Fast, data-assisted simulations of bubble transport in submerged double jets

Thomas Lichtenegger
6th K1MET Simulation Conference, Vienna, 23.4.2025

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Particulate Flow Modelling

Overview

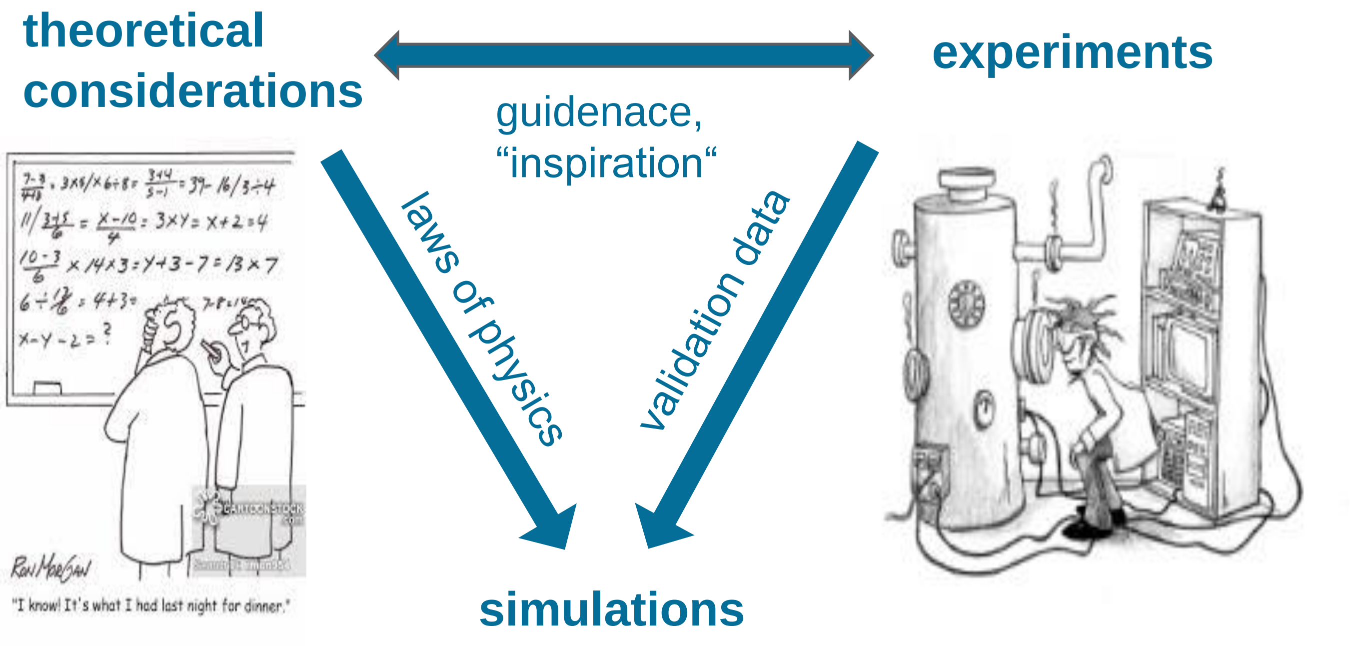
- Why do we need data-assisted simulation methods?
- Application case: Bubble transport in submerged jets
- Current activities: Towards real-time simulations of impurity transport and capture
- Outlook: Prevention of rare events

The need for data-assisted simulations

The importance of process simulations

Many industrial processes exhibt multiscale and multiphysics phenomena:

- complex systems
- difficult to describe accurately
- optimization ?
- novel, ‘green‘ processes ?



