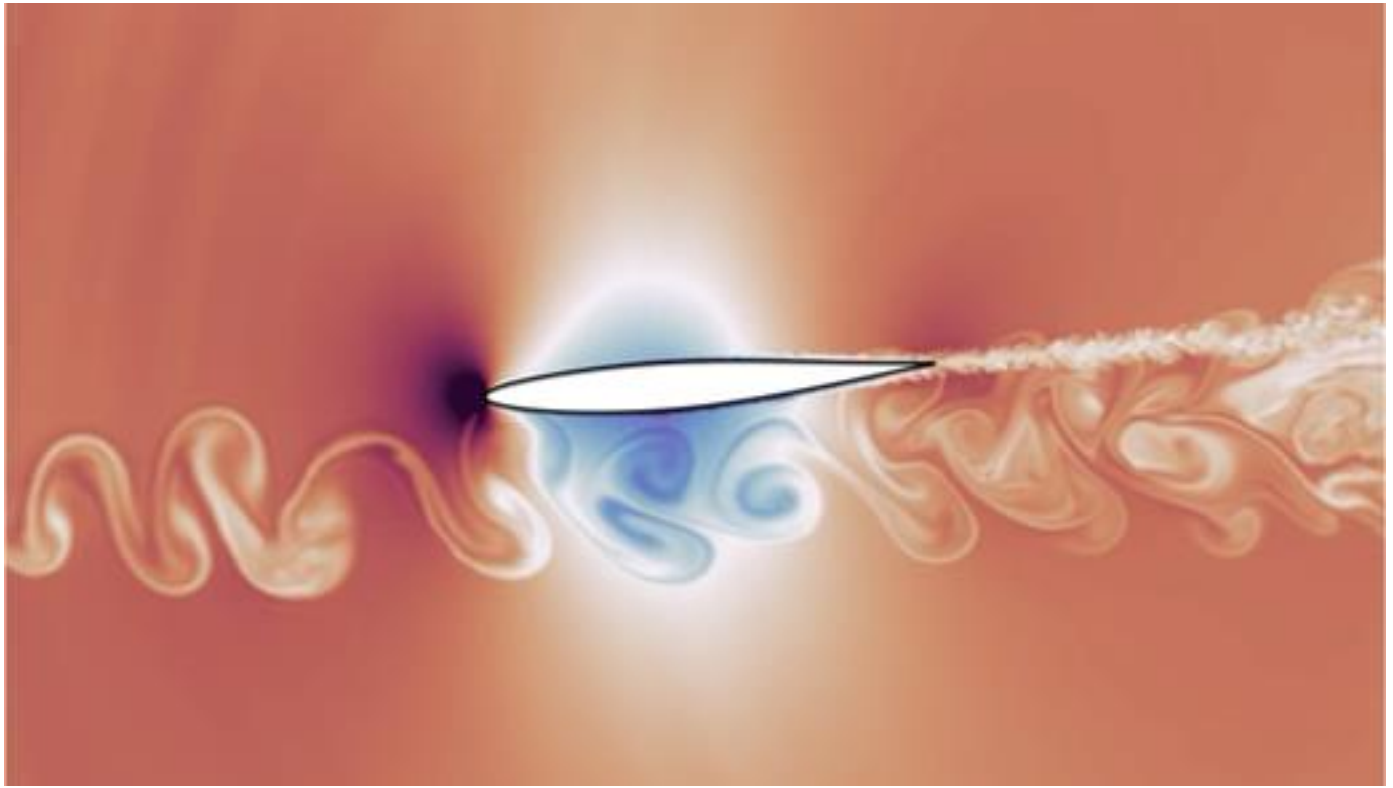


DNS



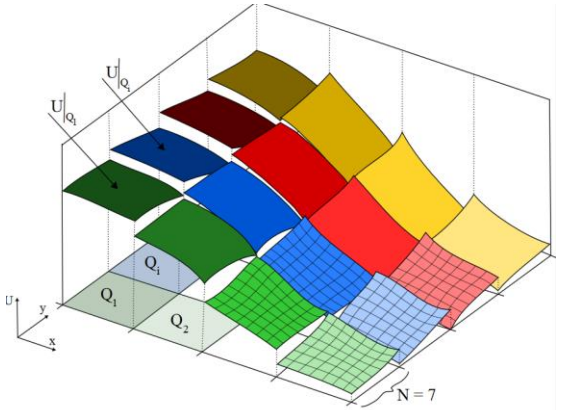
N=15, 64 DOF

- For the same accuracy:
  - 1 Billion DOF with a high order DG scheme
  - 256 Billion DOF with 2nd order FV scheme



Discontinuous Galerkin Schemes

- Different Roads to High Order: Higher Derivatives, wider stencils: From local to global
- Discontinuous Galerkin schemes combine useful properties for multiscale problems
- Basic ideas:
  - High order polynomial basis with compact support
  - L_2 projection is optimal
  - Hybrid FE and FV scheme
- This gives flexibility, locality, conservation and stability (FV) and accuracy (FE)



Discontinuous Galerkin Schemes

- A hyperbolic / parabolic conservation law of the form

$$U_t + \vec{\nabla} \cdot \vec{F}(U, \vec{\nabla} U) = 0$$

- Variational formulation and weak DG form per element

$$\langle J\, U_t, \psi \rangle_E + \left(\widetilde{f}^*\, \vec{n}_\xi, \psi \right)_{\partial E} - \left\langle \tilde{\vec{F}}, \nabla_\xi \psi \right\rangle_E = 0,$$

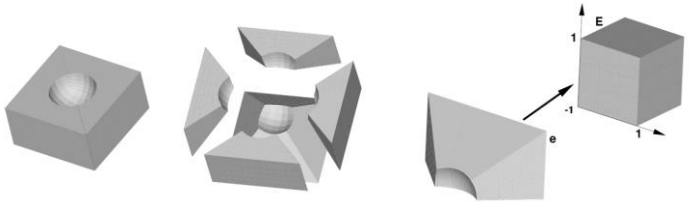
- Local tensor-product basis of Lagrange polynomials, interpolation nodes = quadrature nodes:

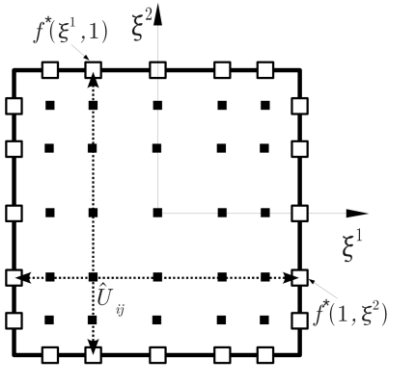
$$(U_i)_t + \frac{1}{J_i} \left[\widetilde{f}^*(1)\hat{\psi}_i(1) - \widetilde{f}^*(-1)\hat{\psi}_i(-1) + \sum_{k=0}^{N} \hat{D}_{ik}\, \widetilde{F}_k \right] = 0$$

- Tensor-product structure in multi-D: line-by-line operations

Simulation software: FLEXI
Discontinuous Galerkin Spectral Element Method (DG-SEM)

- DG-SEM:
  - Type of grid cells: Hexahedrons (curved elements, unstructured, hanging nodes)





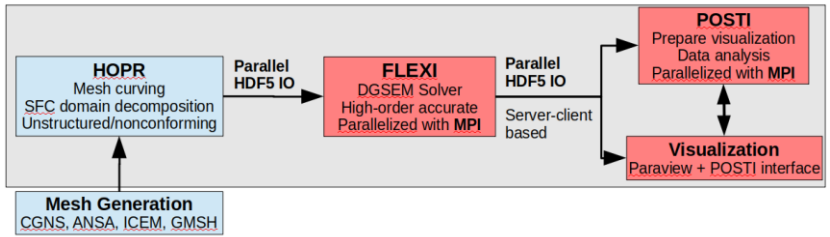
  - Set of basis functions: Tensor product, Lagrange polynomials at Gauß / Gauß-Lobatto points

$$U_h(\xi,t)\sum_{i,j=1}^{N}\hat{U}_{i,j}(t)\psi_i^N(\xi^1)\psi_j^N(\xi^2)$$

  - Numerical integration: Collocation approach (SEM approach)
  - Time approximation: Explicit Runge-Kutta, IMEX
  - Numerical flux: Riemann solver, BR1/2
  - Stability: De-Aliasing, Split form (entropy / energy stable fluxes)
  - Shock-capturing: Finite volume sub-cells, h/p adaptivity

Simulation software: FLEXI

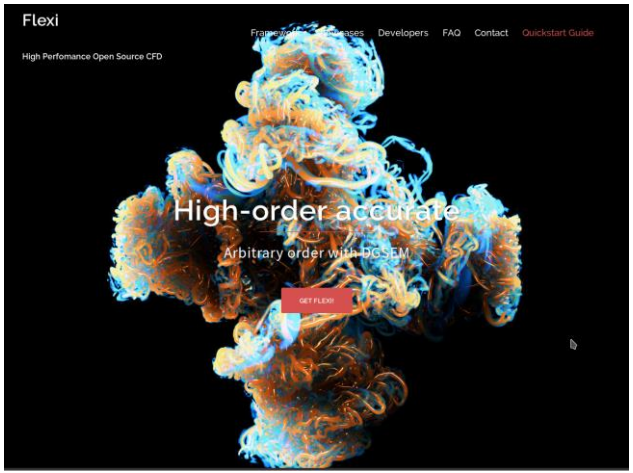
- Under development since 2010
- High order Discontinuous Galerkin SE framework with proven HPC capabilities
- Full framework: Preprocessor HOPR, FLEXI, Postprocessor POSTI and Paraview-Plugin, Blender Pipeline, HPC-UQ-Framework POUNCE, FLEXI-preCICE, FLEXI-OpenFOAM, FLEXI-TAU
- Reproduceability: Regression/unit testing, “compile from file”, Development and Management via gitlab / on github




Computers & Mathematics with Applications
Volume 81, 1 January 2021, Pages 186-219
ELSEVIER

FLEXI: A high order discontinuous Galerkin framework for hyperbolic–parabolic conservation laws

Nico Krais [a], Andrea Beck [a], Thomas Bolemann [a], Hannes Frank [a], David Flad [a], Gregor Gassner [b], Florian Hindenlang [c], Malte Hoffmann [a], Thomas Kuhn [a], Matthias Sonntag [a], Claus-Dieter Munz [a]

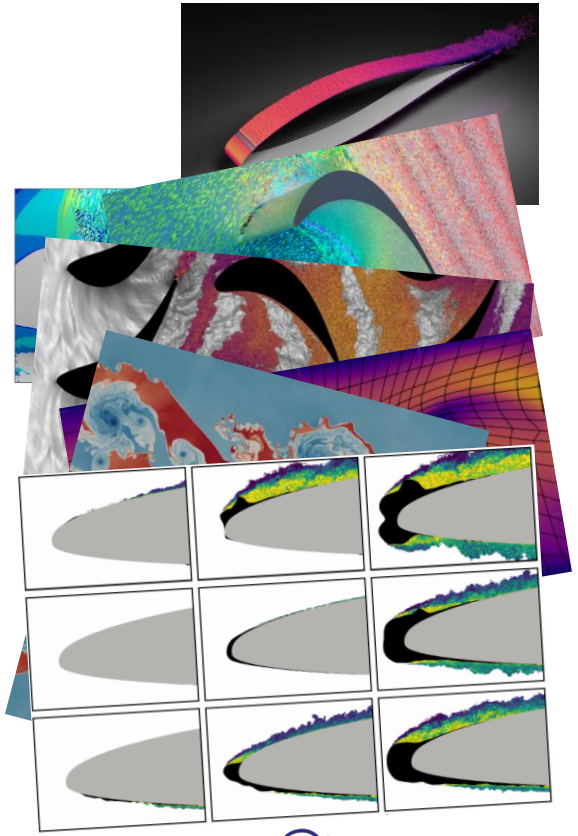


www.hopr-project.org
www.flexi-project.org
https://github.com/flexi-framework/flexi

Simulation software: FLEXI
Some features

[1]www.flexi-project.org

- High-order accurate open source solver[1] with excellent scaling behavior
- Discontinuous Galerkin spectral element method (DG-SEM)
- Written in modern Fortran and optimized for CPU based HPC systems
- Focus on DNS/LES of multiscale- and multi physics problems governed by the compressible Navier-Stokes equations
- Additional features
  - Lagrangian particle tracking (LES/DNS of particle laden flows)
  - Conservative sliding mesh interface for stator/rotor flow
  - Mesh deformation and mesh moving based on ALE formulation
  - hp-adaptivity
  - Intrusive and non-intrusive methods for uncertainty quantification
  - Management framework for optimal scheduling on HPC systems
  - A solver-in-the-loop framework for reinforcement learning

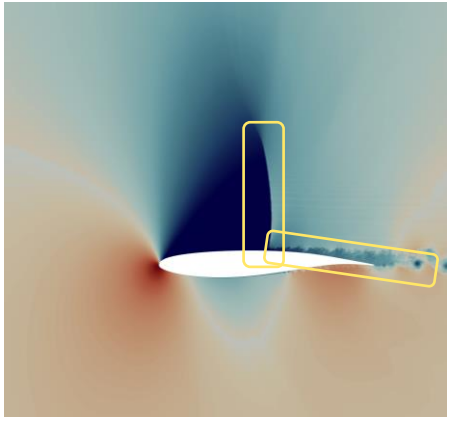


For a smooth solution and a consistent scheme of order N, we have an error bound

$$\|u - u_h\|_{h,\Omega} \leq Ch^{N+1}$$

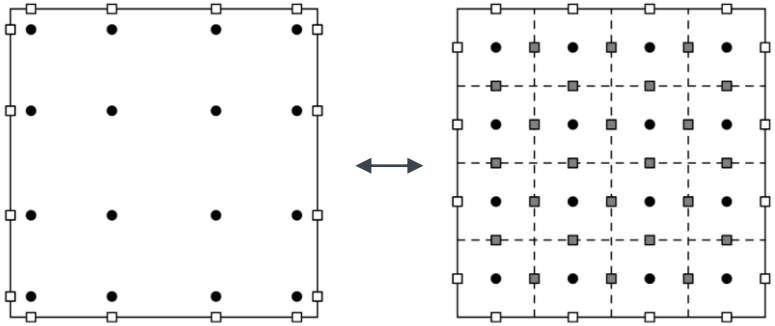
Put differently, HO schemes can leverage the smoothness of the underlying solution

What if the solution is not smooth (enough)?

