

University of Stuttgart



Towards data-driven high fidelity CFD NHR4CES Workshop 23

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$$\begin{split} &\int_{E} J(\vec{\xi}) U_{t} \phi \, d\vec{\xi} = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} J(\vec{\xi}) \left(\frac{\partial}{\partial t} \sum_{r,s,t=0}^{N} \hat{U}_{rst}(t) \psi_{rst}^{N}(\vec{\xi}) \right) \, \psi_{ijk}^{N}(\vec{\xi}) d\vec{\xi^{1}} d\vec{\xi^{2}} d\vec{\xi^{3}} \\ &= \sum_{\alpha,\beta,\gamma=0}^{N} J(\vec{\xi}_{\alpha\beta\gamma}) \left(\frac{\partial}{\partial t} \sum_{r,s,t=0}^{N} \hat{U}_{rst}(t) \underbrace{\ell_{r}^{N}(\xi_{\alpha}^{1})}_{=\delta_{r\alpha}} \underbrace{\ell_{s}^{N}(\xi_{\beta}^{2})}_{=\delta_{s\beta}} \underbrace{\ell_{t}^{N}(\xi_{\gamma}^{3})}_{=\delta_{t\gamma}} \right) \, \psi_{ijk}^{N}(\vec{\xi}_{\alpha\beta\gamma}) \omega_{\alpha} \omega_{\beta} \omega_{\gamma} \\ &= \sum_{\alpha,\beta,\gamma=0}^{N} J(\vec{\xi}_{\alpha\beta\gamma}) \frac{\partial}{\partial t} \hat{U}_{\alpha\beta\gamma}(t) \underbrace{\ell_{i}^{N}(\xi_{\alpha}^{1})}_{=\delta_{i\alpha}} \underbrace{\ell_{j}^{N}(\xi_{\beta}^{2})}_{=\delta_{j\beta}} \underbrace{\ell_{k}^{N}(\xi_{\gamma}^{3})}_{=\delta_{k\gamma}} \omega_{\alpha} \omega_{\beta} \omega_{\gamma} \end{split}$$

High Fidelity CFD: FLEXI

Multiscale Challenges to CFD

- Wide range of interacting scales: Nonlinearity is the source of complexity and sensitivity
- For a smooth solution and a consistent scheme of order N, we have an error bound

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

Number of points per wavelength for a given error: Measure of information efficiency

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
 - L₂ projection is optimal
 - Hybrid FE and FV scheme
- This gives flexibility, locality, conservation and stability (FV) and accuracy (FE)

Simulation software: FLEXI Introduction

- High-order accurate open source solver¹ 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

¹www.flexi-project.org

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:
 - Numerical integration: $U_h(\xi, t) \sum_{i,j=1}^{N} Collocation$
- Time approximation:
- Numerical flux:
- Stability

•

• Shock-capturing:

- Tensor product, Lagrange polynomials at Gauß / Gauß-Lobatto points $U_h(\xi,t) \sum_{i,j=1}^N \hat{U}_{i,j}(t) \psi_i^N(\xi^1) \psi_j^N(\xi^2)$
- Collocation approach (SEM approach)
- Explicit Runge-Kutta, IMEX
- Riemann solver, BR1/2
- De-Aliasing, Split form (entropy / energy stable fluxes)
- Finite volume sub-cells, h/p adaptivity

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

Time

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, FLEXIpreCICE, FLEXI-OpenFOAM, FLEXI-TAU
- Reproduceability: Regression/unit testing, "compile from file", Development and Management via gitlab / on github

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

Nico Krais * 유 편, Andrea Beck * 편, Thomas Bolemann * 편, Hannes Frank * 편, David Flad * 편, Gregor Gassner ^b 편, Florian Hindenlang ^ 편, Malte Hoffmann * 편, Thomas Kuhn * 편, Matthias Sonntag * 편, Claus-Dieter Munz * 편

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

Simulation software: FLEXI Adaptivity and error control – hp-refinement

- h-refinement¹
 - 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-refinement²
 - Local p-adaptivity in smooth solution regions
 - Dynamic Load Balancing (under development)

¹Blind et al., Grid-Adaptation for Wall-Modeled Large Eddy Simulation Using Unstructured High-Order Methods. arXiv preprint ¹⁸ ²Mossier et al., A p-Adaptive Discontinuous Galerkin Method with hp-Shock Capturing. Journal of Scientific Computing, 2022

