AI super-resolution-based models for turbulence and combustion

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Predictive Large-Eddy Simulations (LESs)

- Fighting climate change requires many new/optimized technologies. E.g.:
  - more efficient engines
  - more efficient turbines
  - hydrogen as fuel
  - ammonia as fuel
- ➢ This is only efficiently possible with predictive simulations supporting the development and design process
- ➢ Data-driven subfilter models for LES

- Use high-fidelity direct numerical simulation (DNS) data to train data-driven subfilter models for complex LES
- Examples include simple turbulence data but also more complex data, such as breakup data used to model the fuel injection

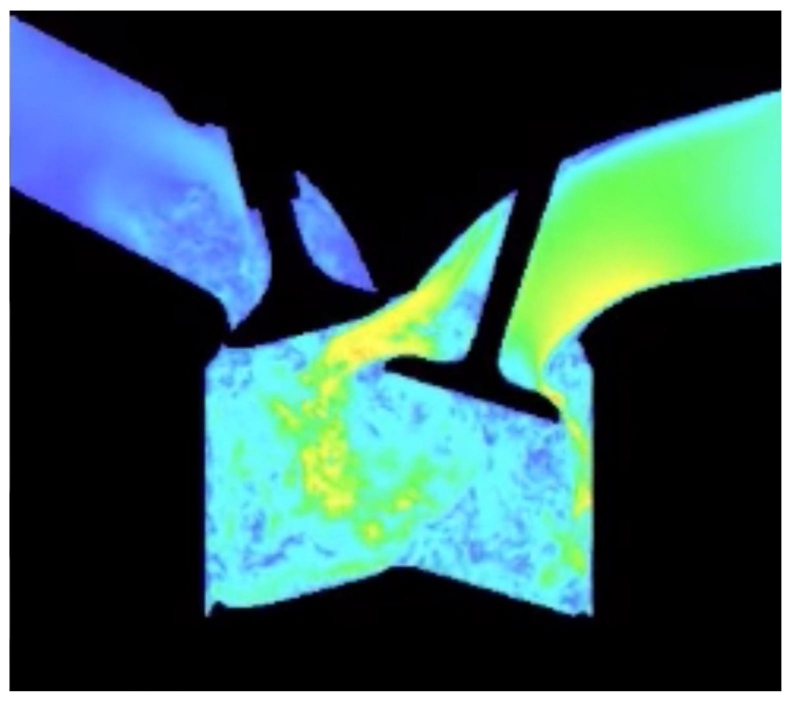


Fig. 1: Visualization of breakup DNS data (left) and complex engine LES (right). The highly-resolved DNS data can be used to train a data-driven subfilter model, which is then used to accurately model fuel injection in the LES.

Closing Algorithm

- Filtered/LES equations contain unclosed terms (red) which need to be modeled

$$(\Phi)_t + \boldsymbol{u}\cdot\nabla(\Phi) = D\nabla^2(\Phi) + \dot{\omega}_\Phi$$

