aPriori: a Python package to process Direct Numerical Simulations

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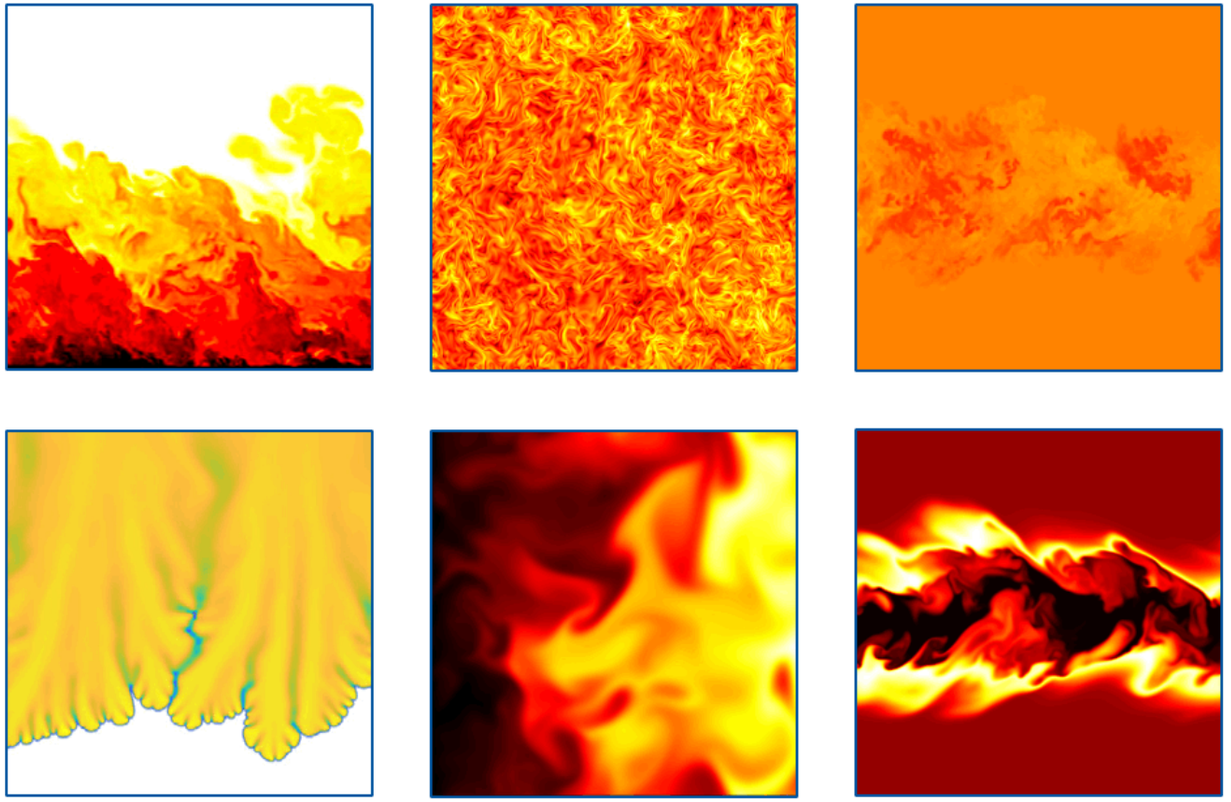
[1] ULB Université Libre de Bruxelles

[2] itv | RWTH Aachen University

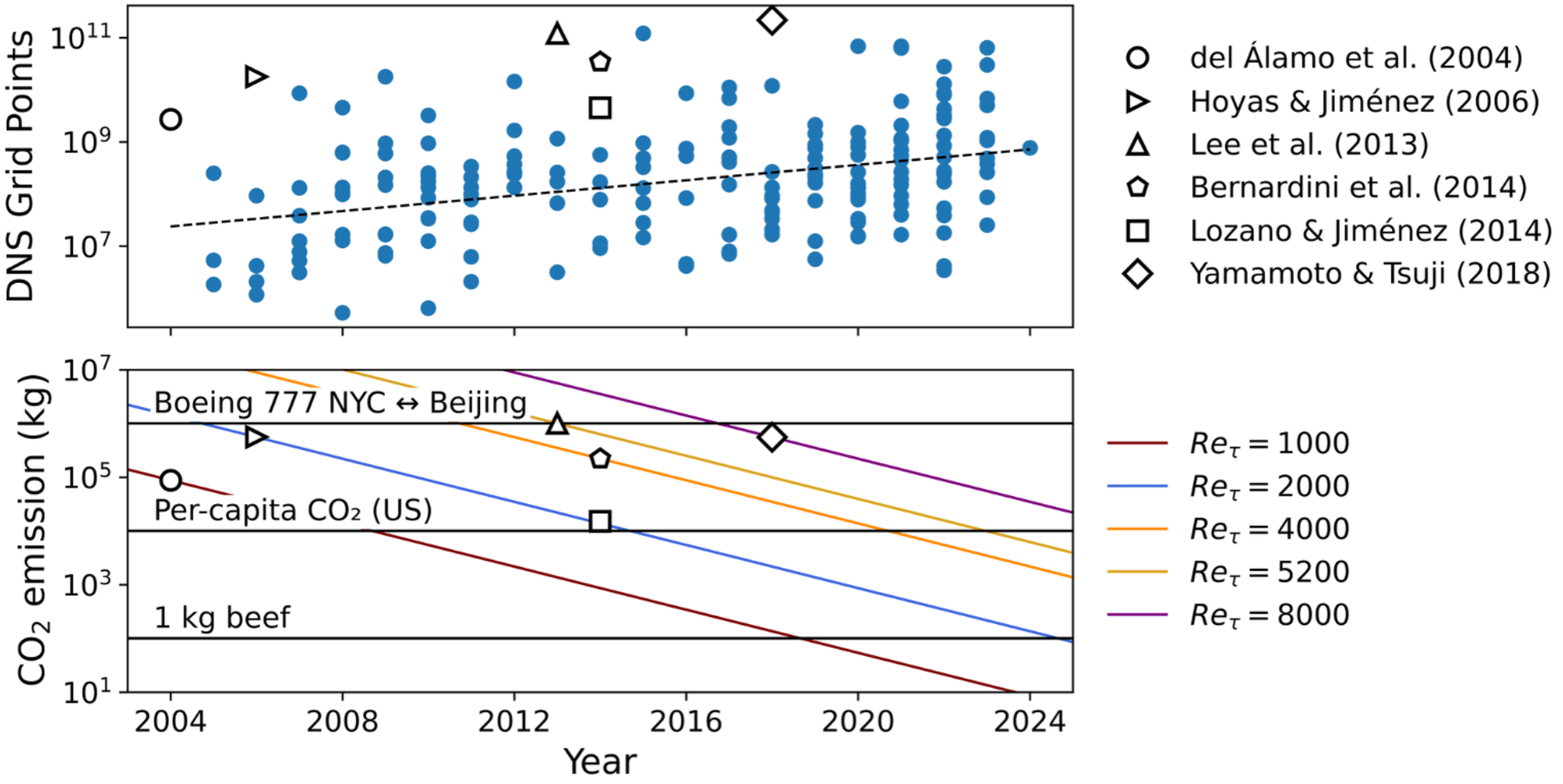
Direct Numerical Simulations (DNS) can provide highly detailed physical insights

- Boundary layer structure [1]
- Homogeneous isotropic turbulence [2]
- Thermo-diffusive instabilities in premixed laminar hydrogen flames [3]
- Soot emissions in methane diffusion flames [4]
- Non-conventional combustion regimes (MILD combustion) [5,6]



[1] Watanabe, T., Zhang, X., & Nagata, K. (2019). . *Computers & Fluids*.
[2] Gauding, M., Thiesset, F., et al. (2022). *Journal of Fluid Mechanics*
[3] Berger, L., Kleinheinz, K., Attili, A., Pitsch, H., (2019) . *Proceedings C. I.*
[4] Attili, A., Bisetti, F., Mueller, M. E., & Pitsch, H. (2014). *Combustion and Flame*
[5] Frascino, L., Scialabba, G., Chu, H., & Pitsch, H. (2025). Zenodo.
[6] Doan, N. A. K., Swaminathan, N., & Minamoto, Y. (2018). *Combustion and Flame*