Simulation software: FLEXI hp-adaptive Multiphase Branch

- 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

(c) $t^* = 4.7$

(e) $t^* = 9.4$

HPC-CFD: FLEXI

- Parallelization with the MPI paradigm
 - Domain decomposition using a space-filling curve
 - Communication latency hiding by local work
 - DGSEM operator requires only com. of surface fluxes
 - Small communication stencil
- Parallel I/O
- Small memory footprint
- Efficient cache usage at about 2000 DOF/core
- Excellent scaling up to over 10⁶ cores
- Transition in HPC architecture requires support of accelerators (e.g. GPUs)

Simulation software: FLEXI Postprocessing & visualization

A UQ-HPC Framework for Icing

Intrusive and Non-Intrusive UQ

(a) Mean

Non-Intrusive / NISP, MLMC

Intrusive / SG

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Uncertainty Quantification for Direct Aeroacoustic Simulations of Cavity Flows

Thomas Kuhn, Jakob Dürrwächter, Fabian Meyer, Andrea Beck, Christian Rohde and

Claus-Dieter Munz

A high-order stochastic Galerkin code for the compressible Euler and Navier-Stokes equations

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(b) Standard Deviation

Fig. 6. Spacecraft: mean and standard deviation; Mach number on spacecraft surface, pressure in slice through flow field. Example 5.4.

Accelerating Monte Carlo

Multilevel MC:

- Cheap models: coarse mesh resolutions
- Driving factor: Mesh convergence

Multifidelity MC:

- Cheap models: arbitrary correlated models
- Driving factor: Model covariance

- Wall-resolved LES of the clean geometry: an HPC problem
- Optimal number of samples is solution dependent!
- HPC challenge: Extreme simulation cost variations
- We need millions of computations

POUNCE (Propagation Of Uncertainties)

DOI: 10.21105/joss.04683

 Fully automated model management framework for UQ on HPC systems (OpenSource)

- runs multiple iterations with different models:
 Optimal stacking according to length and size
- Common MPI Communicator & common IO
- each model includes pre- and post-processing
- focus on efficient machine use: different machines via ssh
- Object-oriented Python, modular Design
- NISP, MLMC, MFMC Hazel Hen, HAWK, local cluster

PoUnce: A framework for automatized uncertainty quantification simulations on high-performance clusters

Jakob Duerrwaechter $^{\bullet\,1\P}$, Thomas Kuhn¹, Fabian Meyer², Andrea Beck^{1,3}, and Claus-Dieter Munz^1

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Structured Grid Algorithm

Grid: Results

Simulation Setup

Baseline Simulation

- Laminar flow airfoil
- 3D wall-resolved LES
- Low Reynolds number
- Minimal required resolution

Parameters	
Re	500.000
AoA	3°
Δy_{wall}^+	≈ 4
n _{elems}	190.000
N_{DG}	5
$t_{ m end}$	$10 d/u_{\infty}$
computation time	\approx 40.000 CPUh

Uncertainty Quantification

• NISP

- Two PCA modes, $N_{stoch} = 4$
- 25 LES
- 0.5 M CPUh
- MLMC
 - 3D $N_{DG} = 5, 3, 1$
 - 16 // 63 // 406 simulations
 - 1 M CPUh
- MFMC
 - 3D $N_{DG} = 5 // 2D N_{DG} = 5, 3, 1$
 - 23 // 174 // 587 // 3676 simul.
 - 1 M CPUh

Iced Airfoil Performance

FLEXICE: towards Multi-X/UQ

ML: SL + FLEXI

Data-informed Shock Capturing for High Order Methods

- Stable numerical approximation through Shock Capturing: improves stability, decreases
 accuracy: use sparingly!
- Detecting the occurrence of shocks: non-trivial, empiricism, many parameters
- For HO methods: Just detecting a "troubled cell" is not good enough: We need localization on the element subscale

Data-informed Shock Capturing for High Order Methods

- Supervised learning of a classifier from analytical smooth and non-smooth data
- Convolutional neural networks for spatial correlations
- About 100,000 samples per class, classes balanced
- Train/validate/test split
- Cross-entropy loss, ADAM optimizer, minibatch GD
- Tensorflow 1.6, coupled to FLEXI
- Resulting F1 score > 0.96

Data-informed Shock Capturing for High Order Methods

- Multiscale-CNNs for edge detection
- Consistent subscale localization, contiguous shock fronts: On different grids, for different problems (same model)
- On "bad but practical" grids: stable & accurate