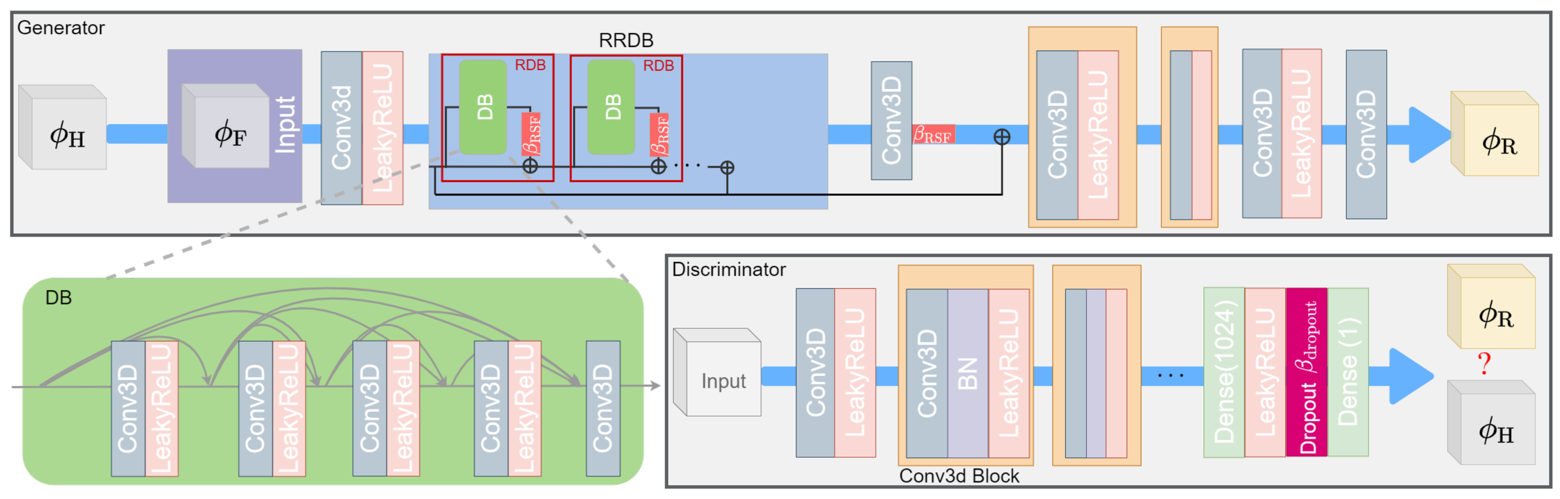
$$\rightarrow (\widetilde{\Phi})_t + \boldsymbol{u}\cdot\nabla(\widetilde{\Phi}) = D\nabla^2(\widetilde{\Phi}) - \widetilde{u''\cdot\nabla(\Phi'')} + \widetilde{\dot{\omega}_\Phi}$$

- Closure is done on reconstructed data fields which are generated by deep learning network called PIESRGAN

1. Use the PIESRGAN to reconstruct Φ_R^n from Φ_{LES}^n.
2. Use Φ_R^n to update the primary species fields of Φ to $\Phi_R^{n;\text{update}}$ by evaluating the source terms and solving the unfiltered scalar equations on the mesh of Φ_R^n.
3. Use $\Phi_R^{n;\text{update}}$ to estimate the unclosed terms Ψ_{LES}^n in the LES equations of Φ by evaluating the local terms with $\Phi_R^{n;\text{update}}$ and applying a filter operator.
4. Use Ψ_{LES}^n and Φ_{LES}^n to advance the LES equations of Φ to Φ_{LES}^{n+1}.

Alg. 1: AI super-resolution closing algorithm.

Phys.-Informed Enhanced Super-Resolution GAN (PIESRGAN)



$$\mathcal{L} = \beta_1 L_{\text{adversarial}} + \beta_2 L_{\text{pixel}} + \beta_3 L_{\text{gradient}} + \beta_4 L_{\text{physics}}$$

Fig. 2: Sketch of PIESRGAN and loss function.