DNS have a non-negligible impact on CO2 emissions



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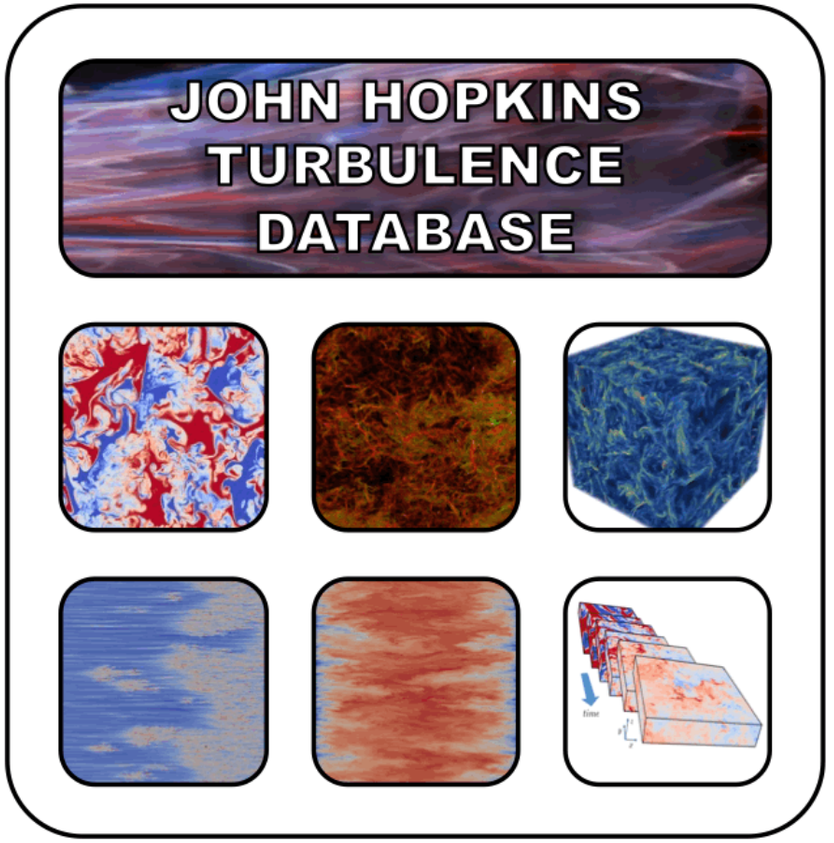
[1] X. Yang, W. Zhang, M. Abkar, W. Anderson. (2024). Journal of Renewable and Sustainable Energy.

Databases reduce the carbon footprint by avoiding redundant computations



- Focus on **non-reactive** cases,
- Large files, lots of timesteps available for **statistics**

~ 3.3 million metric tons of carbon emissions saved [1]

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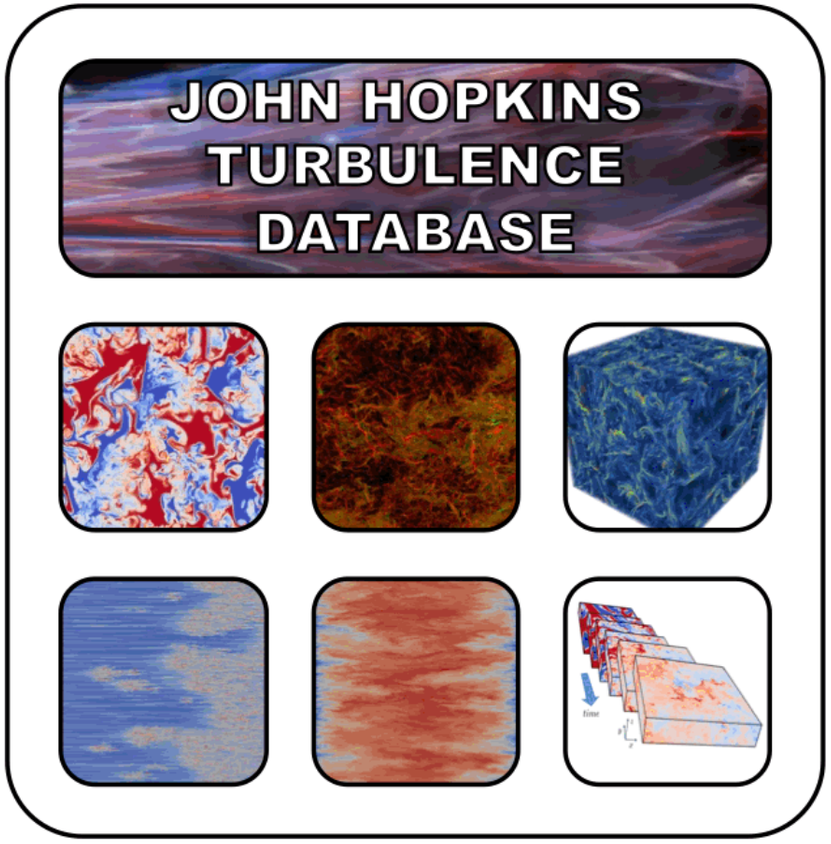

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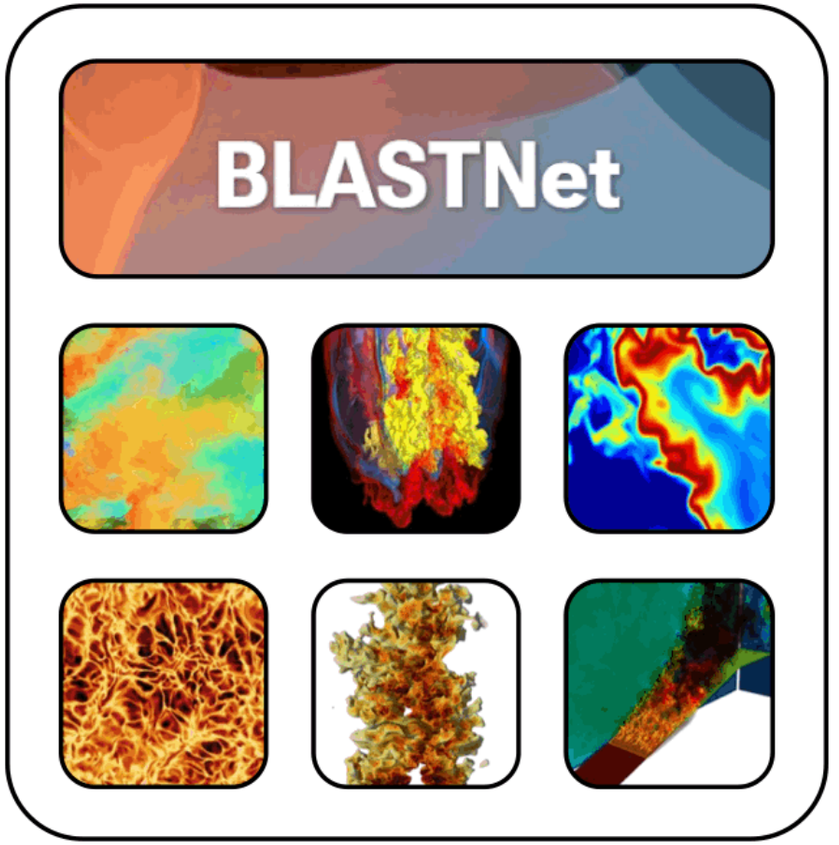

- Focus on datasets **diversity**
- Applications in **machine learning** for **reactive flows**

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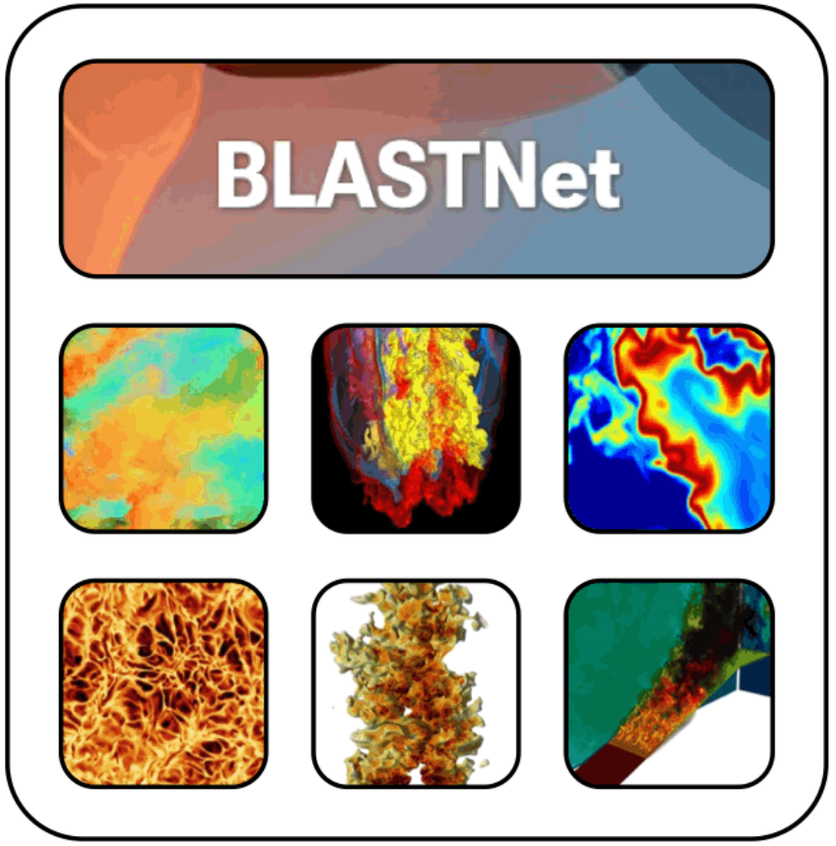
Shared DNS data still require notable post-processing