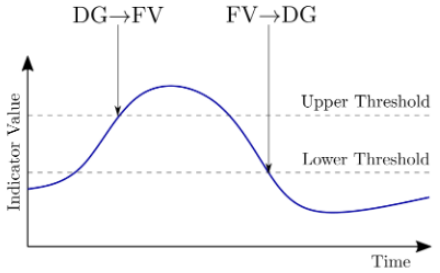


Simulation software: FLEXI
Shock-capturing

- Idea: Combination of DG and FV
  - DG in smooth parts of the flow and FV at shocks
- Oscillation, jump or ML indicators
- Troubled DG cell: $(N+1)^3$ equidistant FV sub-cells
- 2nd order TVD FV scheme on sub-grid
- Same number of degrees of freedom
- Concurrent calculation of FV and DG data
- Convex combination of FV and DG operator

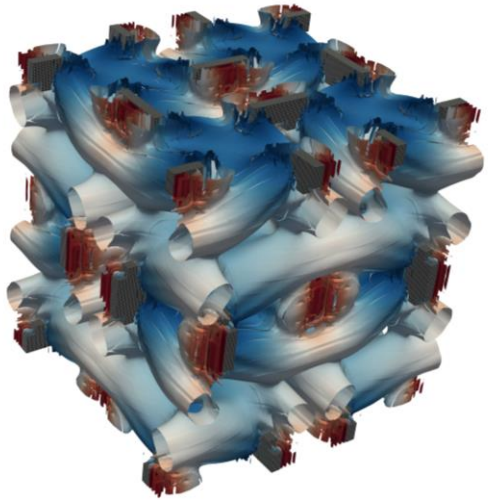


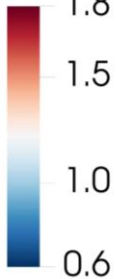
DG FV

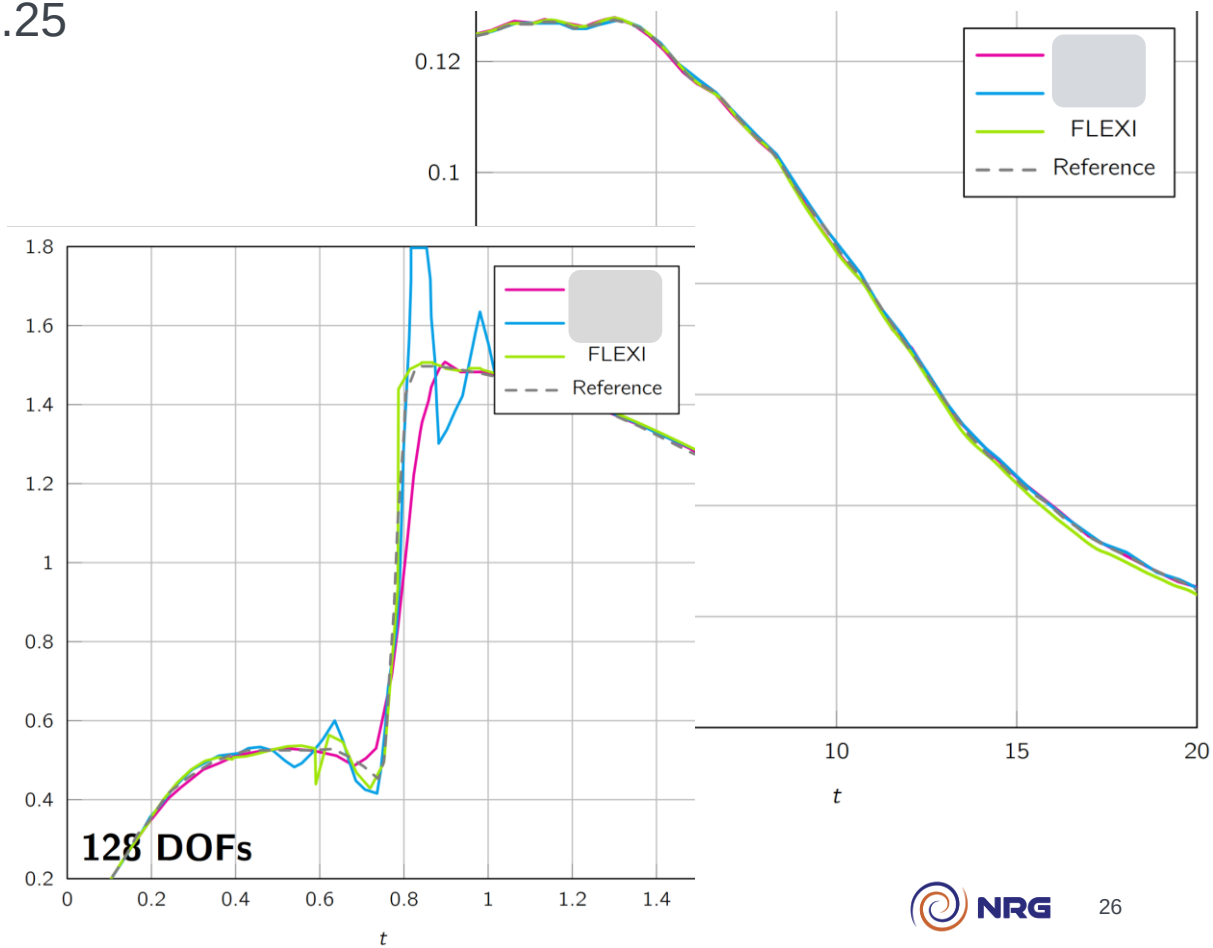


Hybrid DG / FV scheme for compressible turbulence

Taylor-Green vortex at Ma=1.25



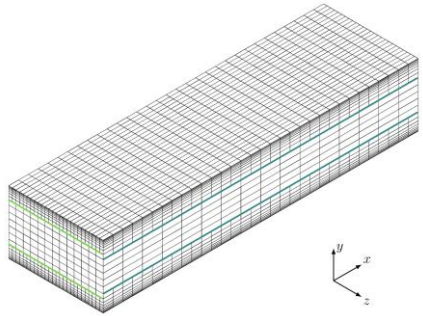


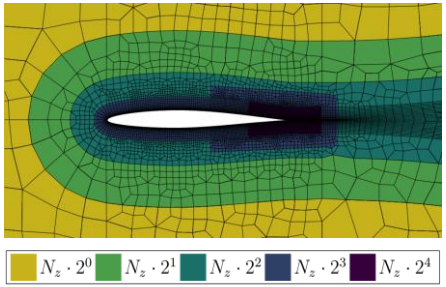


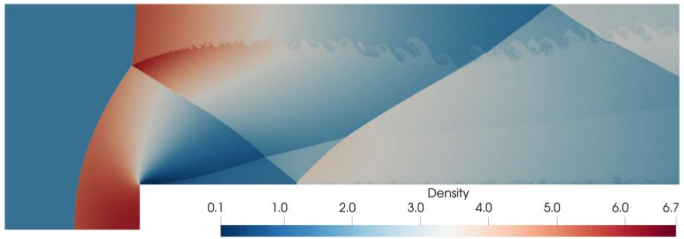
Simulation software: FLEXI

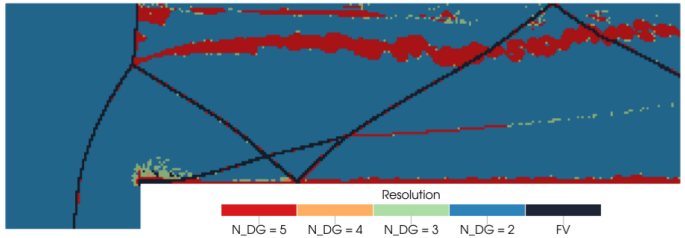
Adaptivity and error control – hp-refinement

- h-refinement[1]
  - Mortar interfaces with hanging nodes for optimal grids
  - Local grid-adaptation and grid-adaptation algorithm required
  - Up to 50% lower cost compared to human-generated grids
  - Residual estimation procedure
- p-refinement[2]
  - Local p-adaptivity in smooth solution regions