Results

Dec. turbulence | Spray | Premixed | Non-Premixed

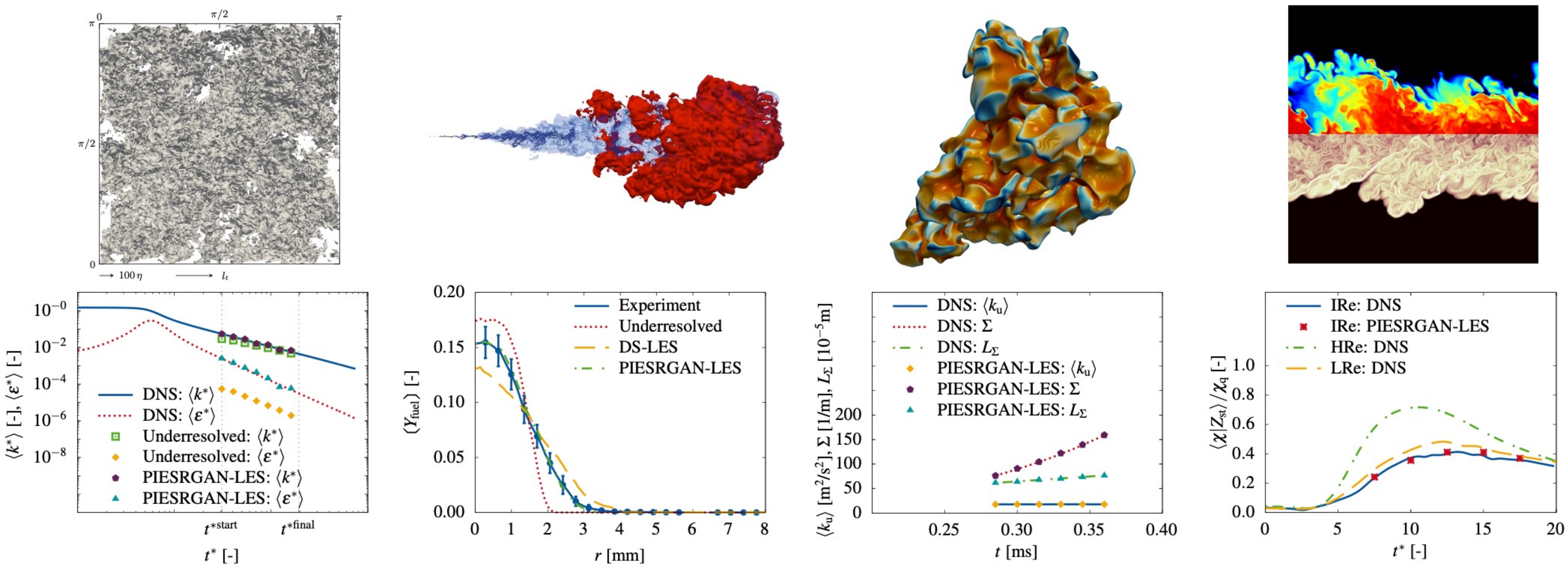


Fig. 3: Demonstration of PIESRGAN-subfilter accuracy in a posteriori tests of multiple complex flows.

Achievements & Conclusions

- Generality
- Efficiency
- Robustness
- Accuracy
- "Universality"

- PIESRGAN was developed and applied to multiple complex flows
- PIESRGAN-LESs result in predictive simulations with higher accuracy than classical LES for lower computational cost on state-of-the-art supercomputers
- As example, cycle-to-cycle variation in engine flame kernels were computed with PIESRGAN-LES as simulations were cheaper than DNS
- Training convergence is still the main challenge and subject to current work

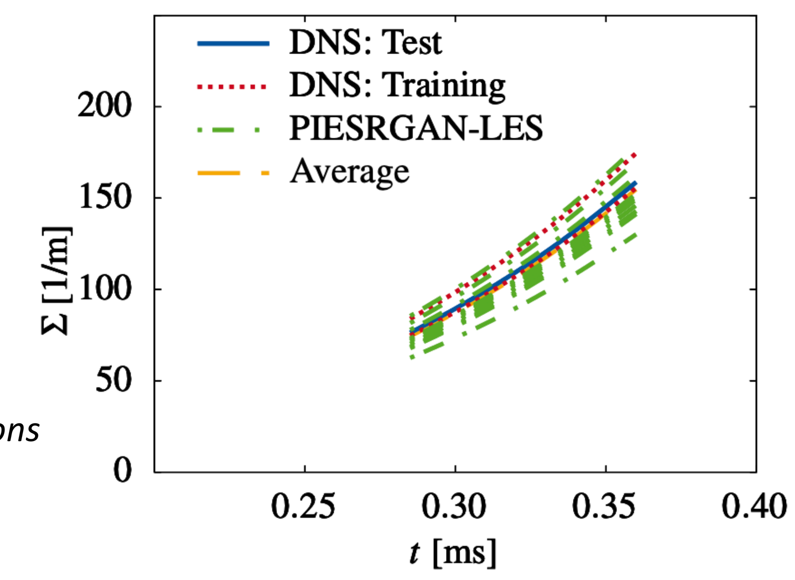


Fig. 4: Evaluation of cycle-to-cycle variations in engine flame kernels with PIESRGAN.

References (selection)

- Bode et al., Using physics-informed enhanced super-resolution generative adversarial networks for subfilter modeling in turbulent reactive flows, PROCI, 2021
- Bode et al., Applying Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks to Turbulent Premixed Combustion and Engine-like Flame Kernel Direct Numerical Simulation Data, PROCI, 2022
- Bode, Applying Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks to Finite-Rate-Chemistry Flows and Predicting Lean Premixed Gas Turbine Combustors, CNF (submitted)
- Bode, Applying Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks to Turbulent Non-Premixed Combustion on Non-Uniform Meshes and Demonstration of an Accelerated Simulation Workflow, CNF (submitted)

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