- **Ready to use**, labeled data
- Easy to handle, **accessible** dataset

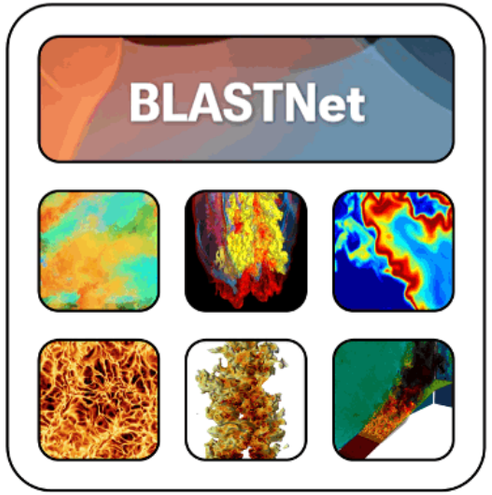


- Data to be **processed** (e.g. sub-filter closures)
- Large dimensions (up-to **100s GB**)

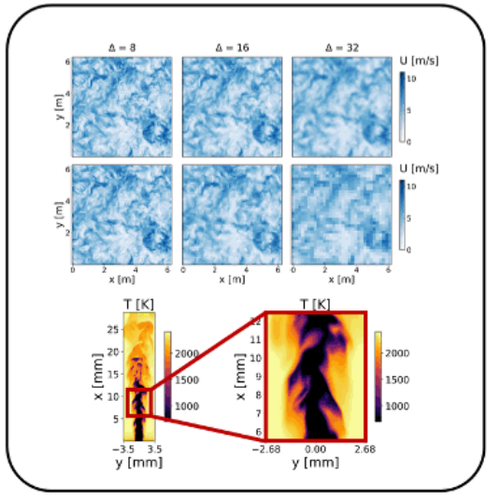
aPriori is an open-source python library to enhance DNS data accessibility

aPriori

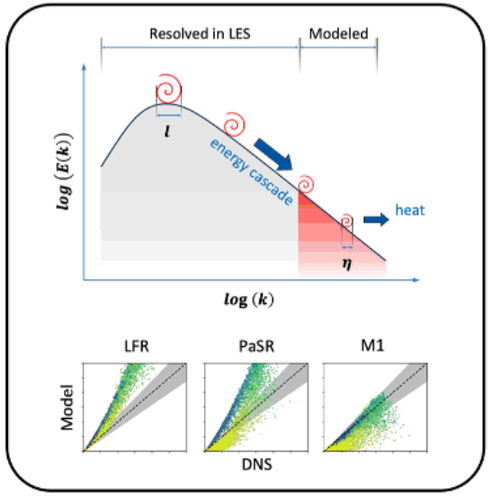
1. Handling large datasets from open-source repositories



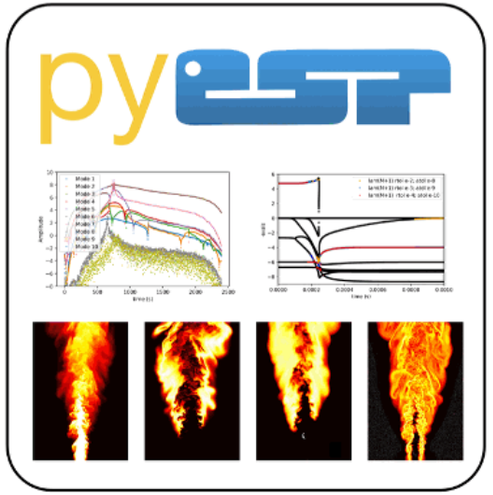
2. Filtering, downsampling, and sub-domain extraction



3. Sub-filter quantities and model assessment

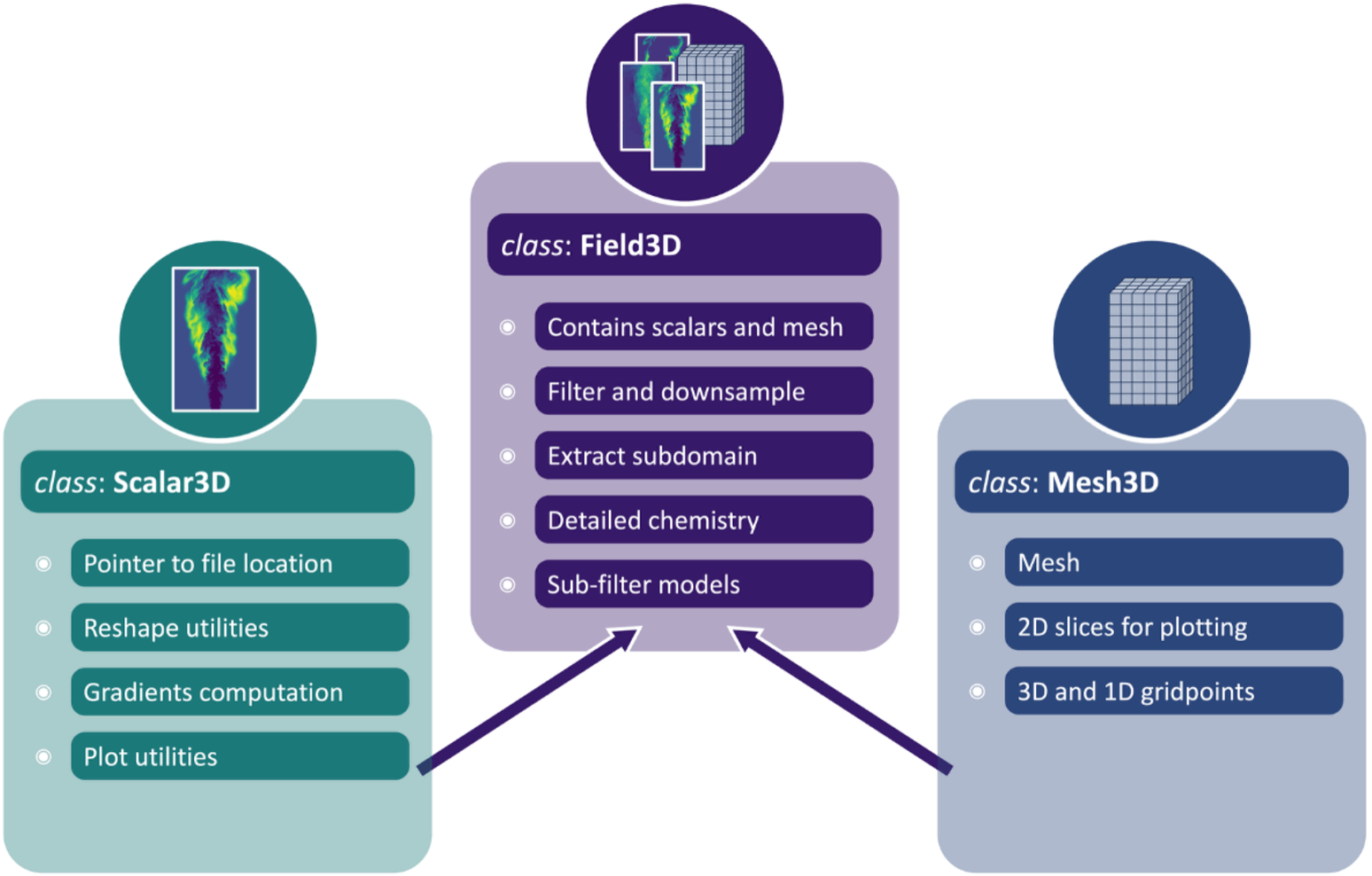


4. CSP and complex chemical analyses for reactive flows



The software architecture is modular and object-oriented

```
├── chem_thermo_tran
│   └── li_h2.yaml
├── data
│   ├── P_Pa_id000.dat
│   ├── RHO_kgm-3_id000.dat
│   ├── T_K_id000.dat
│   ├── UX_ms-1_id000.dat
│   ├── UY_ms-1_id000.dat
│   ├── UZ_ms-1_id000.dat
│   ├── YH2O2_id000.dat
│   ├── YH2O_id000.dat
│   ├── YH2_id000.dat
│   ├── YHO2_id000.dat
│   ├── YH_id000.dat
│   ├── YN2_id000.dat
│   ├── YO2_id000.dat
│   ├── YOH_id000.dat
│   └── YO_id000.dat
├── grid
│   ├── X_m.dat
│   ├── Y_m.dat
│   └── Z_m.dat
└── info.json
```