The challenge of multiscale flows

≈ 10^{-6} ... 10^{-3} m

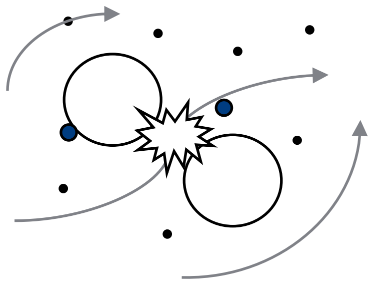
length scale

≈ 10^{0} ... 10^{1} m

time scale

≈ 10^{-6} s

EOMs known only at small scales

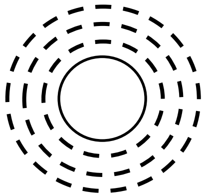


large N, V =
- large comp. costs
- lack of small-scale info

?

small Δt = short observations
current limit: a few minutes

≈ 10^{3} s



chem. reactions,
heat transfer

www.voestalpine.com

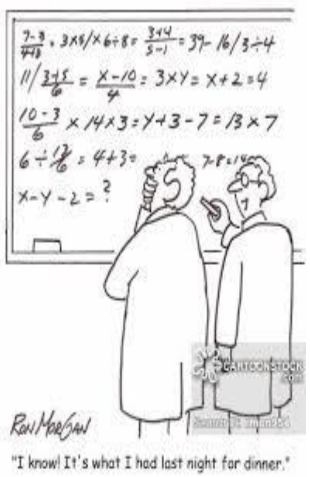
The importance of data for process simulations

Many industrial processes exhibit multiscale and multiphysics phenomena:

- complex systems
- difficult to describe accurately
- optimization ?
- novel, ‘green‘ processes ?

Microscopic EOMs not sufficient: data allow us to include meso and macro behavior!

theoretical considerations



experiments

guidenace, “inspiration“

laws of physics

validation data

online data

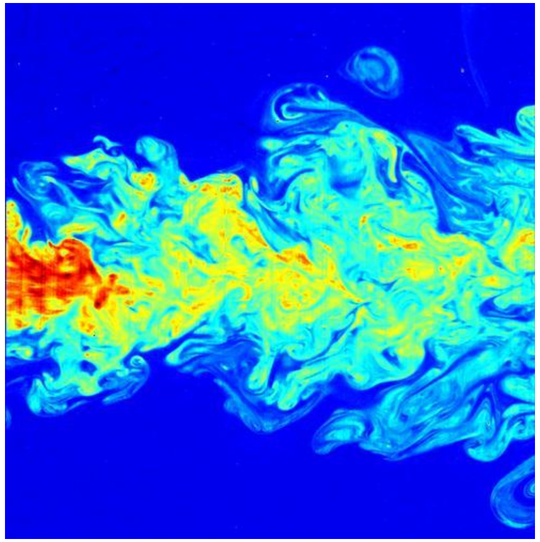
simulations:

real-time simulation

high-fidelity data

Strongly separated time scales

turbulence

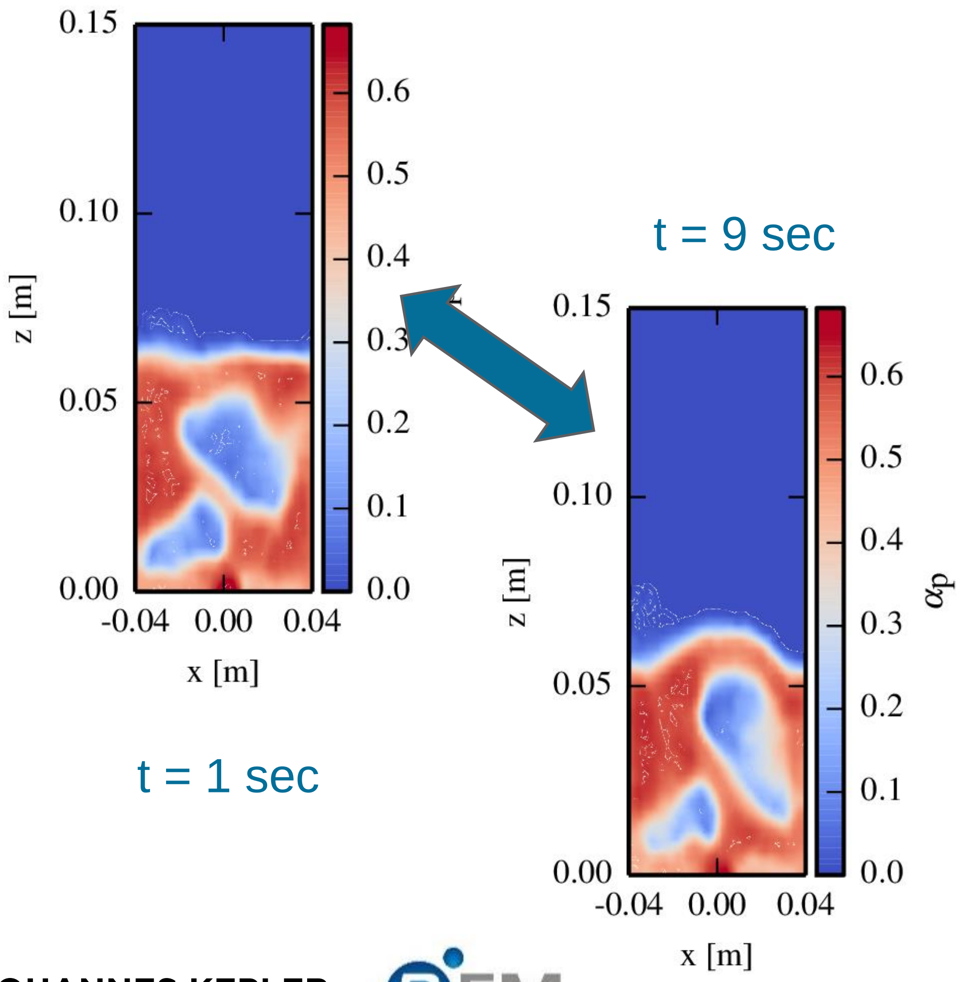


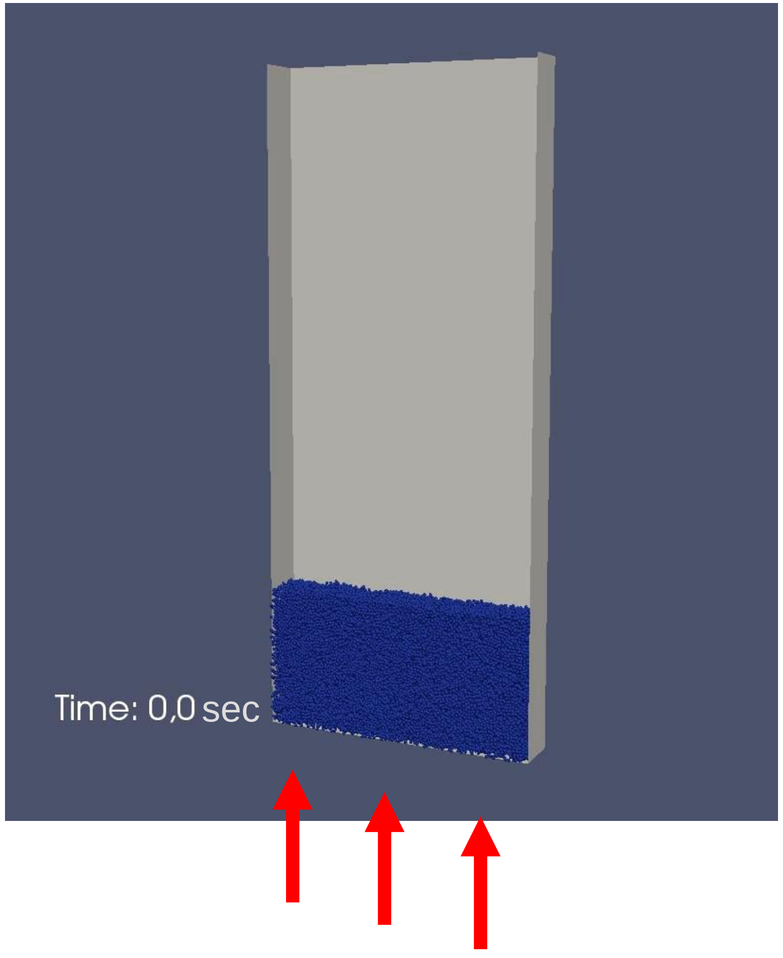
bubbly flows

particulate flows

common feature of many flows with separated time scales: **(transio-)recurring patterns**