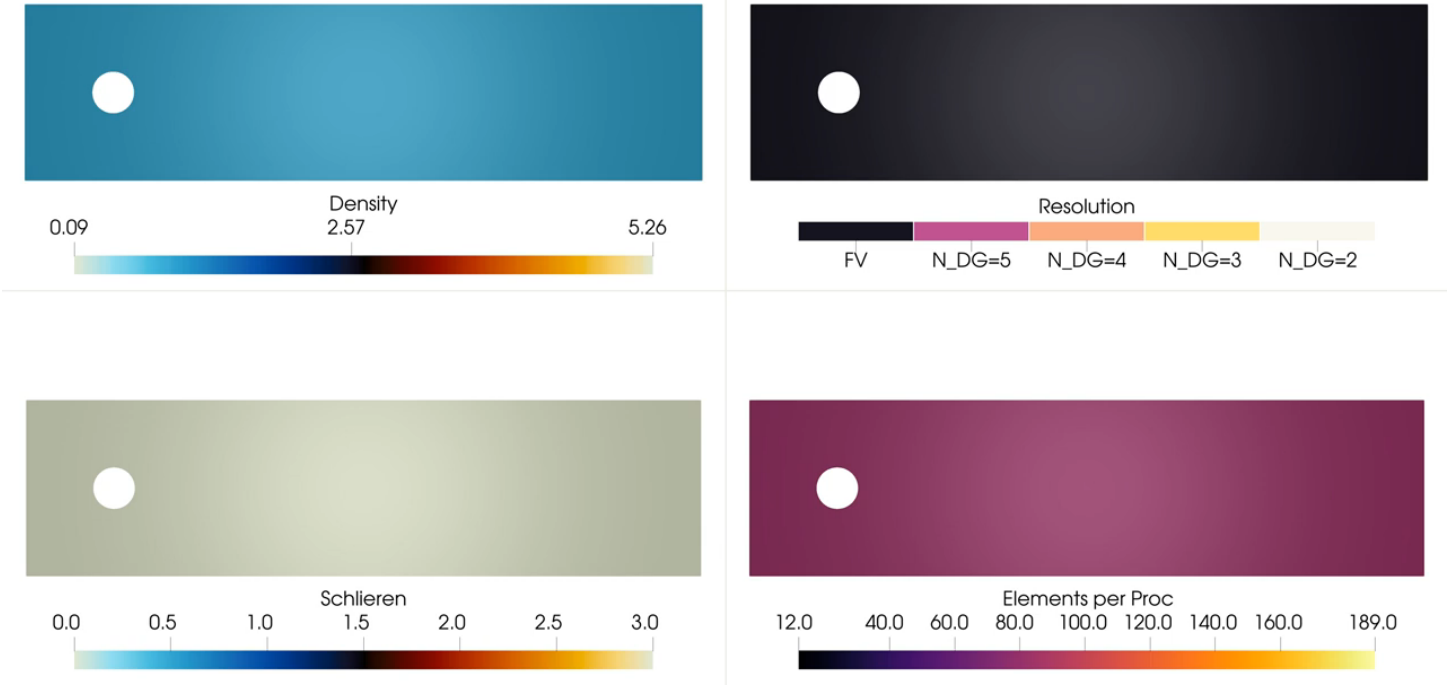




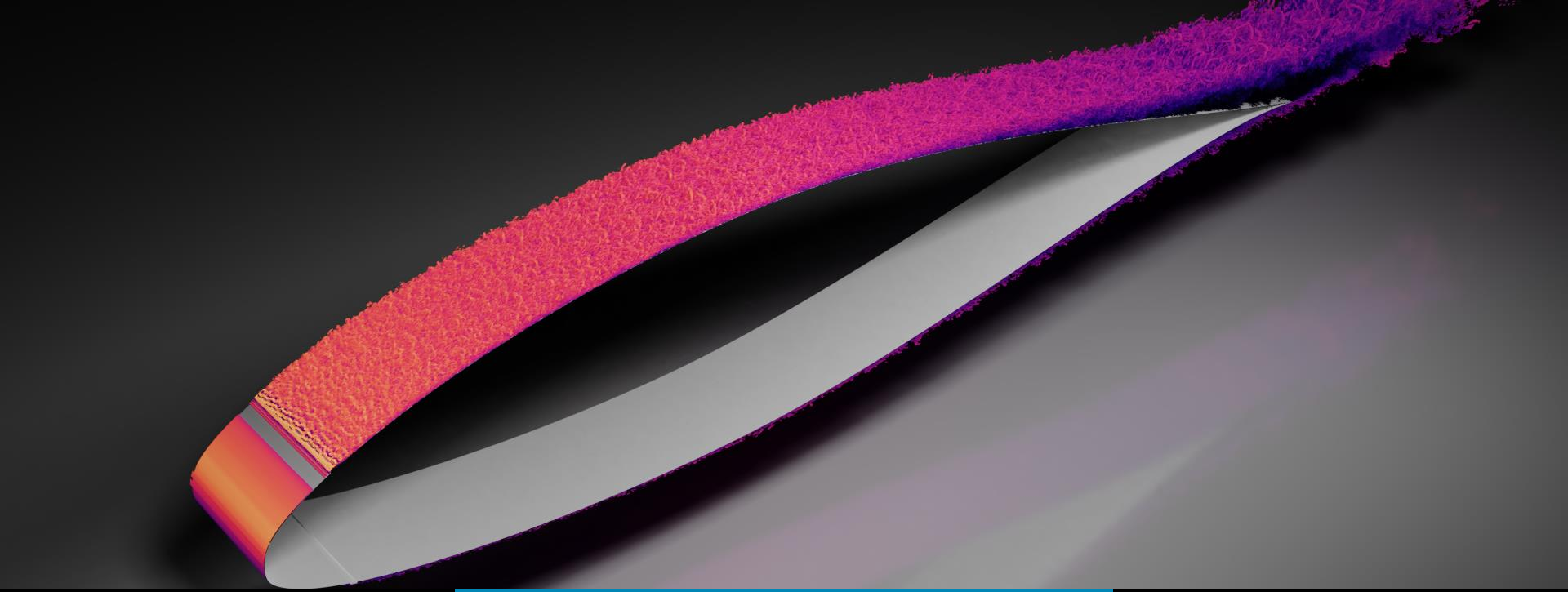


[1]Blind et al., Grid-Adaptation for Wall-Modeled Large Eddy Simulation Using Unstructured High-Order Methods. arXiv preprint
[2]Mossier et al., A p-Adaptive Discontinuous Galerkin Method with hp-Shock Capturing. Journal of Scientific Computing, 2022

Simulation software: FLEXI
Shock-capturing, DLB and p-adaptivity



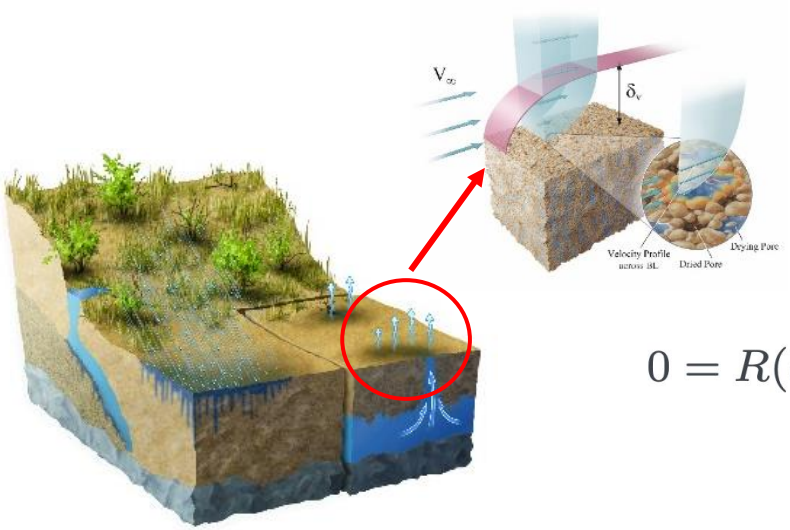
Multi-X simulations require flexible and adaptive discretization schemes: h/p adaptivity, unstructured grids, submodels…



LES closures from data

The Scale Gap

- Multiscale problems: Formulations on micro, meso, macro, … scales
- Definition of a coarsening operator (1) → (2) possibly ambiguous
- Solving coarse-scale equations plus models for the closure terms $M(U_h)$



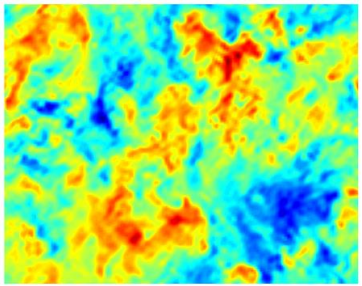
$$\underbrace{R(U_l, x_l) = 0}_{\text{Governing Equations at level l}} \quad (1)$$

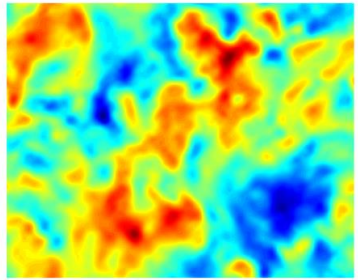
$$0 = R(U_h, x_h) + C(U_l, U_h) \approx \underbrace{R(U_h, x_h,) + \mathbf{M(U_h)}}_{\text{"Closed" Equations at level h}} \quad (2)$$

LES – Basic Formalism

- Coarsening operator (1) → (2)

$$\overline{u(x)} = \int_{-\Delta x}^{\Delta x} u(r) G(x-r) dr$$

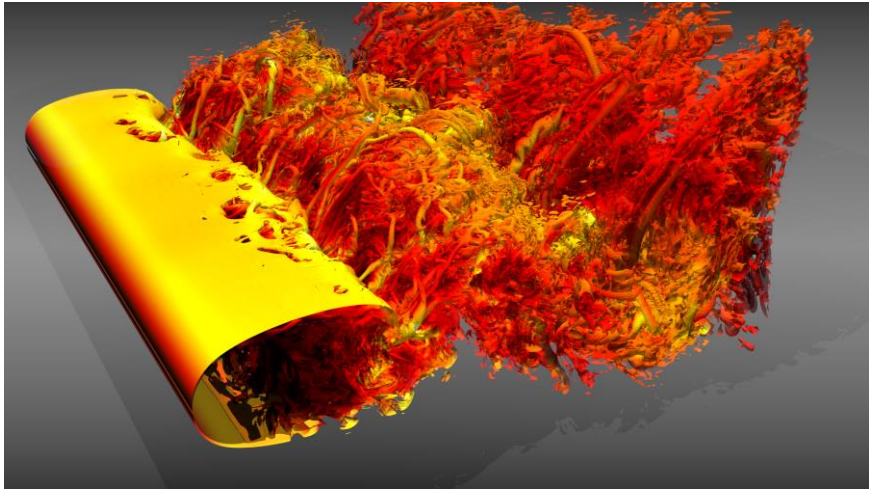


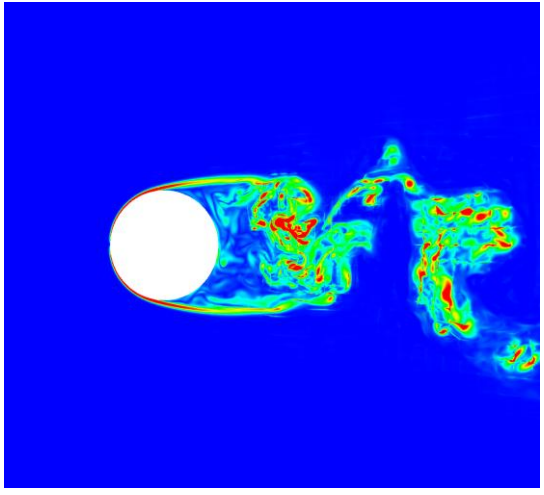


- Solving coarse-scale equations plus models for the Closure terms M(U_h)

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{u}_i \overline{u}_j\right) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + 2\nu \frac{\partial}{\partial x_j}\bar{S}_{ij} - \frac{\partial \tau_{ij}}{\partial x_j}$$

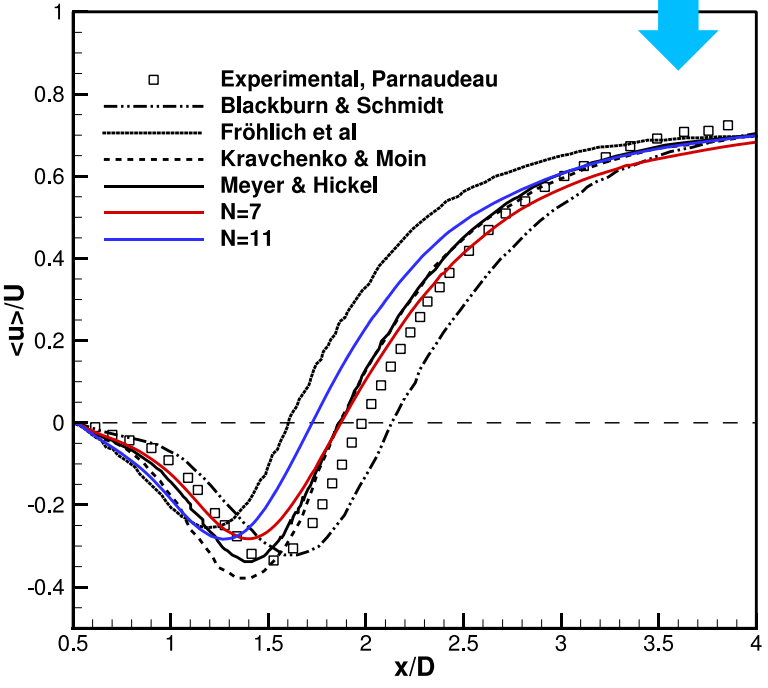
$$\overline{u_i u_j} = \tau_{ij} + \overline{u}_i \overline{u}_j$$





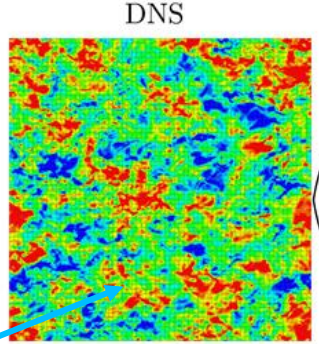
"It is the model's fault!"

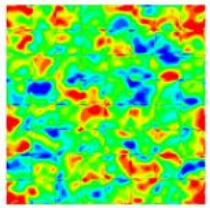
"Same equations, domains, …"

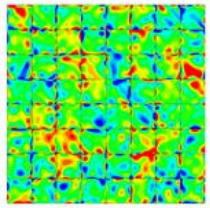


Can we find better models through data?

LES Closure Terms through supervised learning







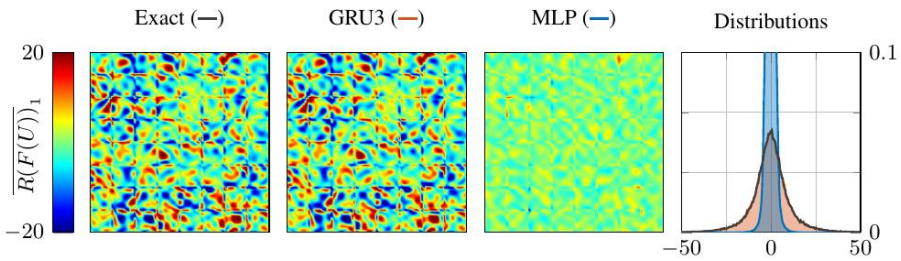
NN: $\min_\theta \left\| \hat{Y} - \hat{M}(\hat{X}, \theta) \right\|$

$$\underbrace{R\left(U_l, x_l, t_l\right) = 0}_{\text{Governing Equations at level l}}$$

$$\underbrace{R\left(U_L, x_L, t_L\right)}_{\text{Governing Equations at level L}} + \overbrace{\overline{M\left(U_l, U_L\right)}}^{\text{Influence of level l on L}} = 0$$

Supervised Learning for LES models in a nutshell

- SL finds mappings from inputs to outputs: it extracts existing knowledge
- SL requires a lot of a priori knowledge in the form of labeled data
- For well-defined data sets, it works well: Data-driven SGS models exist for canonical LES cases
- Incorporation of physical constraints improves stability
- But…



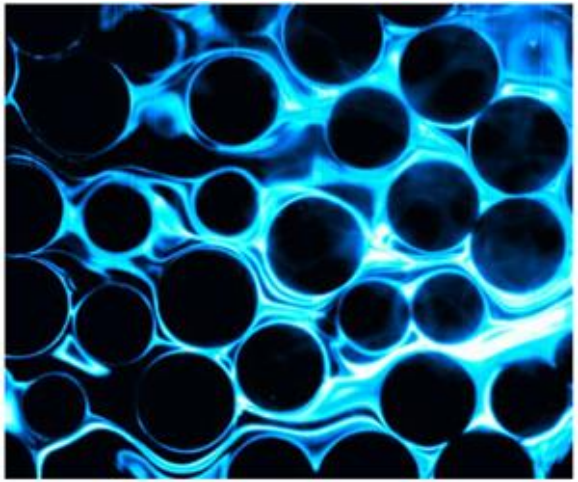
ELSEVIER
Journal of Computational Physics
Volume 398, 1 December 2019, 108910