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  YH2_id000.dat
  YHO2_id000.dat
  YH_id000.dat
  YN2_id000.dat
  YO2_id000.dat
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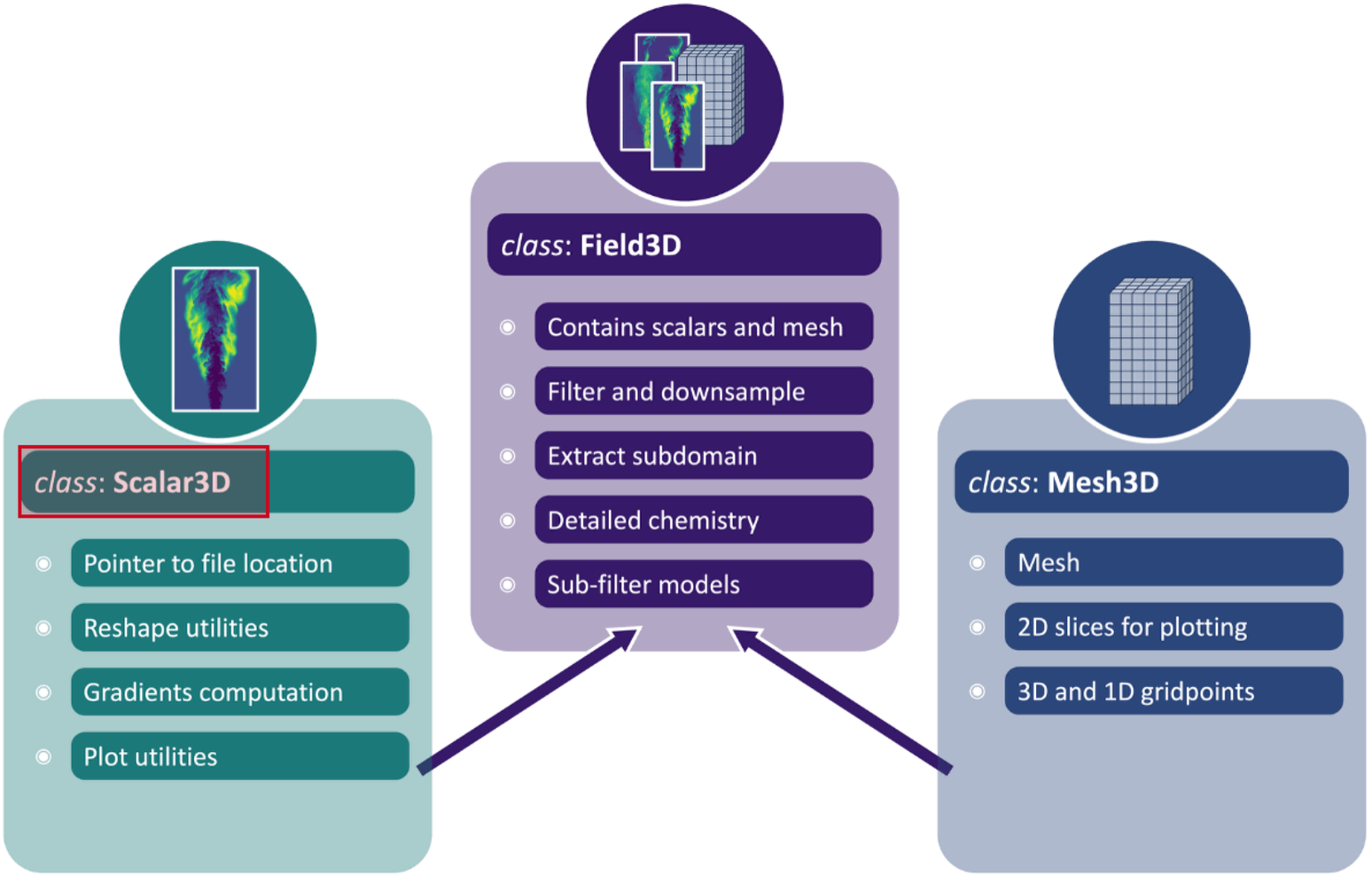

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  YH_id000.dat
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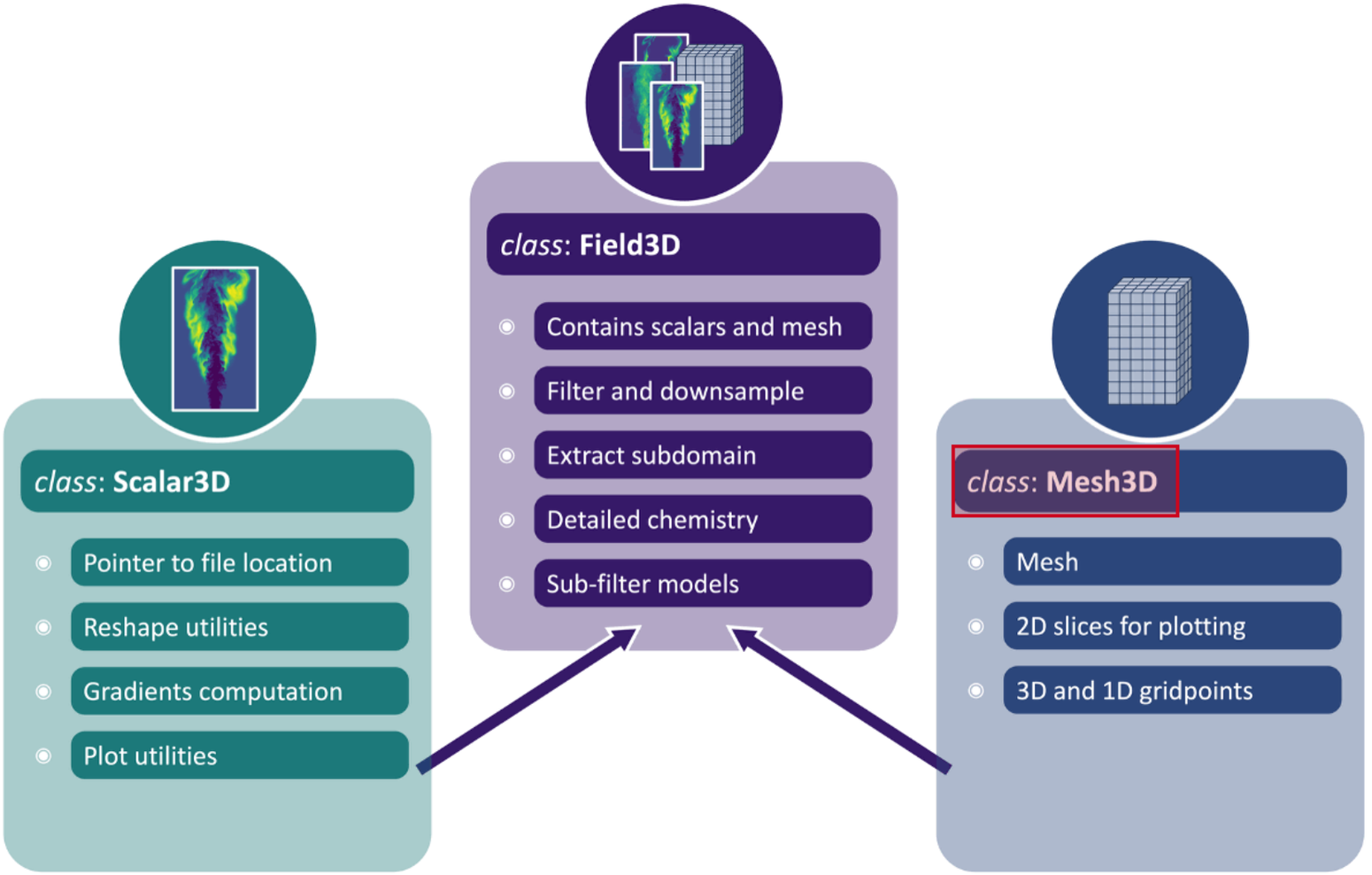

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  YH2O_id000.dat
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  YHO2_id000.dat
  YH_id000.dat
  YN2_id000.dat
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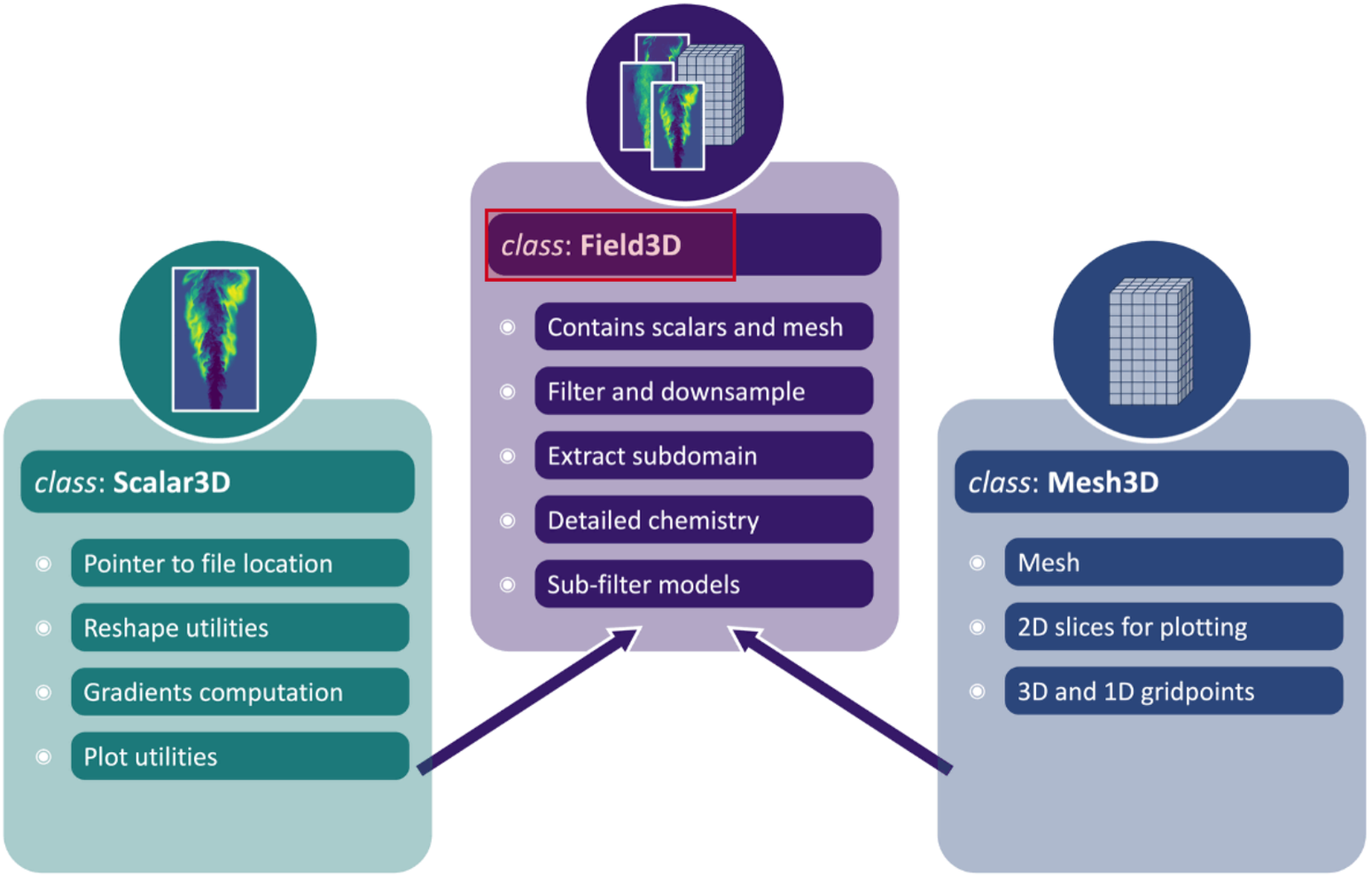