Localized AV for shock capturing

 Use prediction of "shocked nodes" (binary edge map) and smooth with high order Radial Basis functions (RBF) interpolation

$$\mu_a(ec{x}) = \mu_{a ext{scale}} \sum_{i=1}^{n_s} lpha_i \phi_r \left(\|ec{x} - ec{x}_{s_i}\|_2
ight),$$

- With ϕ being the chosen RBF, α_i as interpolation coefficients and the spatial position of the inner-element solution nodes labeled "shocks" as \vec{x}_{s_i}
- This leads to a global, but weakly coupled Vandermonde matrix.
- Solve linear system with PETSc or approximate as local problems (compact support)

ML: RL + FLEXI

The Scale Gap in Turbulence

Large Eddy Simulation - Definition

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

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

- Joined Δr and h
- Implicit filtering: $h \not\rightarrow 0$
- Discretization scheme defines filter kernel

99.5% on google scholar, 100% for "industrial" LES

"Same equations, domains, models..."

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

 Commutation introduces errors: IFF isotropy, homogeneity, linearity of the filter are given and grid and filter are completely separated, then the closure term is:

LES Closure Terms: Supervised learning

- Turbulence is a non-local phenomena: Pointwise data only not sufficient
- LES closure term prediction from spatial (CNN) or temporal (GRU/LSTM) data
- 99.99% CC, error < 0.01%

LES Closure Terms: Supervised learning

- Directly close LES equations with ML-learned Reynolds forces
- Implicitly filtered LES: Expected stability problems
- Incorporating physical constraints and ML stabilization for uncertainty estimation helps

LES Closure Terms: Supervised learning

- Turn the ML prediction into a useful model:
 - include dissipation constraint from TKE in cost function
 - project forces prediction on stable basis
- Eddy viscosity approach with adaptive viscosity in space and time

 $\widetilde{R}(F(\overline{U^{i}})) - \overline{R(F(U^{i}))} \approx \mu_{ANN} \ \widetilde{R}(F^{visc}(\overline{U^{i}}, \nabla \overline{U^{i}}))$

Control Problems

 How to model decisions in dynamical systems under uncertainty?

Credit: Department Safety Critical Systems & Systems Engineering, DLR

Learning for dynamical systems

Learning for dynamical systems

- Simulations are (discrete) dynamical systems
- RL is a different paradigm from ML: Learning to take optimal actions in a dynamical system from experience (on the coarse level)
- Supervised learning has two problems: How do we define a lot of true data and make models robust?
- Reinforcement Learning is the method behind the recent successes: Self-Driving Cars, Autonomous Robots, AlphaGo, Starcraft, ...

$$\widetilde{R}\left(U_{L}, x_{L}, t_{L}
ight) = -\widetilde{M}\left(U_{L}
ight)$$

ML with Solver-in-the-loop: discretization-awareness

An Example: RL for LES closures

- Turbulence is a prime example of the scale gap
- We need models to augment the coarse-grained equations (LES & RANS)
- We can formulate this as an RL problem: Find a strategy for choosing the best model

Formulation

Environment

 a_t

Environment

- Implicitly filtered LES with High-Order DG scheme.
- Homogeneous Isotropic Turbulence ("Turbulence-in-a-box"), $Re_{\lambda} = 180$
- Periodic boundaries
- Forcing for statistically stationary flow

Reward

- Reward based on error in spectrum of turbulent kinetic energy
- Spectrum of precomputed DNS as target
- Reward scaled to $\mathbf{r_t} \in [-1,1]$ with exponential function

Simulation software: FLEXI Reinforcement learning framework – ReLeXI¹

- Distribution on hybrid HPC systems via the SmartSim Library²
- 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
- Easily extendable to other codes

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

Relexi Framework

- The framework scales well over many parallel runs
- We can efficiently evaluate each policy to get reliable gradients
- We can run many samples in parallel

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.

Results

Results

Results

• Optimal model for different discretizations

Summary

- Supervised learning of models with guarantees can successfully augment CFD codes
- Examples: Data-driven shock capturing for DG, turbulence closures
- Learning tasks that can be framed as MDPs: Reinforcement learning
- RL can learn from uncertainty, non-linear environments but needs lots of runs to gather experience: HPC
- We have developed a framework for coupling PDE solvers with RL on HPC systems in a plug-and-play style
- With this, we can derive optimal, discretization-specific strategies for turbulence closure
- Generally: an optimizable PDE solver

More Information

- UQ
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- Supervised Learning

- Reinforcement Learning •
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Thank you!