Deep neural networks for data-driven LES closure models

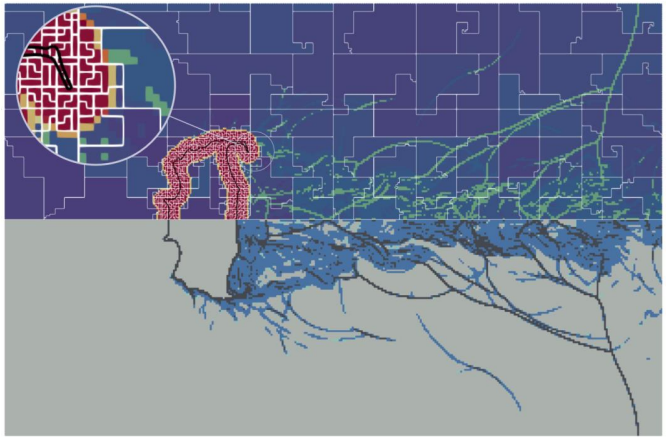
Andrea Beck, David Flad, Claus-Dieter Munz

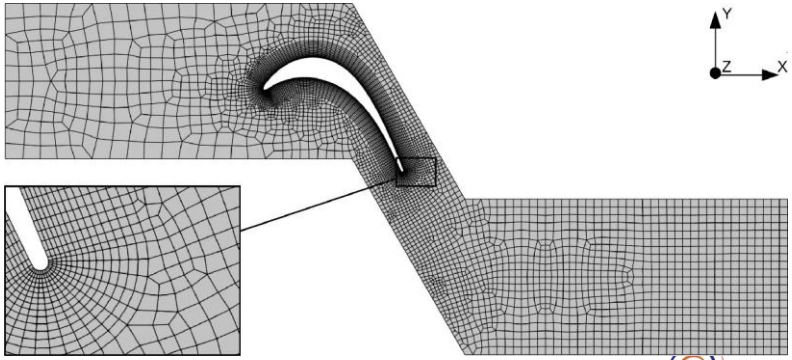
We want LES models that work for …

- Adaptive discretizations
- Unstructured grids
- All kinds of flows across Re, Ma, Sc, …
- SL: Data-rich but efficiency-poor?









Revisiting the LES problem: Implicit vs. Explicit

$$u = \overline{u}(x,t) + u(x,t)' \Rightarrow \overline{u}(x,t) = \int_{\Delta r} u(r,t)G(x-r)dr$$

- What is the relationship between the filter kernel size and the discretization?

- Separate Δr and h
- Explicit filtering: $h \to 0$
- Discretization scheme not relevant
- Caveat: homogeneity and isotropy, boundary conditions, realizability, commutation…

0.5% on google scholar

- Joined Δr and h
- Implicit filtering: $h \not\to 0$
- Discretization scheme defines filter kernel
- $\Leftarrow$ plus discretization parameters and errors

99.5% on google scholar, 100% for “industrial” LES

We derive the LES equations and the closure terms for a convolution with a known, homogenous, linear filter kernel with commutation

$$\overline{\psi}(x) := F(\psi(x)) = \int_{\infty}^{\infty} k(\xi - x, \Delta)\psi(\xi)d\xi,$$

Use Burgers equations as the simplest model for non-linearity

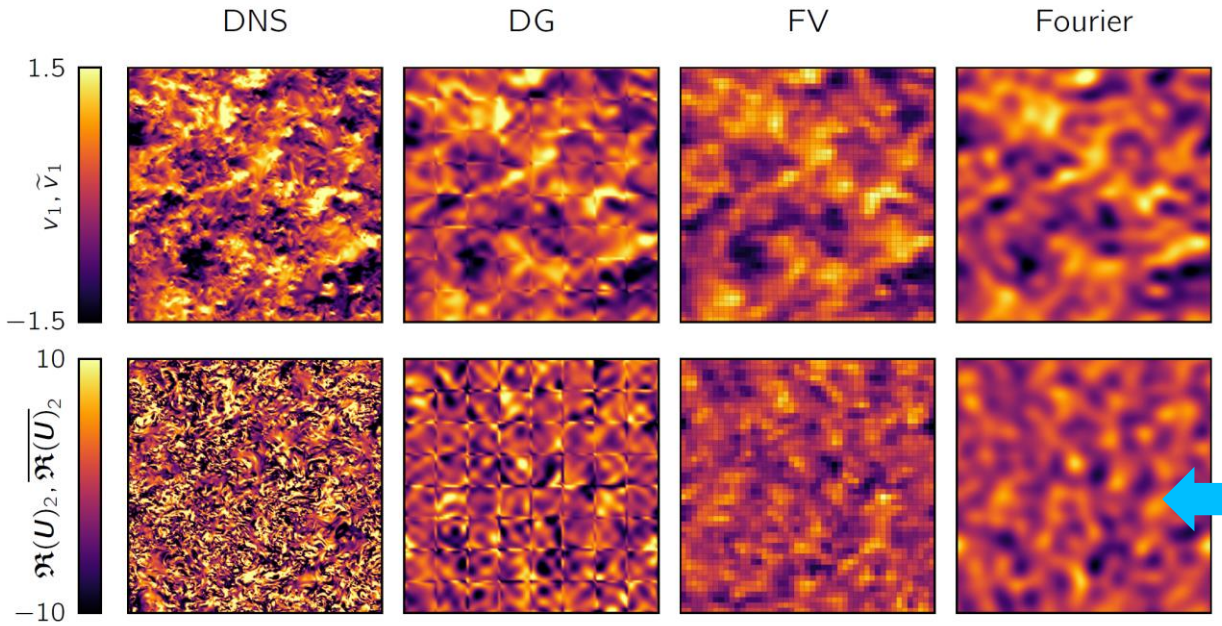
$$R(u) = \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0,$$

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\partial \overline{u^2}}{\partial x} = \frac{1}{2}\underbrace{\left(\frac{\partial \overline{u^2}}{\partial x} - \frac{\overline{\partial u^2}}{\partial x}\right)}_{C_1[F;\frac{\partial}{\partial x}](u^2)}$$

$$= \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\partial \overline{u}\,\overline{u}}{\partial x} = C_1 + \frac{1}{2}\underbrace{\left(\frac{\partial \overline{u}\,\overline{u}}{\partial x} - \frac{\partial \overline{u^2}}{\partial x}\right)}_{C_2[F;()^2](u)},$$

- “the” unclosed term per textbook

Almost all practical LES: filtering is implicit, through grid / operator / discretization:
1.) Discretization characteristics induce filter shape



The induced filter results in different SF stresses

2.) Resolved and represented scales

$$h \approx \Delta$$

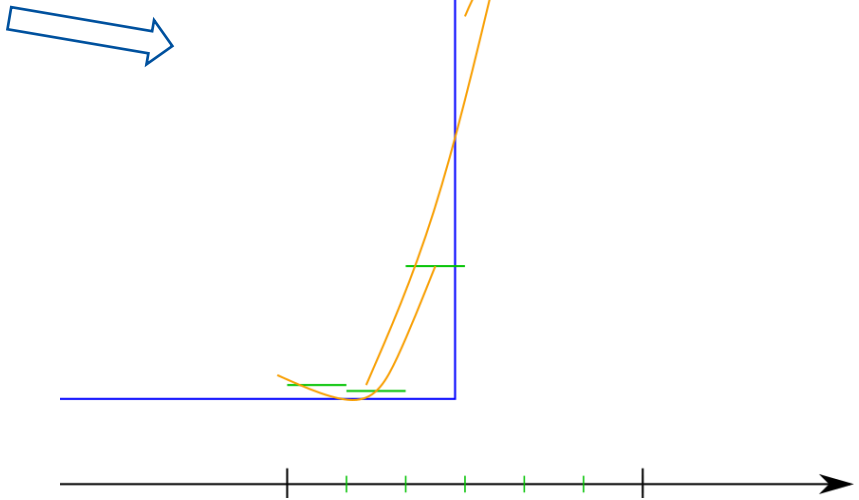
Discrete flux operator induces computational subgrid stresses

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\underbrace{\left(\frac{\delta \overline{u}\,\overline{u}}{\delta x} - \frac{\partial \overline{u}\,\overline{u}}{\partial x}\right)}_{C_3[\partial_x;\delta_x]},$$

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\frac{\partial}{\partial x}\underbrace{\left(\widehat{\overline{u}\,\overline{u}} - \overline{u}\,\overline{u}\right)}_{C_3^*[\widehat{\cdot};\cdot]}; \; \delta_x f = \partial_x \hat{f}$$

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\left(\frac{\delta \overline{u}\,\overline{u}}{\delta x} - \frac{\partial \overline{u}\,\overline{u}}{\partial x}\right),$$

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\frac{\partial}{\partial x}\underbrace{\left(\widehat{\overline{u}\,\overline{u}} - \overline{u}\,\overline{u}\right)}_{C_3^*[\widehat{\cdot};\cdot]}; \quad \delta_x f = \partial_x \hat{f}$$

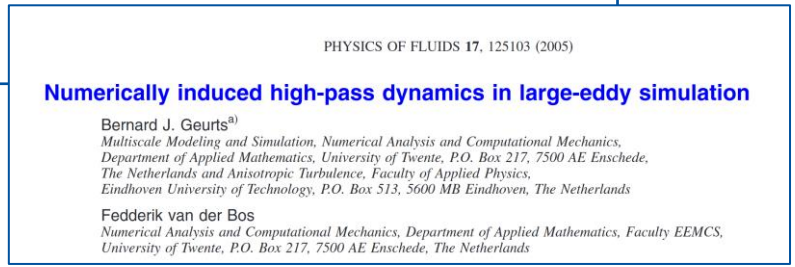


Linear numerical schemes for solving partial differential equations, having the property of not generating new extrema (monotone schemes), can be at most first-order accurate.

Think: Upwinding schemes, characteristic based schemes, WENO, SUPG, …

"… the computational large-eddy closure typically contains an important contribution that is sensitive to the adopted spatial discretization"

"… considerable improvements of practical large-eddy simulation may be achieved in case the closure problem in the modified equation is made to explicitly account for the coarseness as well as the type of discretization."



PHYSICS OF FLUIDS **17**, 125103 (2005)

Numerically induced high-pass dynamics in large-eddy simulation

Bernard J. Geurts[a)]
Multiscale Modeling and Simulation, Numerical Analysis and Computational Mechanics, Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands and Anisotropic Turbulence, Faculty of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

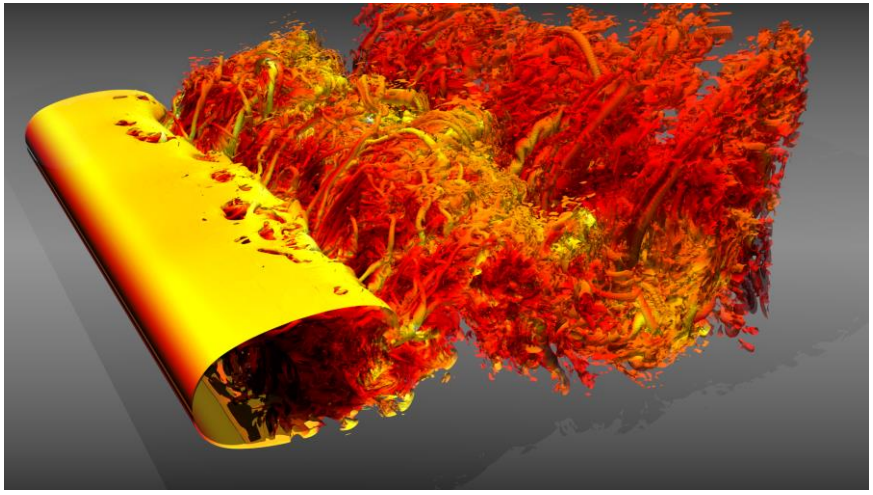
Fedderik van der Bos
Numerical Analysis and Computational Mechanics, Department of Applied Mathematics, Faculty EEMCS, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

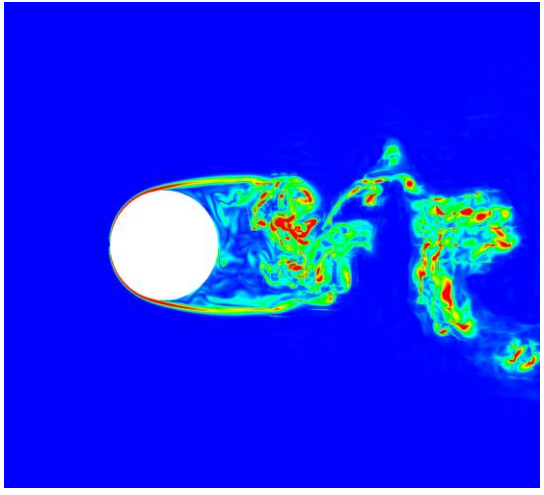
We derive the LES equations and the closure terms for a known, homogenous, linear filter kernel with commutation…

… Scale Separation filtering in practical LES is done implicitly with a partially unknown, inhomogeneous, possibly anisotropic and often non-linear filter kernel

What makes LES uncertain? More non-linearities.