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    YHO2_id000.dat
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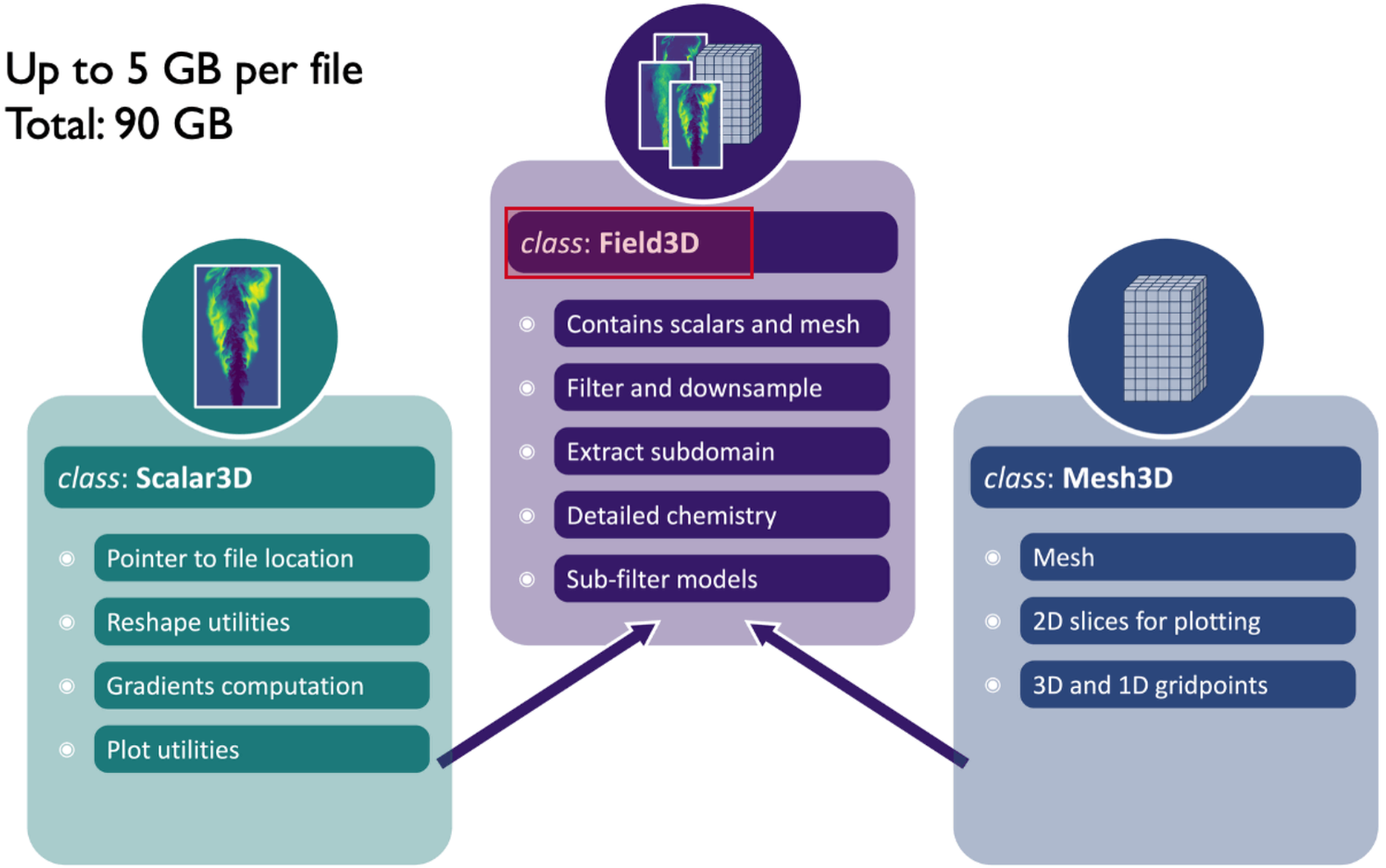
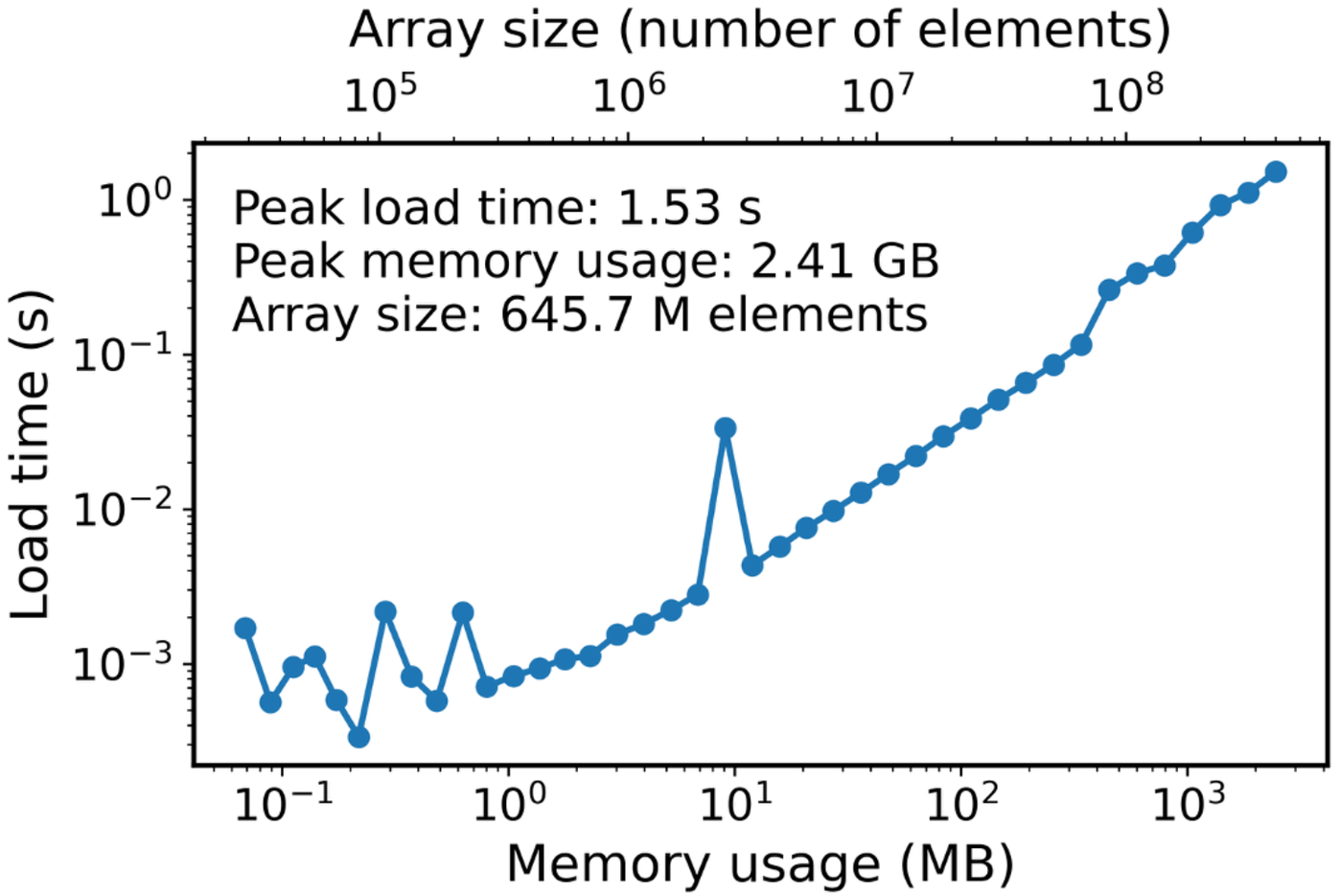
```

Up to 5 GB per file
Total: 90 GB



The load time for typical datasets sizes is in the order of seconds



Smagorinsky model assessment example