An illustrative example: Fluidized particle beds



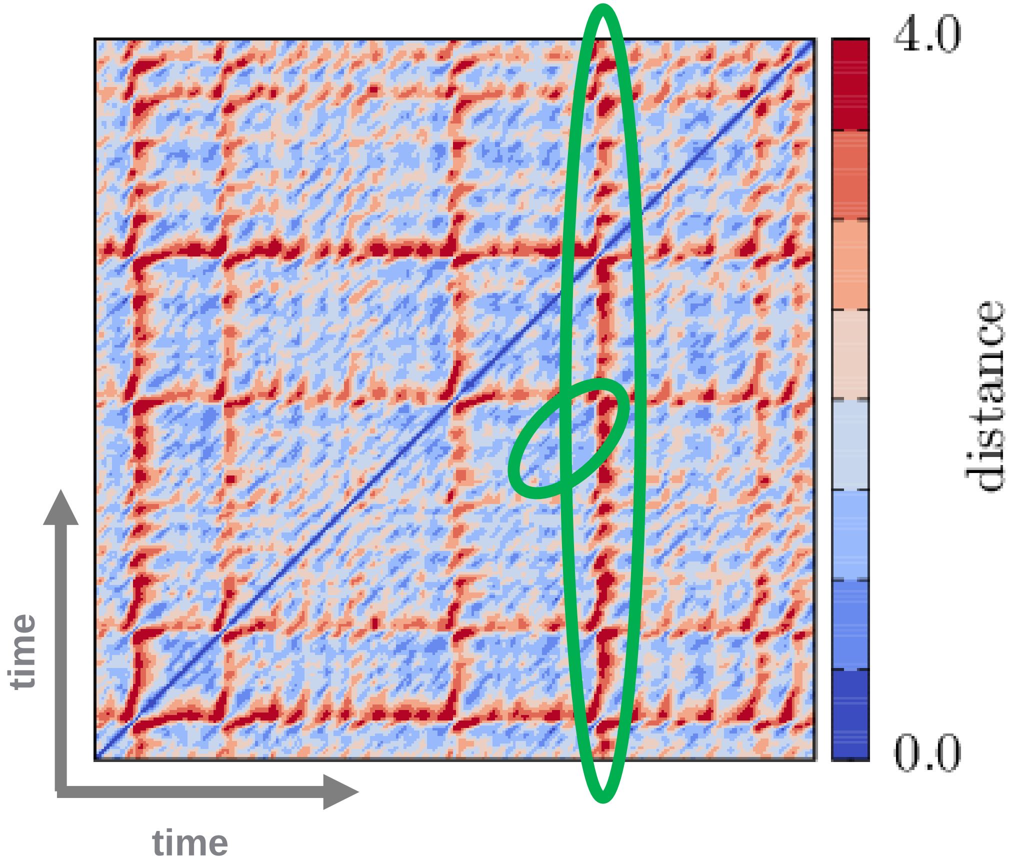


Extrapolation of recurrent dynamics

Recurrence plots[1] compare a system at two times based on some metric, e.g.

$$D(t_1, t_2) \propto \int d^3r \left(\alpha_\mathrm{p}(\mathbf{r}; t_1) - \alpha_\mathrm{p}(\mathbf{r}; t_2)\right)^2$$

visual representation of recurrences, rare events etc.