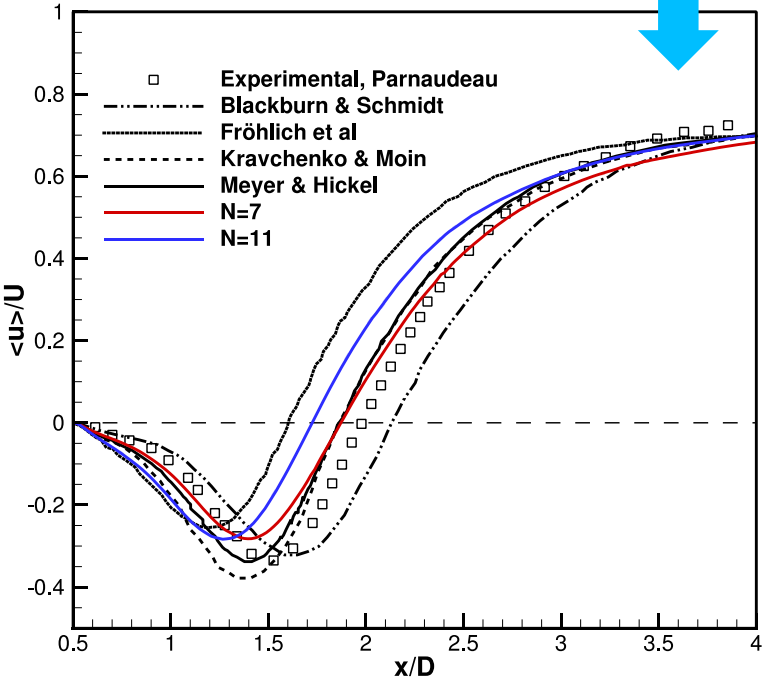






"Is it the model's fault? Did we account for C1 and C3?

"Same equations, domains, …"



Challenges for data-driven modelling

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\underbrace{\left(\frac{\delta \overline{u}\,\overline{u}}{\delta x} - \frac{\partial \overline{u}\,\overline{u}}{\partial x}\right)}_{C_3[\partial_x;\delta_x]},$$

Make SL models scale-aware

Train SL models on Reynolds stresses from DNS or Exp.

$$\delta^n = \delta(\overline{u}^n), \quad \overline{u}^{n+1} = \overline{u}(\delta^n)$$

Knowable a priori

Not knowable a priori

Challenges for data-driven modelling

- For implicitly-filtered LES, the closure terms are defined a posteriori. They are…
  - A function of the local discretization operator
  - A function of the local solution

- How can we find discretization-consistent models? Supervised learning requires a priori knowledge.

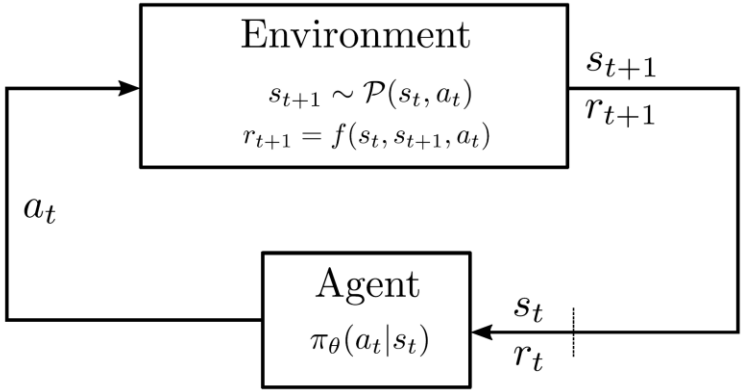
- “Tune the Smagorinsky constant to the flow”: A priori bad models can do “good”, a priori great models can fail miserably a posteriori

How can we learn from data for discretized PDEs in a posteriori manner?

Learning for dynamical systems: An Alternative to SL

- LES simulations solve discrete dynamical chaotic systems
- Supervised learning has two problems: How do we define a lot of true data and make models robust?
- Reinforcement learning is a different paradigm from ML: Learning to take optimal actions in a dynamical system from experience
- Submodels need to be consistently integrated with the discretization: a simple gradient looks very different for a FD, FV, FE scheme
- Putting the PDE solver in the loop

RL on a single slide





$$\pi = S \times A \to \mathcal{R}, \langle s, a \rangle \to [0, 1]$$

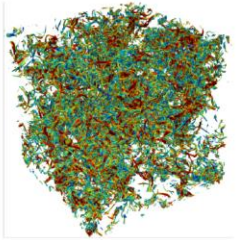
$$\max_\theta E_\theta \Big(\sum_{k=1}^{T} \gamma^k r_k \Big), \text{ subject to } \langle S, A, P(\cdot), R(\cdot) \rangle$$

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau \sim \pi_\theta} \Big[\underbrace{\Big(\sum_{k=1}^{N} \gamma^k r_k \Big)}_{\text{Cum. reward over } \tau} \underbrace{\nabla_\theta \log \pi_\theta(\tau)}_{\text{Grad. of the policy}} \Big]$$

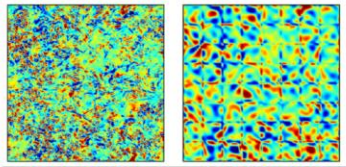
- “Play many games, track rewards, explore and exploit”

LES Closures as an MDP

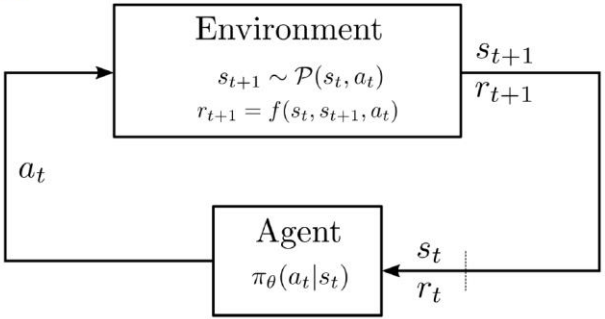
Forced LES of HIT

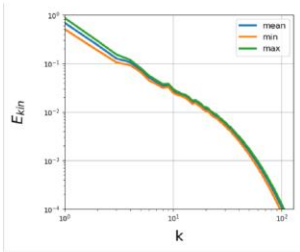


Implicitly filtered LES with a HO DGSEM

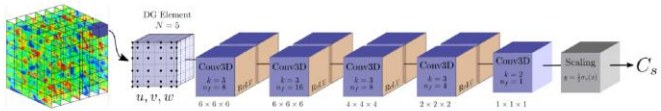


FLEXI iLES





Expected Spectrum



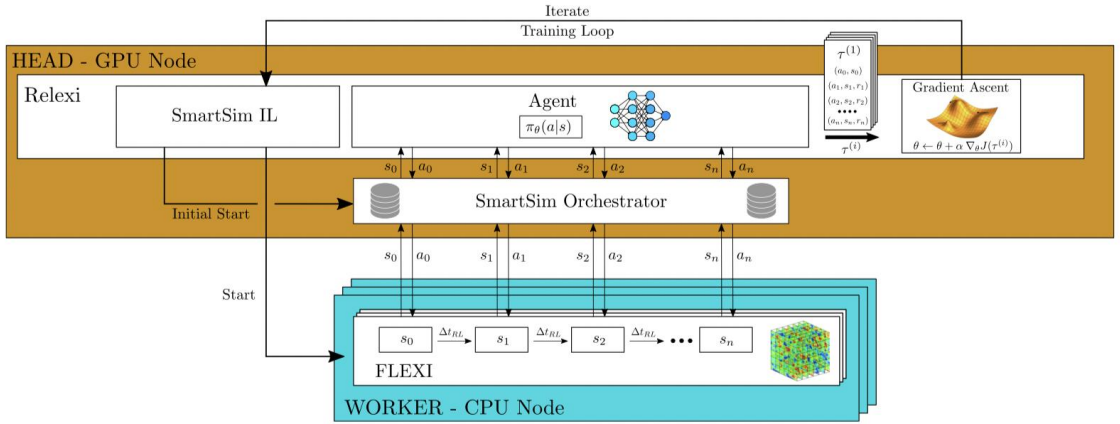
Policy net predicts C_s

- "Play many games, track rewards, explore and exploit"

Incorporate physics, optimize under discretization

Reinforcement learning framework – ReLeXI[1]: IAG, HLRS & HPE

- Distribution on hybrid HPC systems via the SmartSim Library[2]
- Dedicated GPU node („Head“) for training and model evaluation
- FLEXI instances interactively distributed across multiple CPU nodes („Workers“)
- Communication via in-memory database with the Redis library



[1]Kurz et al., Relexi—A scalable open source reinforcement learning framework for high-performance computing. Software Impacts, 2022
[2]https://github.com/CrayLabs/SmartSim

Relexi Framework

- The framework scales well over many parallel runs
- LES solver strong scaling essentially unaffected by coupling
- We can efficiently evaluate each policy to get reliable gradients
- We can run many samples fast
- We can run many samples in parallel

Journal of Computational Science
Volume 65, November 2022, 101884

Deep reinforcement learning for computational fluid dynamics on HPC systems

Marius Kurz [a 1], Philipp Offenhäuser [b 1], Dominic Viola [b], Oleksandr Shcherbakov [c], Michael Resch [c], Andrea Beck [a]

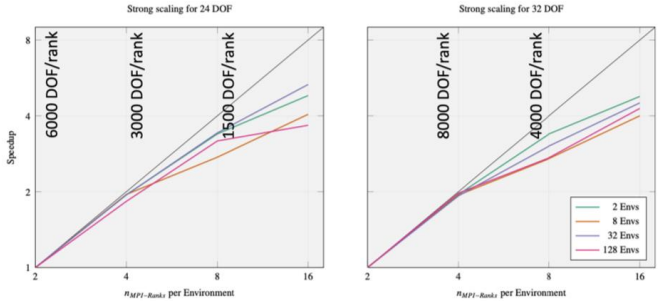


Figure 4: Strong scaling of FLEXI within the Relexi framework for the HIT test case with 24 DOF and 32 DOF for 2, 4, 8 and 16 MPI ranks per FLEXI instance. For clarity, only the runs for 2, 8, 32 and 128 parallel FLEXI environments are shown. The black line indicates perfect scaling.

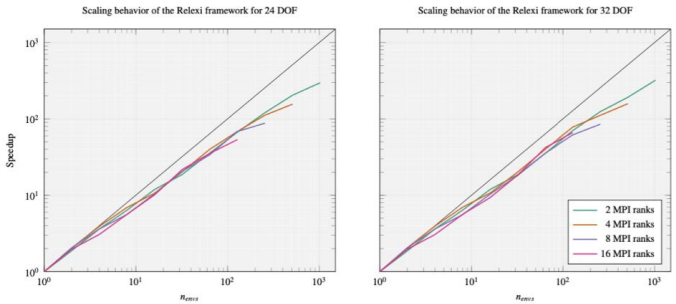
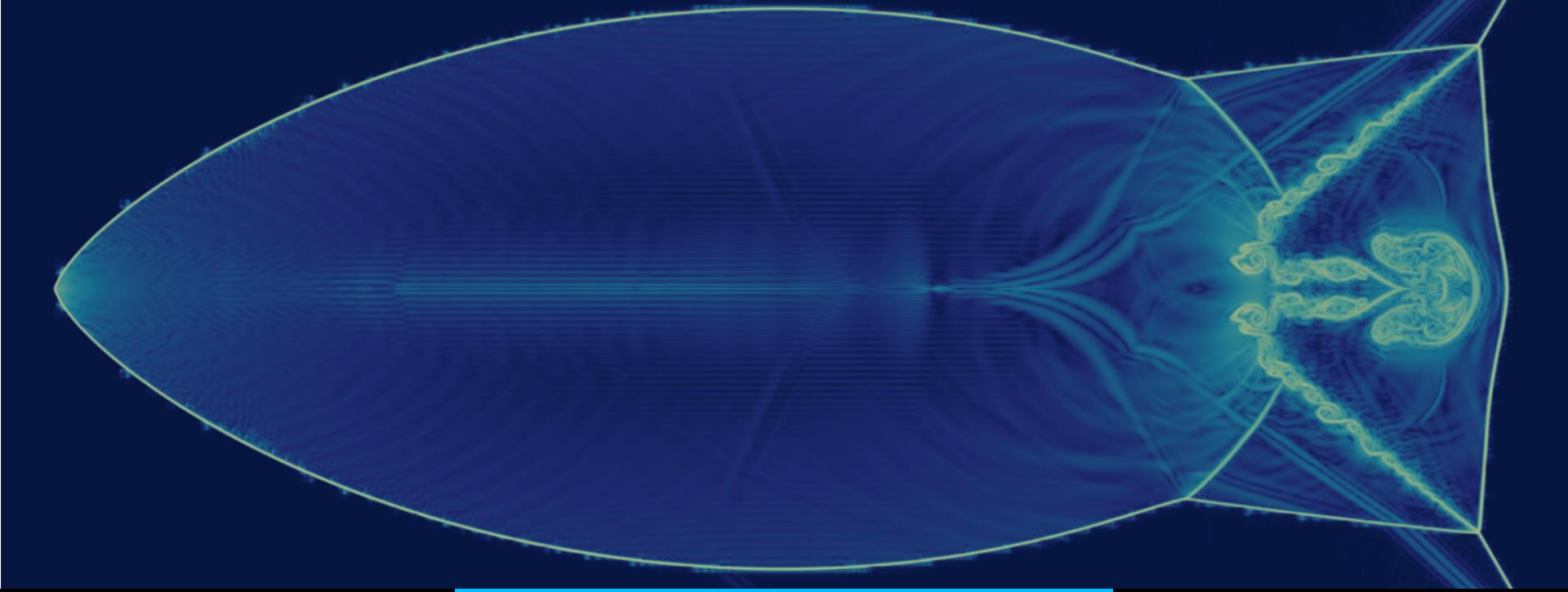
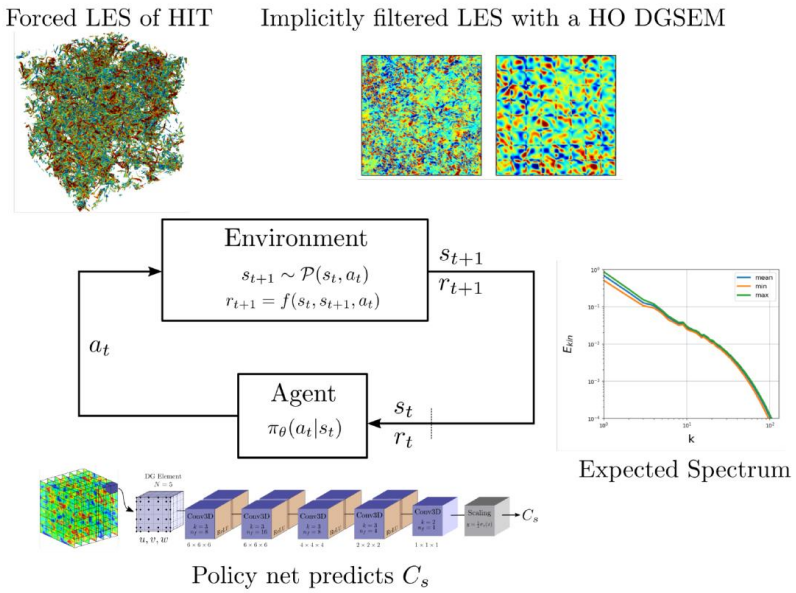