```
DNS_field = ap.Field3D('DNS_data')
```

```
DNS_data
└── data
    ├── P_Pa_id000.dat
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    ├── UY_ms-1_id000.dat
    ├── UZ_ms-1_id000.dat
    └── Y_id000.dat
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[1] Gauding, M., Thiesset, F., Varea, E., & Danaila, L. (2022). *Journal of Fluid Mechanics*

Smagorinsky model assessment example

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    ├── Y_id000.dat
    └── S_DNS_s-1_id000.dat
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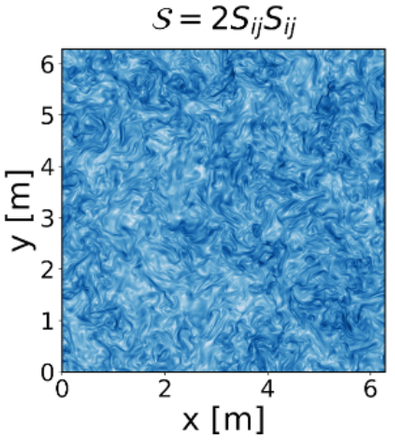

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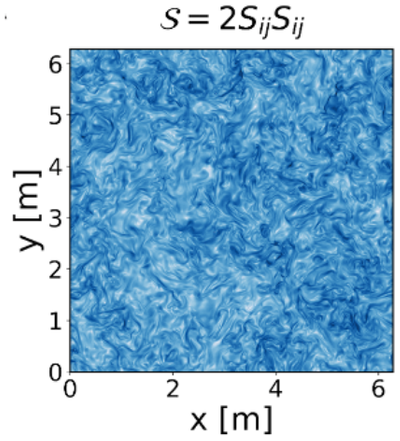