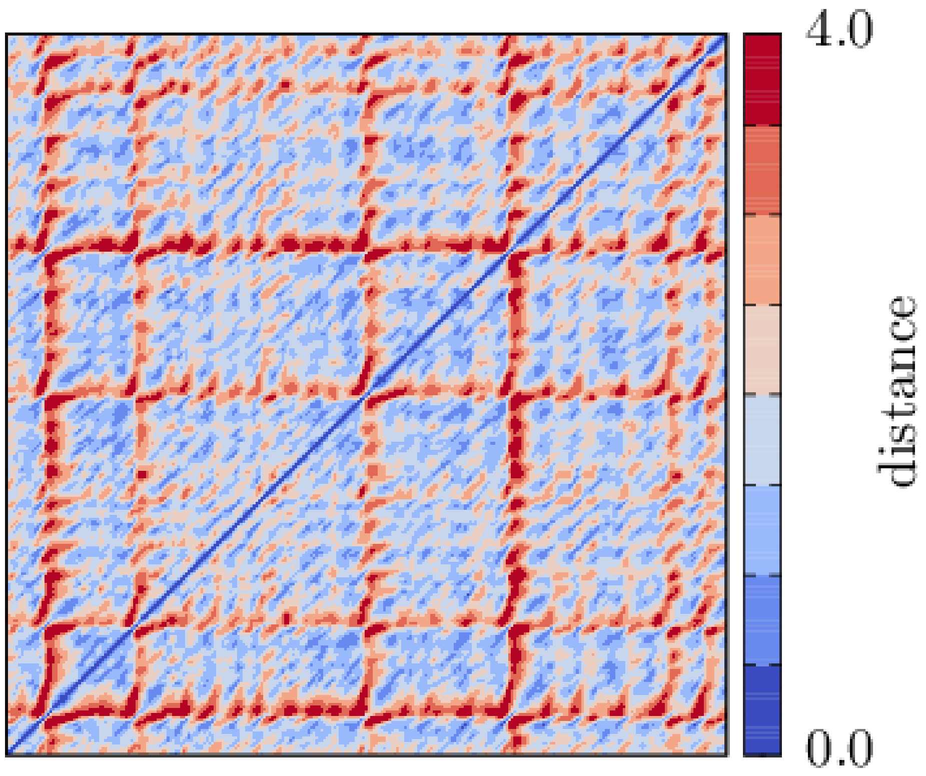


1. Eckmann et al. Europhys. Lett. 4 (1987)

Extrapolation of recurrent dynamics

Recurrence CFD[1] in a nutshell

0.) Create a short, high-fidelity time series of flow fields.



1. TL and Pirker, Chem. Eng. Sci. 153 (2016)

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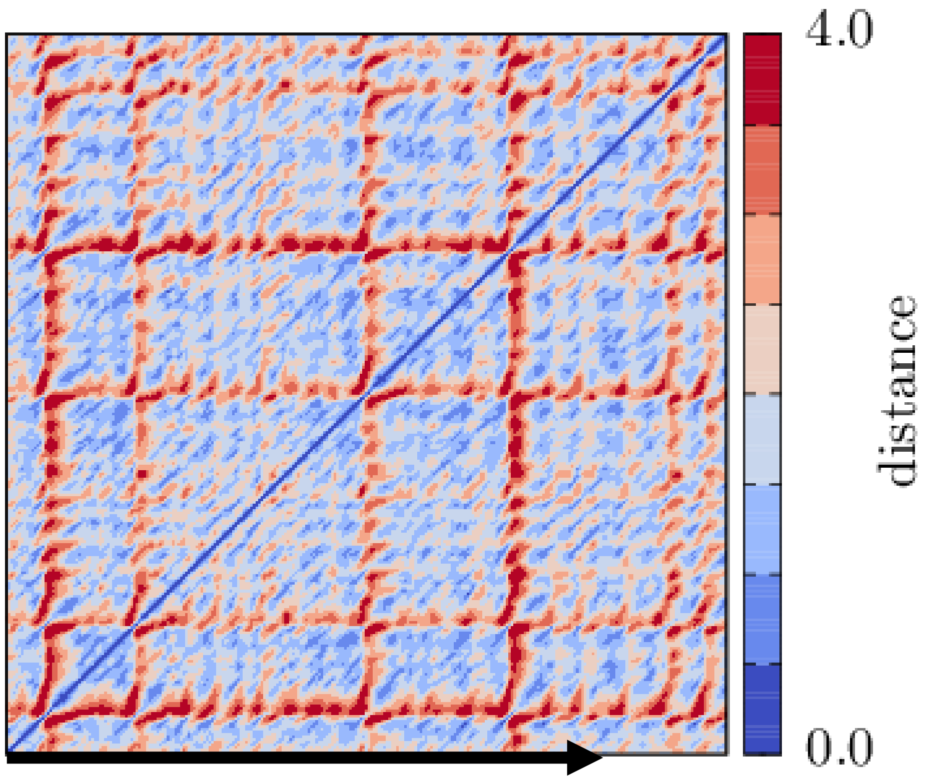
Extrapolation of recurrent dynamics

Recurrence CFD[1] in a nutshell

0.) Create a short, high-fidelity time series of flow fields.