Figure 3: Scaling behavior of the Relexi framework on up to 16 Hawk compute nodes (2048 MPI ranks) and one Hawk-AI node for the HIT test case with 24 DOF and 32 DOF for 2, 4, 8 and 16 MPI ranks per FLEXI instance. The black line indicates perfect scaling.



RL for discretization consistent LES closures

Details



- Environment: Implicitly filtered HO DGSEM of FHIT
- Reward / Goal: Spectrum up to cut-off wavenumber
- Agent: Convolutional / Residual NN
- Method: Proximal Policy Optimization
- No DNS data; optimization requires LES runs only
- Implement as hybrid CPU/GPU parallel code in SmartSim on HAWK-AI
- Training wall clock time: 24h

Policy: Find explicit or implicit closure strategy

$$\overline{R(u)} = \frac{\partial \overline{u}}{\partial t} + \frac{1}{2}\frac{\delta \overline{u}\,\overline{u}}{\delta x} = C_1 + C_2 + \frac{1}{2}\frac{\partial}{\partial x}\underbrace{\left(\widehat{\overline{u}\,\overline{u}} - \overline{u}\,\overline{u}\right)}_{C_3^*[\widehat{\cdot};\cdot]}; \; \delta_x f = \partial_x \hat{f}$$

- **Complete,** discretization-consistent closure model for full SGS / SFS terms

Optimized eddy viscosity

Optimized dissipative properties

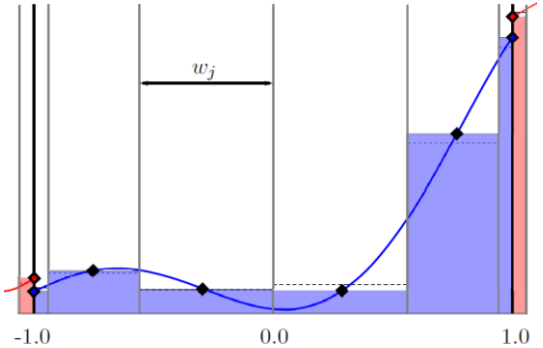
Formulate modelling strategy as an MDP, solve with RL

Things to note

- We find models for the complete closure terms C1...C3 (and others)
- We do not need to know C1…C3 a priori: We do not need DNS data, only a statistic
- Instead, “training” means running a number of LES simulations
- We optimize the solution of the overall PDE (i.e. the LES), not individual terms
- We discover new modelling schemes through RL: RL itself is not a model

Two modelling scenarios

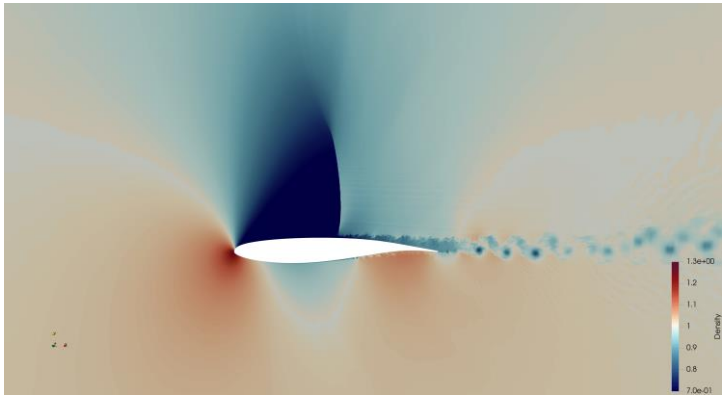
Implicit and explicit SGS modeling: Optimal Operator Blending

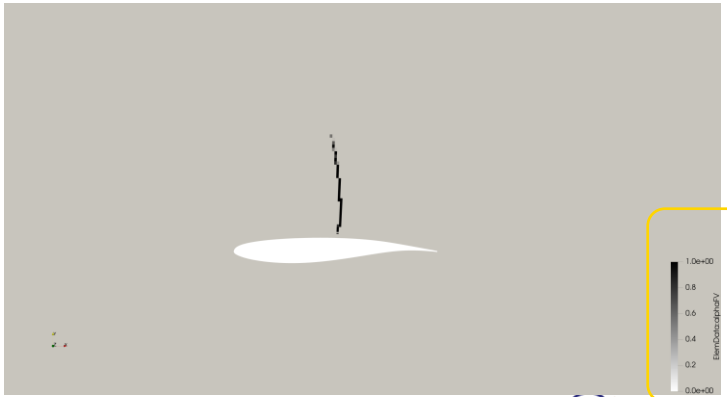


$$\dot{\underline{u}}^{BL} = \dot{\underline{u}}^{DG}\,(1-\alpha) + \dot{\underline{u}}^{FV}\,\alpha$$

A0: For each grid element q_{rst} with $r,s,t \in [1, nElems] : \alpha_s^q = \alpha(t)$

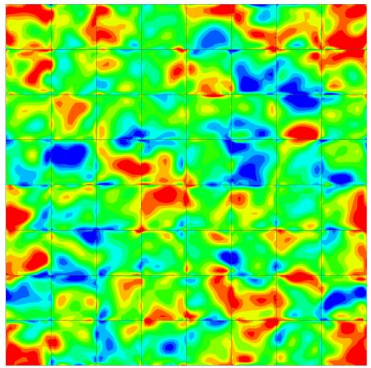
A2: For each grid element q_{rst} with $r,s,t \in [1, nElems] : \alpha_s^q = \sum_{i,j,k=0}^{2} a_i(t) L_i(x) L_j(y) L_k(z)$





Two modelling scenarios

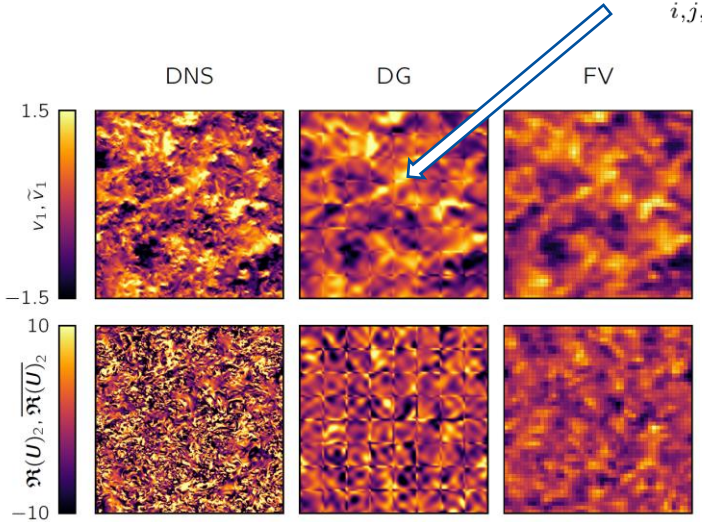
Implicit and explicit SGS modeling: Optimal Smagorinsky constant



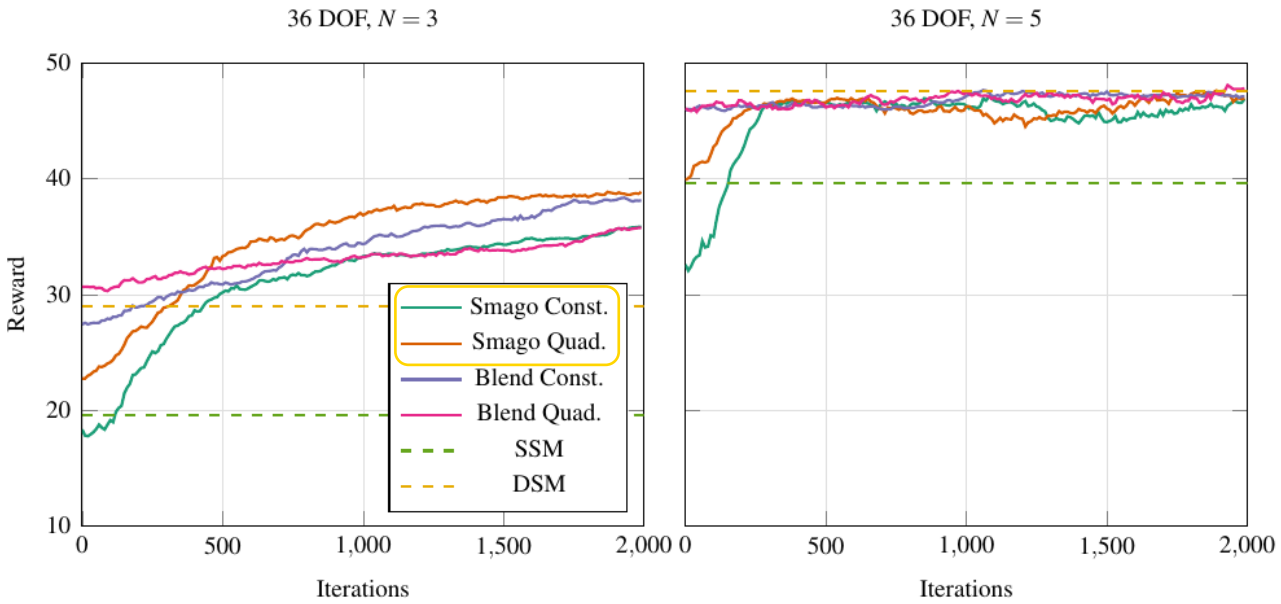
SSM: For each grid element q_{rst} with $r,s,t \in [1, nElems] : C_s^q = C_s = const.$

Cs0: For each grid element q_{rst} with $r,s,t \in [1, nElems] : C_s^q = C_s(t)$

Cs2: For each grid element q_{rst} with $r,s,t \in [1, nElems] : C_s^q = \sum_{i,j,k=0}^{2} c_i(t) L_i(x) L_j(y) L_k(z)$