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Filter8Gauss
└── data
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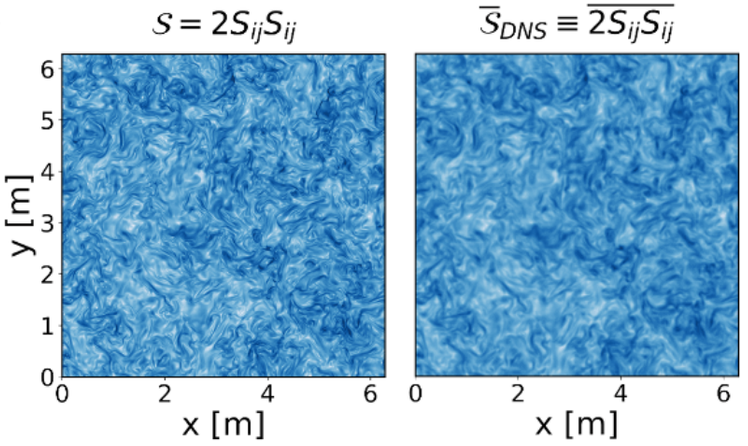
```

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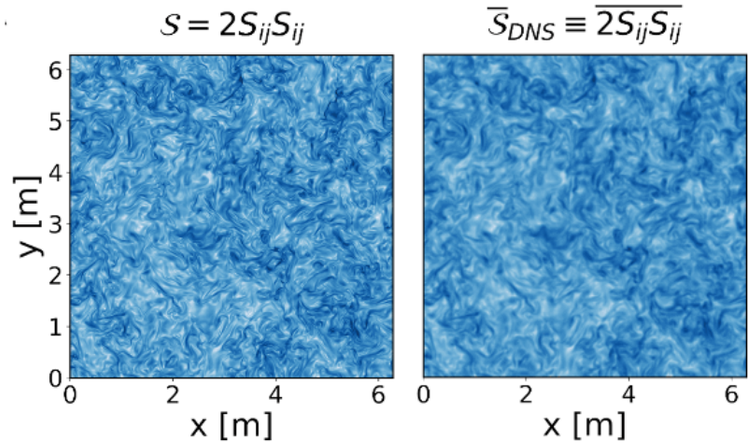


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    ├── P_Pa_id000.dat
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    ├── UZ_ms-1_id000.dat
    ├── Y_id000.dat
    ├── S_DNS_s-1_id000.dat
    └── S_LES_s-1_id000.dat
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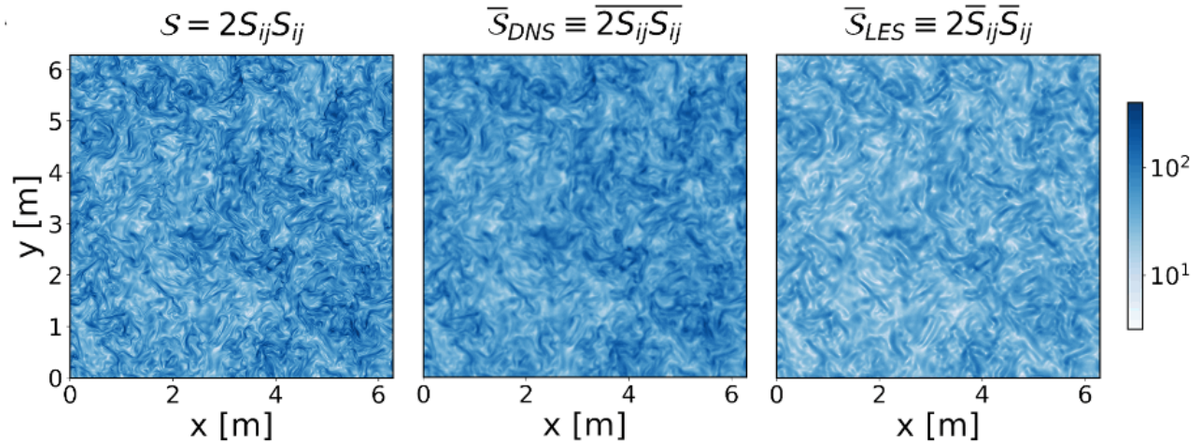


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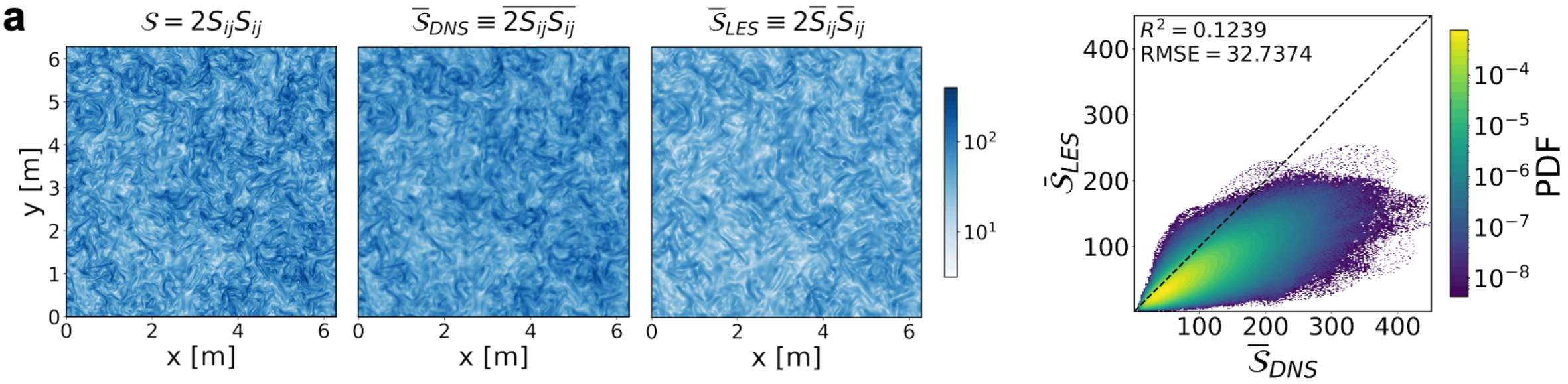

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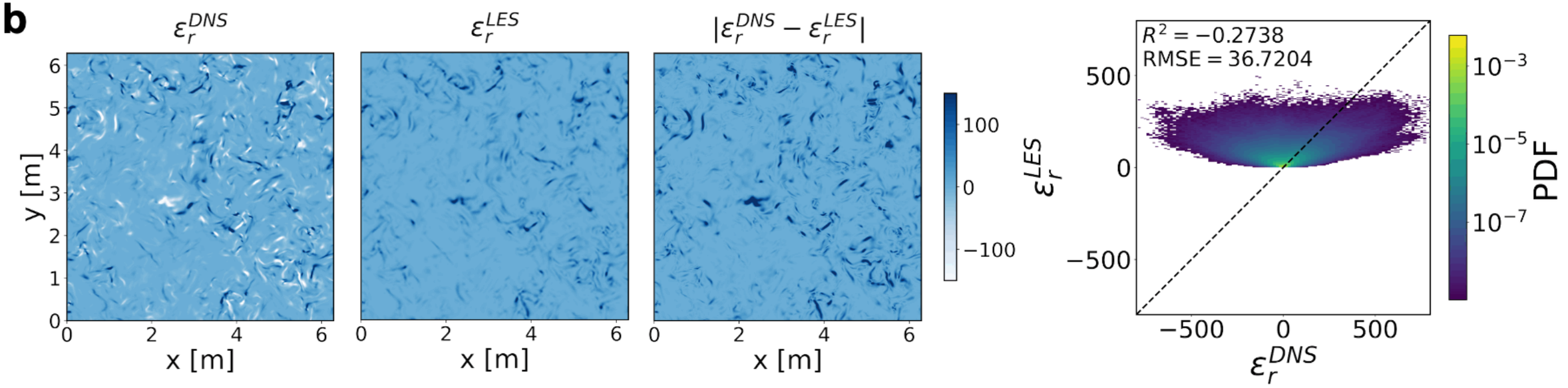

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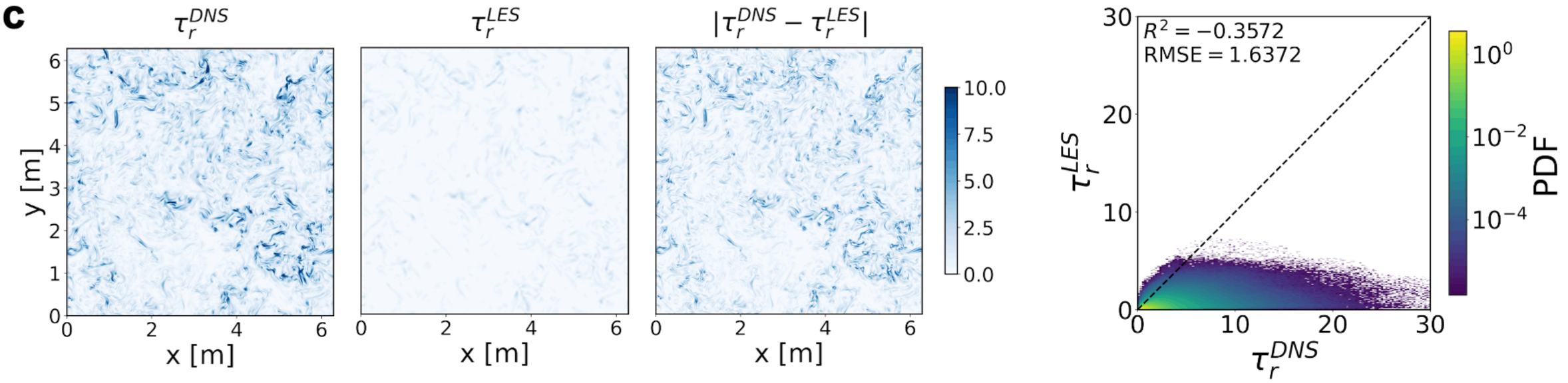

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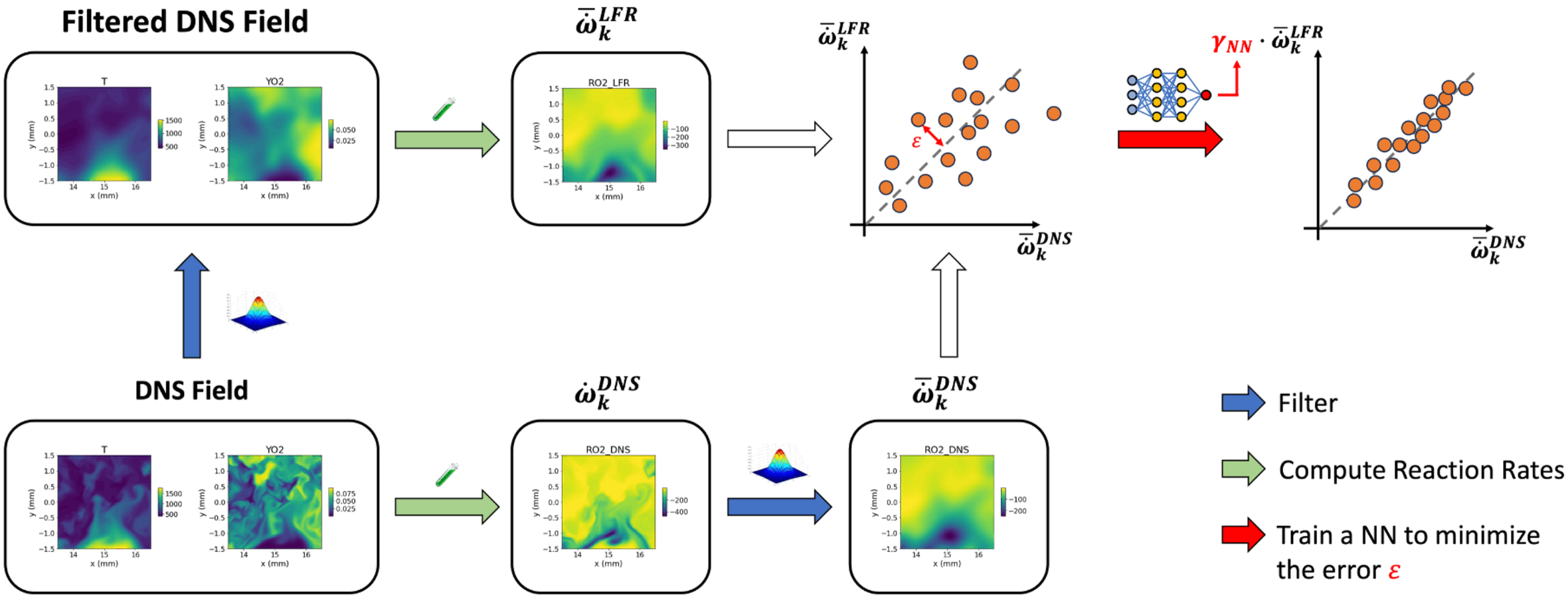
Turbulent combustion modeling with machine learning

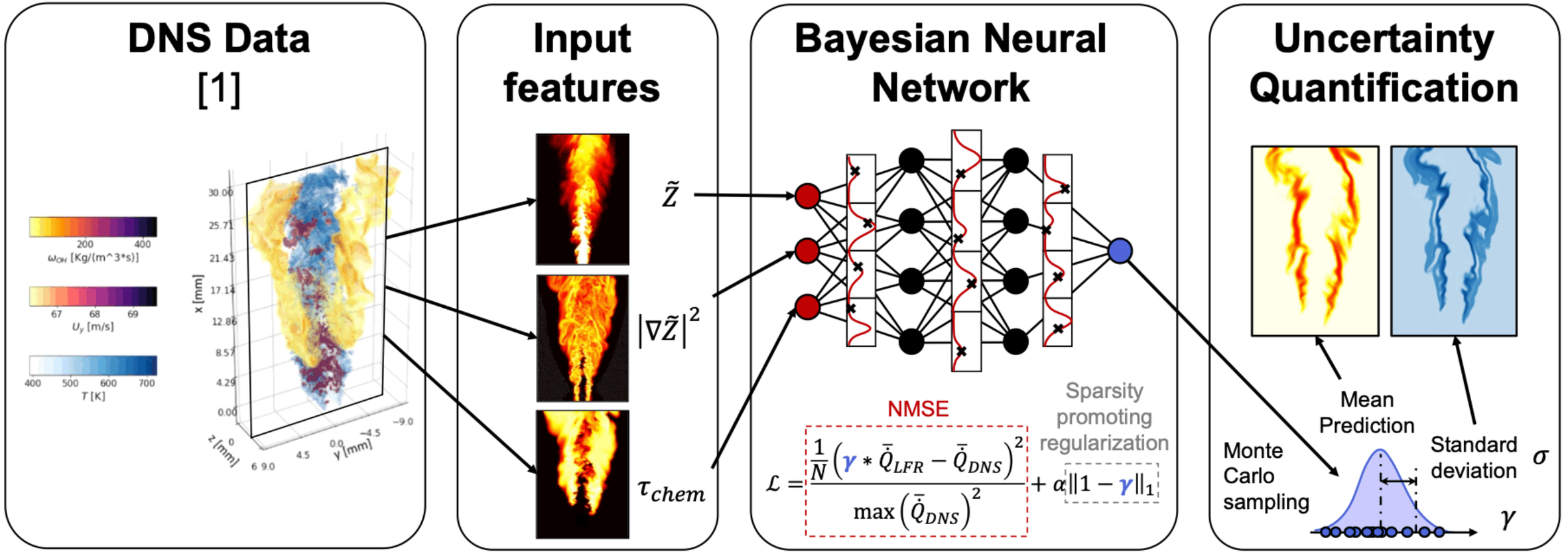


Filter

Compute Reaction Rates

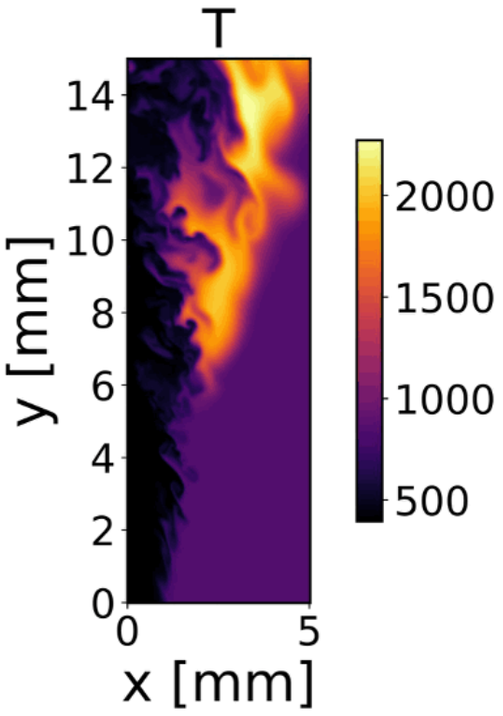
Train a NN to minimize the error ε

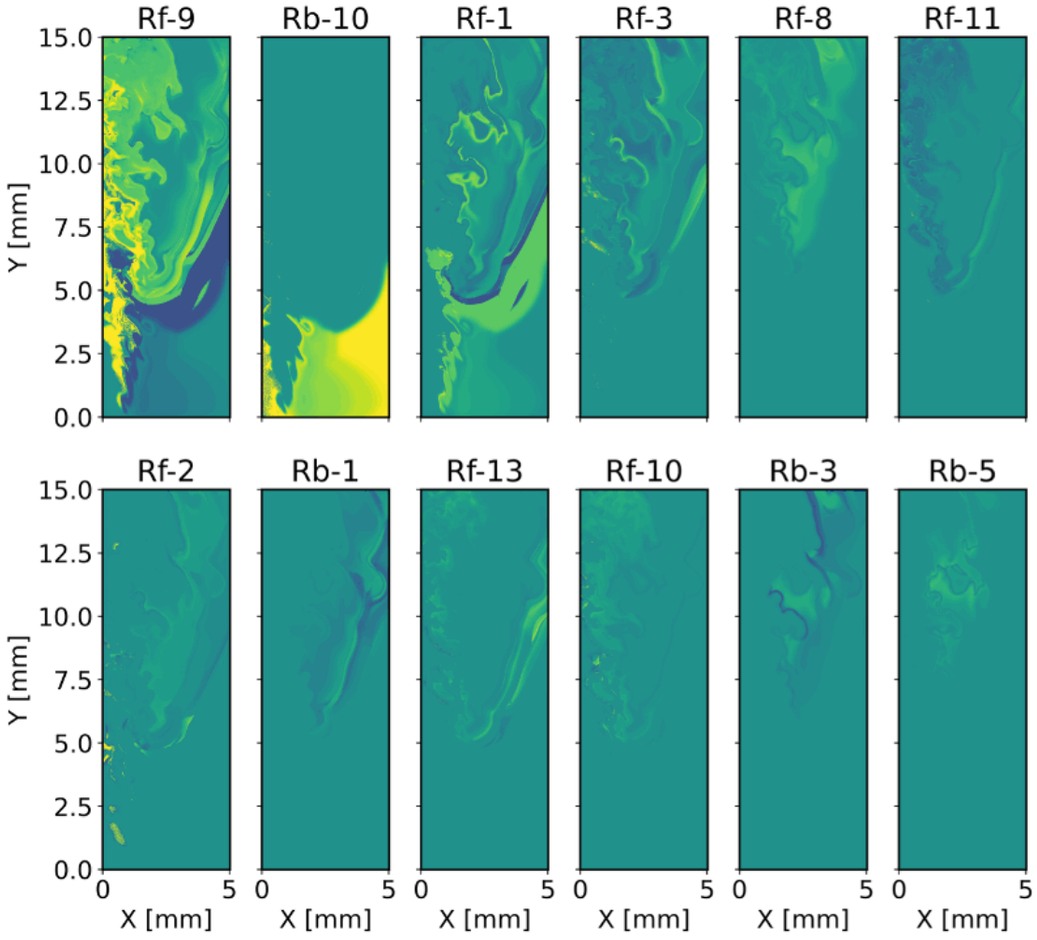
The library was used to process reactive DNS in previous research work

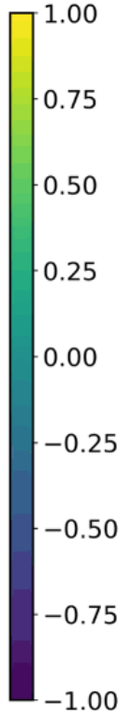


[1] Jung, K. S., Kim, S. O., Lu, T., Chen, J. H., & Yoo, C. S. (2021). Combustion and Flame.
[2] Piu, L., Péquin, A., Iavarone, S., Freitas, R. S. M., Jung, K. S., Chu, H., Pitsch, H., & Parente, A. (Year). 12th European Combustion Meeting.

Coupling with pyCSP allows complex chemical analyses







(Rf-9) H + O2 (+M) <=> HO2 (+M)

(Rb-10) H + HO2 <=> H2 + O2

(Rf-1) H + O2 <=> O + OH

(Rf-3) H2 + OH <=> H + H2O

(Rf-8) H + OH + M <=> H2O + M

(Rf-11) H + HO2 <=> 2 OH

(Rf-2) H2 + O <=> H + OH

(Rb-1) H + O2 <=> O + OH

(Rf-13) HO2 + OH <=> H2O + O2

(Rf-10) H + HO2 <=> H2 + O2

(Rb-3) H2 + OH <=> H + H2O