1.) Take time-ordered sequence of fields.



1. TL and Pirker, Chem. Eng. Sci. 153 (2016)

Extrapolation of recurrent dynamics

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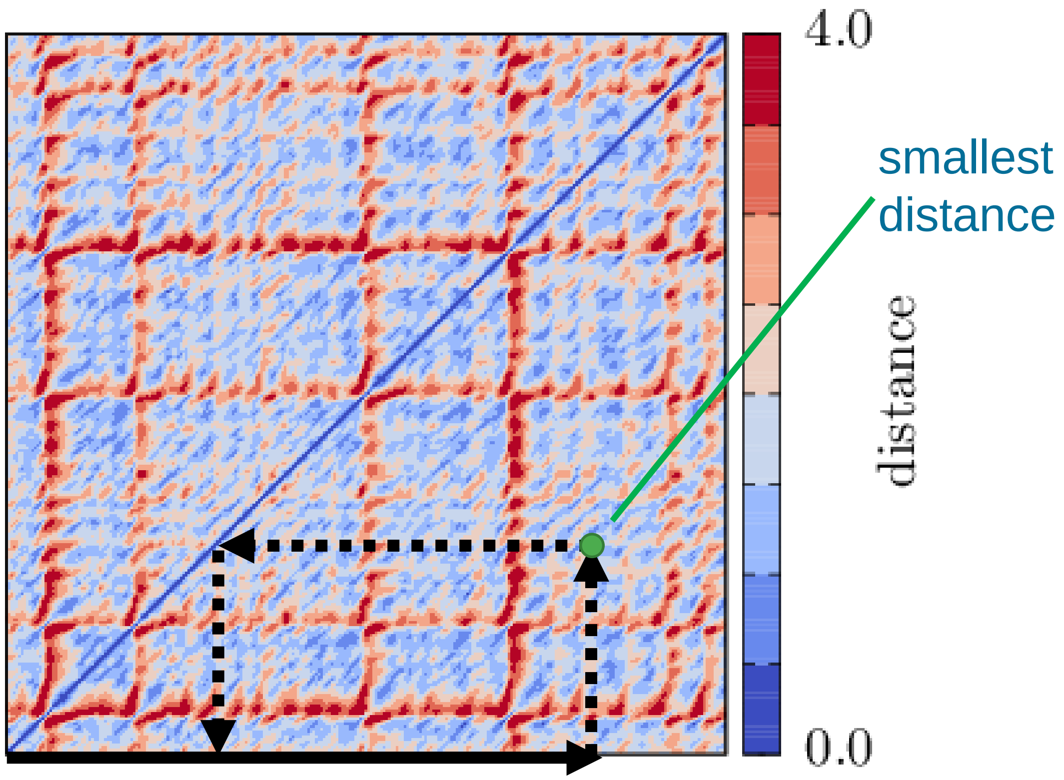
0.) Create a short, high-fidelity time series of flow fields.

1.) Take time-ordered sequence of fields.

2.) Jump to most similar state in the past.