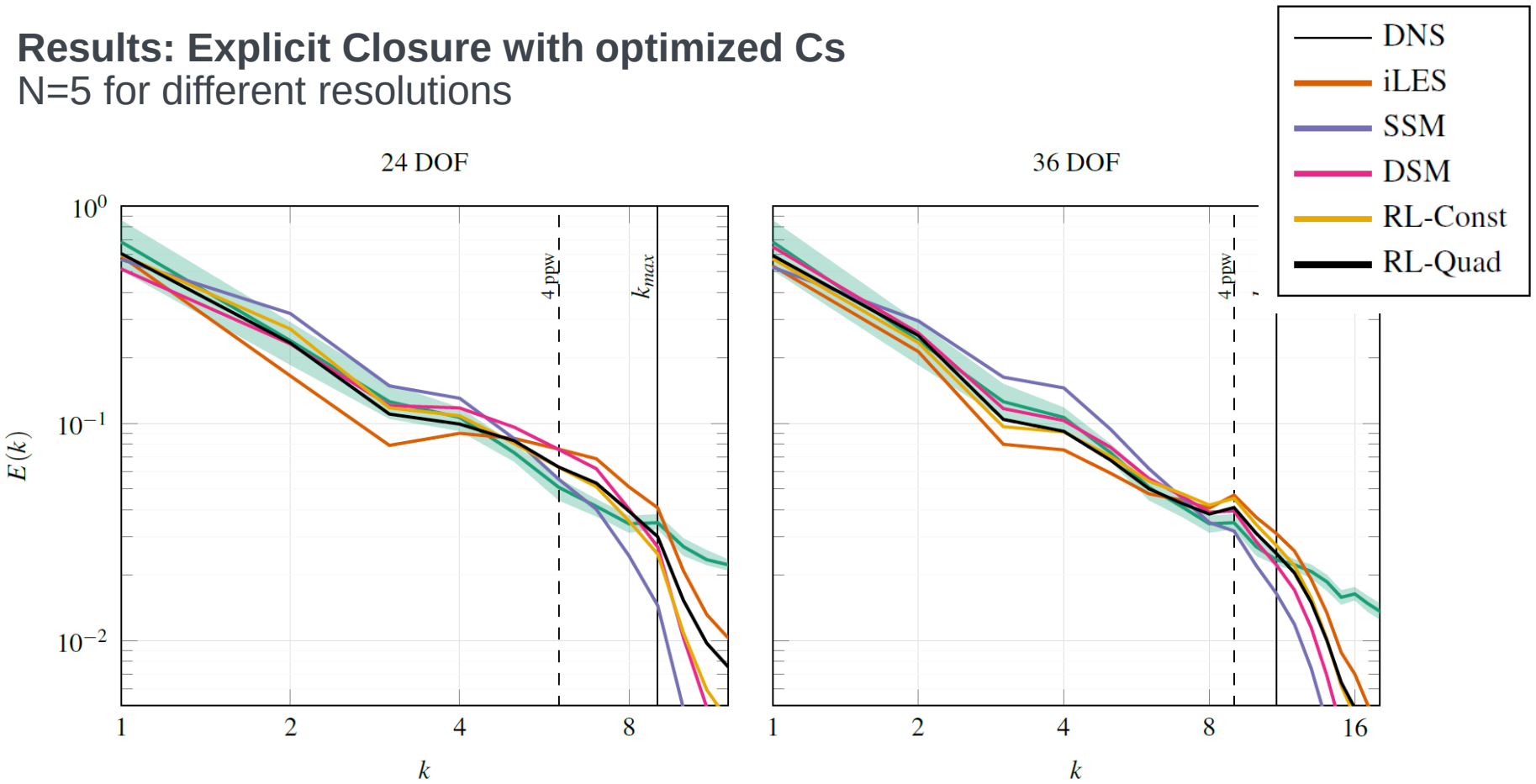


Results: Explicit Closure with optimized Cs



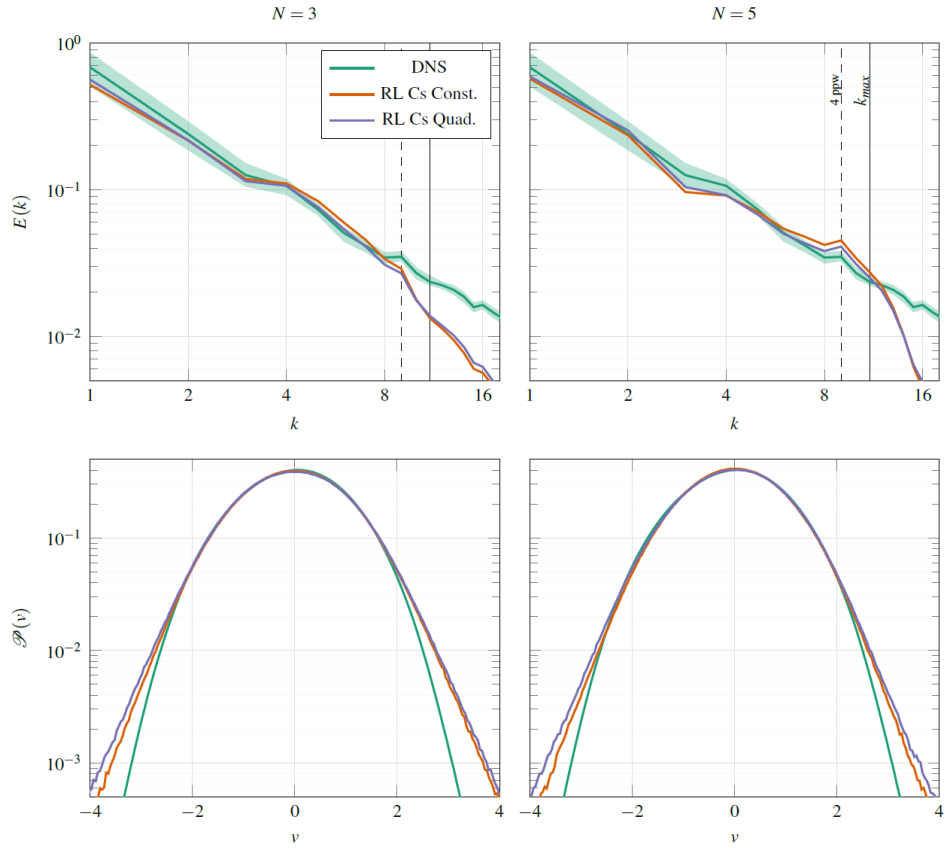
Results: Explicit Closure with optimized Cs

N=5 for different resolutions



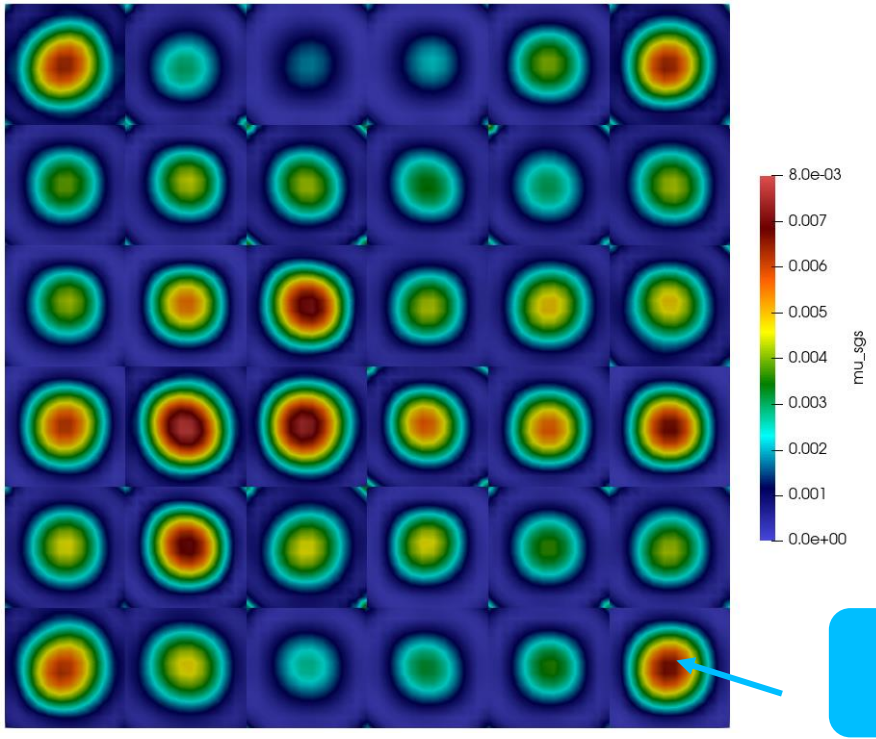
Results: Explicit Closure with optimized Cs

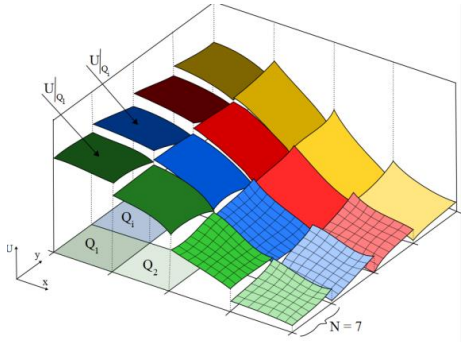
Different operators, same resolution

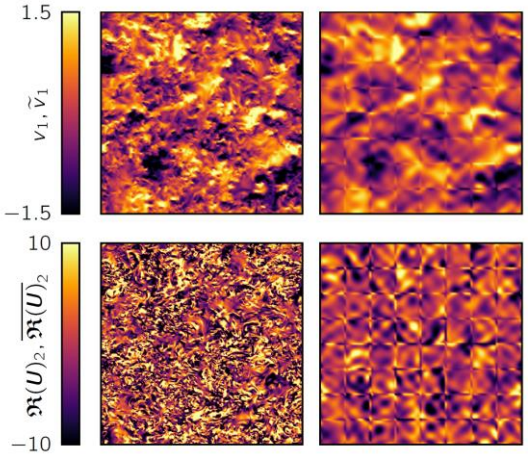


Results: Explicit Closure with optimized Cs

Mean Eddy viscosity field for Cs2



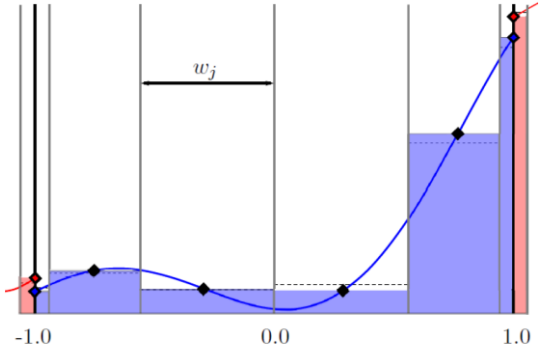




The discretization / induced filter footprint

Two modelling scenarios

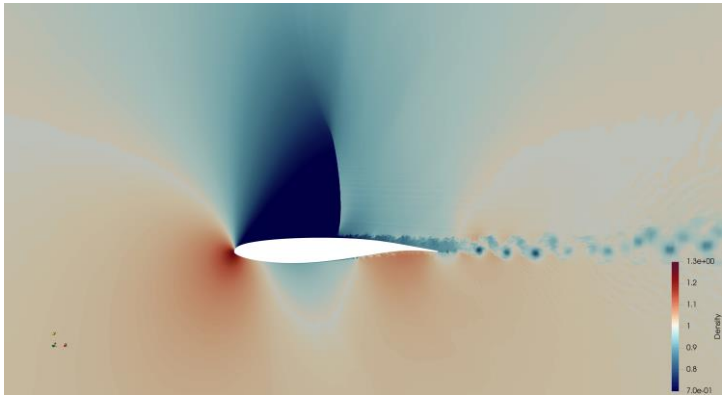
Implicit and explicit SGS modeling: Optimal Operator Blending

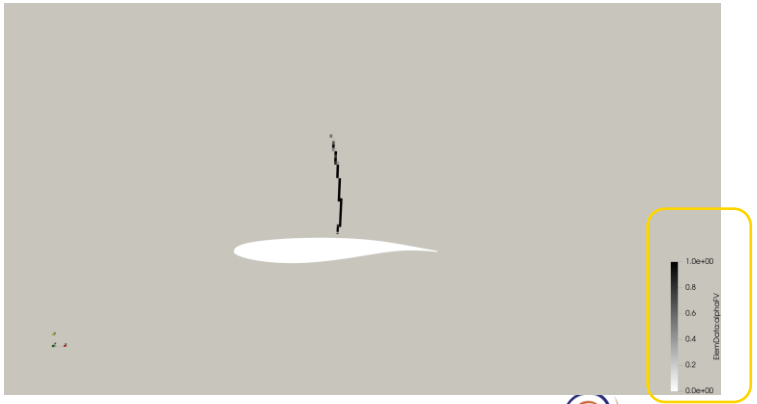


$$\underline{\dot{u}}^{BL} = \underline{\dot{u}}^{DG}\,(1-\alpha) + \underline{\dot{u}}^{FV}\,\alpha$$