(Rb-5) H2 + M <=> 2 H + M

Institute for Combustion Technology, Université Libre de Bruxelles

[1] Jung, K. S., Kim, S. O., Lu, T., Chen, J. H., & Yoo, C. S. (2021). Combustion and Flame
[2] Malpica Galassi, R. (2022). Computer Physics Communications

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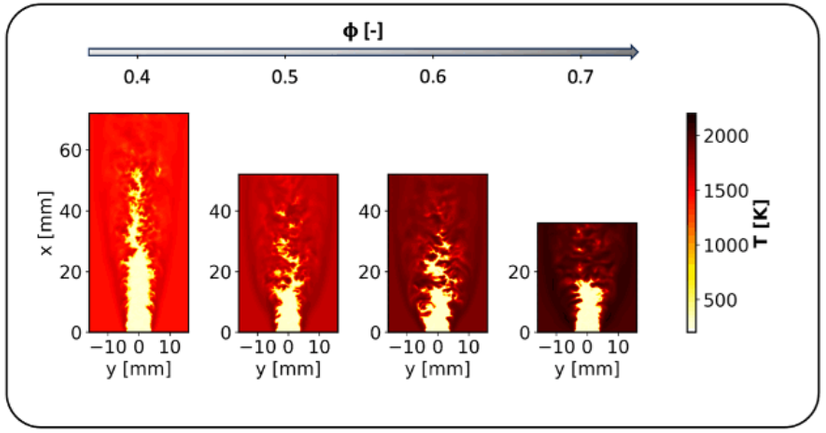
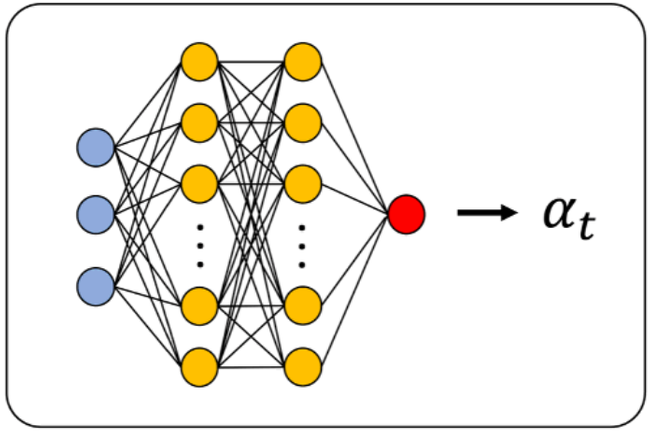
aPriori was largely employed to develop the CYPHER ML challenge (Friday)

Codabench

1. Training data processing



2. Online model training



3. Closure model evaluation

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{C}\right) + \nabla \cdot \left(\bar{\rho}\tilde{\boldsymbol{u}}\tilde{C}\right) =$$

$$\nabla \cdot \left[\bar{\rho}(\alpha_C + \alpha_t)\nabla\tilde{C}\right] + \bar{\rho}\dot{\omega}_C$$

The library aims at solving four main issues

1. Create a tool for BlastNet users to **streamline post-processing** and *a priori* sub-filter models validation

2. Enlarge big **data accessibility** leveraging pointers

3. Creating a Python **interface** which bridges the gap between CFD solvers (C++, Fortran) and modern statistics and machine learning libraries (Python-based). This allows connectivity with other libraries (Matplotlib, PyCSP…)

4. Perform **complex chemical computations** such as CSP or reactor-based models for sub-filter closures, thanks to the data-chunking implementation

Further improvements

- Enhance **gradient computation**
  - Implement more accurate and flexible gradient computation schemes
- Expand **visualization** capabilities
  - Add 3D visualization utilities
- Increase **modularity**
  - Support more abstract data types (e.g., vectors and tensors)
- Emphasize **open-source evolution**
  - aPriori is designed to evolve with community needs
  - Invites contributions and encourages a user-driven roadmap

Thank you for your attention 😃

Documentation website

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