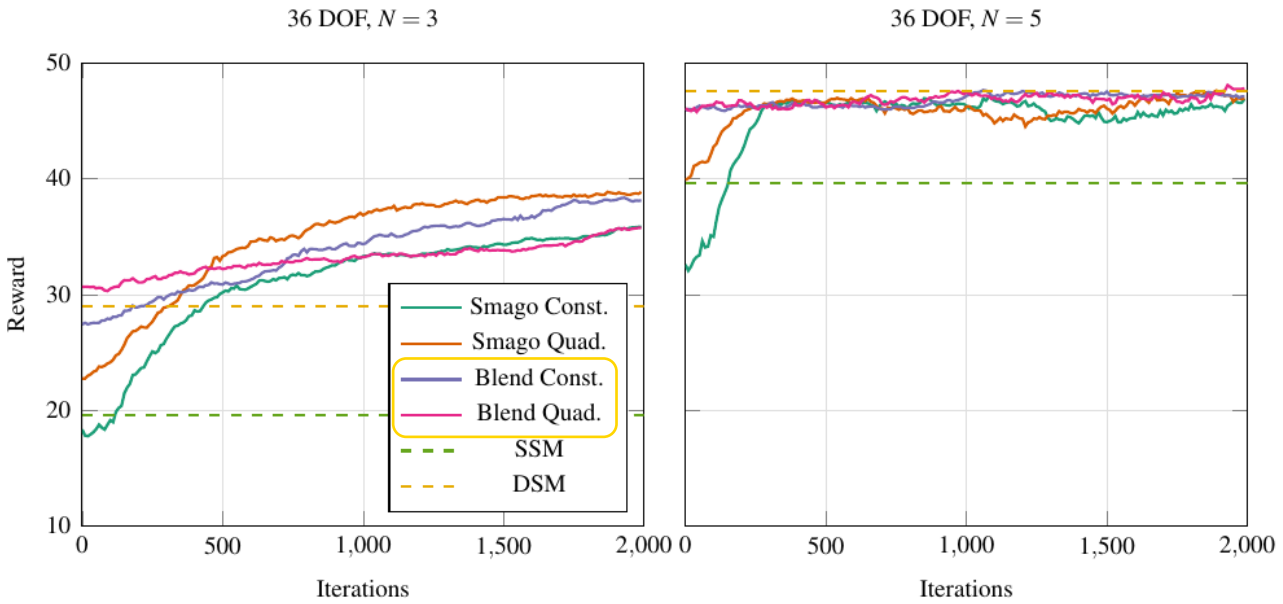
A0: For each grid element q_{rst} with $r,s,t \in [1, nElems] : \alpha_s^q = \alpha(t)$

A2: For each grid element q_{rst} with $r,s,t \in [1, nElems] : \alpha_s^q = \sum_{i,j,k=0}^{2} a_i(t) L_i(x) L_j(y) L_k(z)$



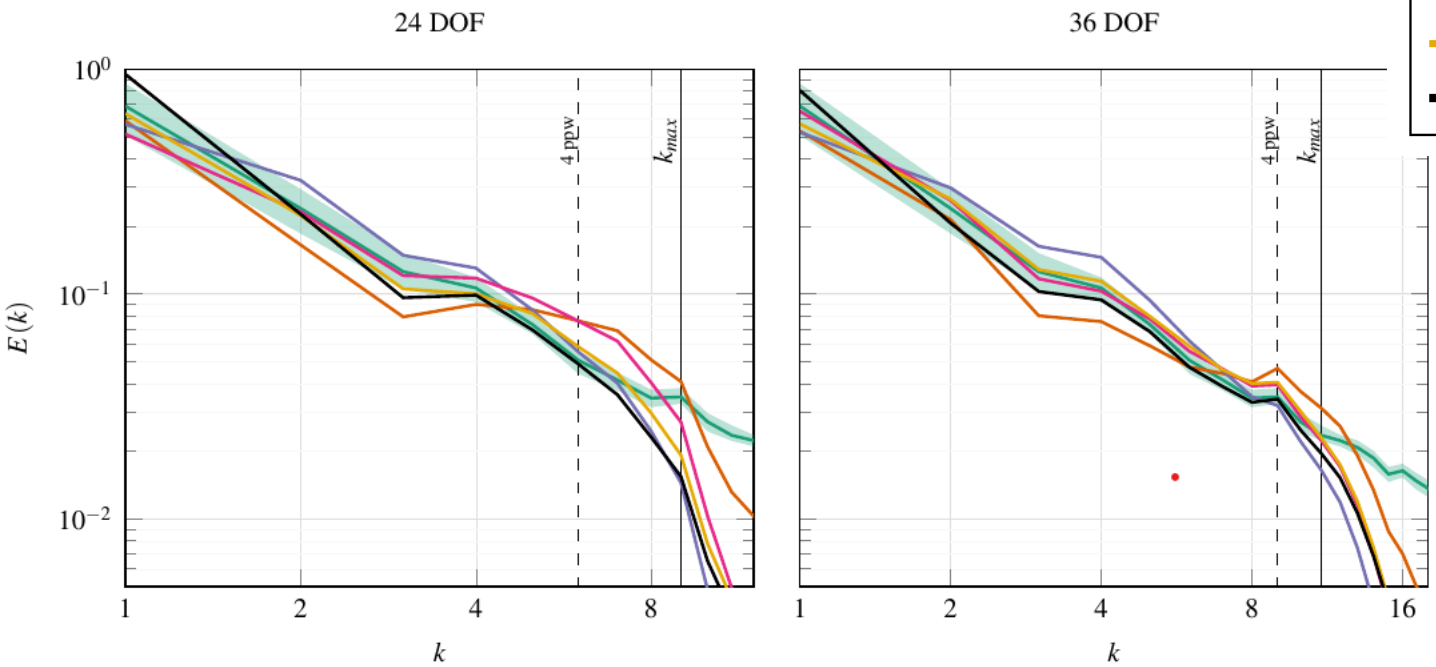


Results: Implicit Closure with optimized Blending



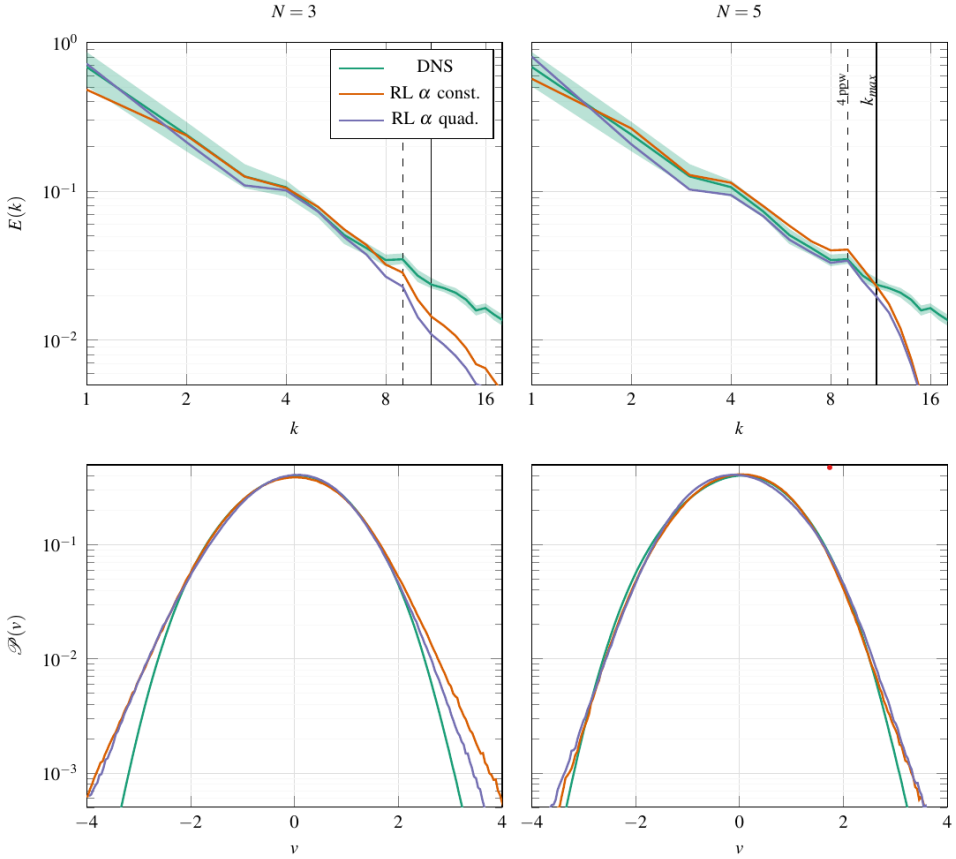
Results: Implicit Closure with optimized Blending

N=5 for different resolutions

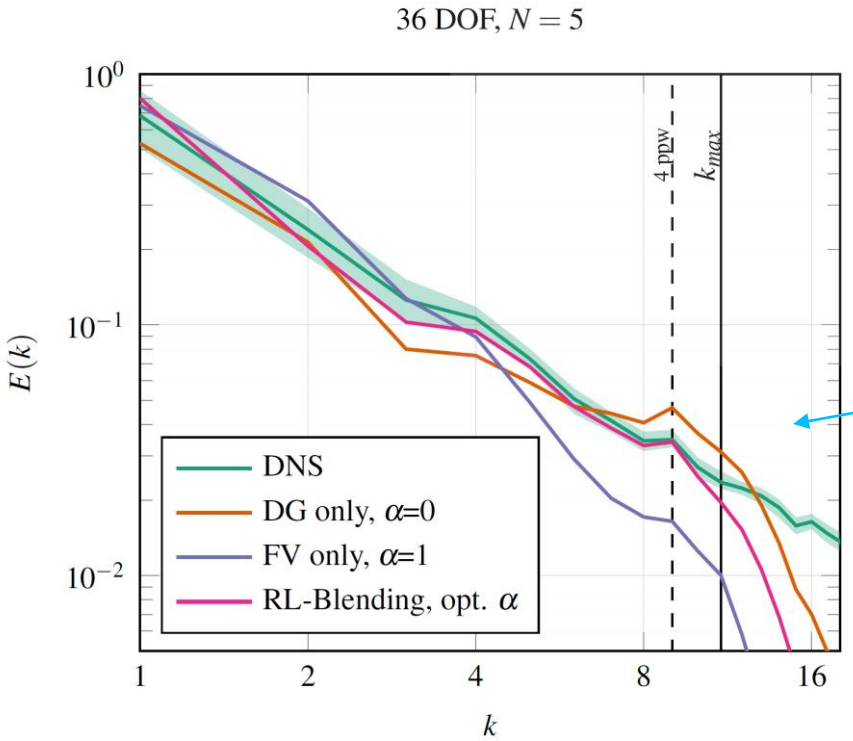


Results: Implicit Closure with optimized Blending

Different operators, same resolution



Results: Implicit Closure with optimized Blending



Implicit LES model through non-linear combination of HO and TVD scheme: A scheme for compressible turbulence?



Summary

Summary

- Multiscale problems require multi-X numerical schemes
- SL works great if one can define good data a priori
- The classical LES formulation omits the challenges of “real life” LES: C1…C3
- Reinforcement learning with a PDE solver in the loop: Versatile, inclusive optimization environment for flow control and modelling
  - RL does not need fine scale data (like DNS), but statistics. Training happens on the coarse (LES) level: Huge computational savings
  - RL allows to optimize and discover new closures, it is not a model itself: All the knowledge about a “good” model is still applicable
  - RL is an alternative to adjoints or differentiable solvers: It approximates gradients of the cost function through sampling
  - RL is ML: it has hyperparameters and we lack theory in parts

Our publications on data-driven CFD

- Journal of Computational Physics 398, 108910
- GAMM-Mitteilungen 44
- Journal of Computational Physics 313, 1-12
- Journal of Computational Physics, 423, 109824
- Electronic Transactions on Numerical Analysis, 56, 117–137
- International Journal of Heat and Fluid Flow 99, 109094
- Journal of Theoretical and Computational Acoustics 27, 1850044
- Journal of Computational Physics 441, 110475
- SIAM Journal on Scientific Computing 42 (4), B1067–B1091
- Journal of Computational Science 65, 101884
- Journal of Computational Physics 408, 109303
- Software Impacts 14, 100422
- Computers & Fluids 228, 105039
- Wear 508, 204476
- Journal of Open Source Software 8 (82), 4683
- PAMM 23 (1), e202200207
- Toward Discretization-Consistent Closure Schemes for Large Eddy Simulation Using Reinforcement Learning arXiv:2309.06260v1

University of Stuttgart
Institute of Aerodynamics and Gas Dynamics

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Thank you!



Andrea Beck

e-mail beck@iag.uni-stuttgart.de
phone +49 711 685-60218
www.iag.uni-stuttgart.de
numericsresearchgroup.org

- Kurz, Marius, Philipp Offenhäuser, and Andrea Beck. "Deep reinforcement learning for turbulence modeling in large eddy simulations." *International Journal of Heat and Fluid Flow* 99 (2023): 109094.
- Kurz, Marius, et al. "Relexi—A scalable open source reinforcement learning framework for high-performance computing." *Software Impacts* 14 (2022): 100422.
- Mossier, Pascal, Andrea Beck, and Claus-Dieter Munz. "A p-adaptive discontinuous Galerkin method with hp-shock capturing." *Journal of Scientific Computing* 91.1 (2022): 4.
- Schwarz, Anna, et al. "A Reinforcement Learning Based Slope Limiter for Second-Order Finite-Volume Schemes." *Proceedings in Applied Mathematics and Mechanics* 7 (2022): 10.
- Kopper, Patrick, et al. "Boundary-Layer Dynamics in Wall-Resolved LES Across Multiple Turbine Stages." *AIAA Journal* 59.12 (2021): 5225-5237.
- Dürrwächter, Jakob, et al. "A high-order stochastic Galerkin code for the compressible Euler and Navier-Stokes equations." *Computers & Fluids* 228 (2021): 105039.
- Beck, Andrea, and Marius Kurz. "A perspective on machine learning methods in turbulence modeling." *GAMM-Mitteilungen* 44.1 (2021): e202100002.

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Thank you!

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