1. TL and Pirker, Chem. Eng. Sci. 153 (2016)

Extrapolation of recurrent dynamics

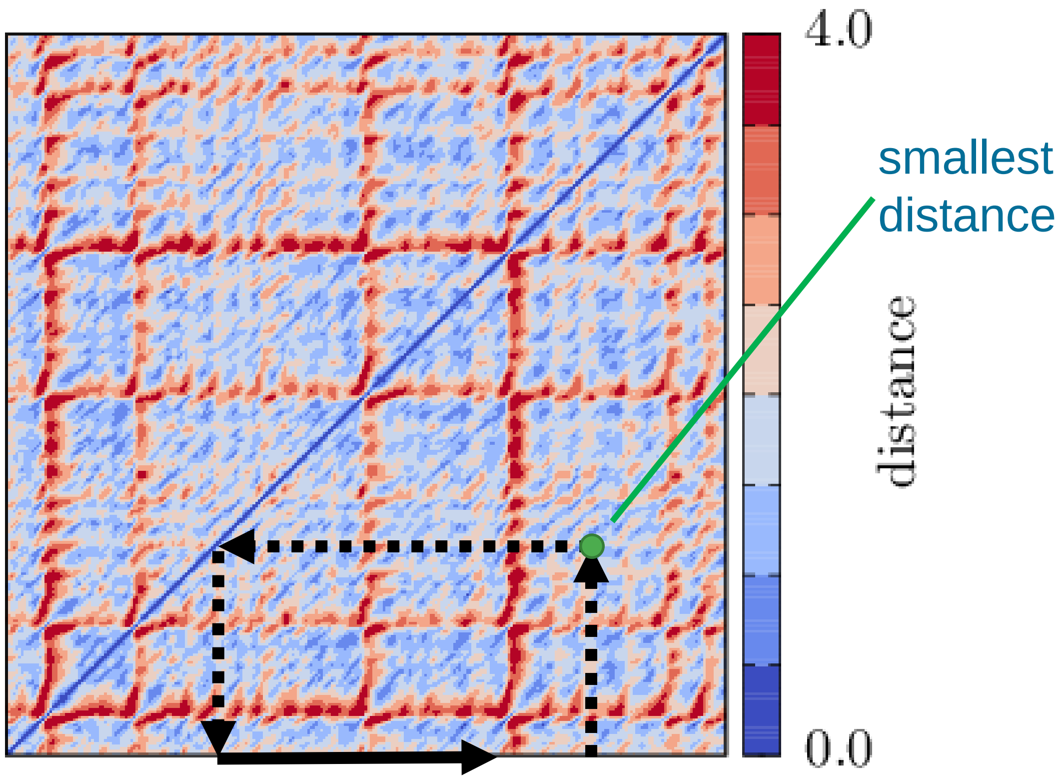
Recurrence CFD[1] in a nutshell

0.) Create a short, high-fidelity time series of flow fields.

1.) Take time-ordered sequence of fields.

2.) Jump to most similar state in the past.

3.) go to 1.)



rCFD = iterated nearest-neighbor search

realized e.g. as Markov process: $t_l \rightarrow \begin{cases} t_l + \Delta t_{\mathrm{rec}} & \text{with prob. } 1 - P_{\mathrm{jump}} \\ t_{\mathrm{nn}(l)} + \Delta t_{\mathrm{rec}} & \text{with prob. } P_{\mathrm{jump}} \end{cases}$

1. TL and Pirker, Chem. Eng. Sci. 153 (2016)

Wait a minute ...

Is this “trivial“ time-extrapolation accurate?

☹ chaotic dynamics: can‘t get single trajectory right

☺ BUT: smooth series of physically valid flow fields, correct spatially resolved mean and variance[1]

resilience against long-term accumulation of prediction errors

Why should it work?

☺ Long-term dynamics is often recurrent with surprisingly short return times!

😐 BUT: bound to database – can deal with transio-recurrent conditions *somehow*[2]...

How is it useful?

fast dynamics + slow, long-term process ➔ **rCFD can help!** But no new info about dynamics...

time-extrapolation

conventional simulation

1. TL, Abbasi, Pirker, Chem. Eng. Sci. 259 (2022)
2. TL et al., Chem. Eng. J. 364 (2019)

Recurrence CFD and its flavors (1)

"**Field-based**" rCFD: conventional transport in time-extrapolated fields

Continuous: Passive transport

$$\frac{\partial}{\partial t}\alpha^{(\mathrm{rec})}(\mathbf{r},t)c(\mathbf{r},t) + \nabla\cdot\alpha^{(\mathrm{rec})}(\mathbf{r},t)\mathbf{u}^{(\mathrm{rec})}(\mathbf{r},t)c(\mathbf{r},t) - \nabla\cdot\alpha^{(\mathrm{rec})}(\mathbf{r},t)D\nabla c(\mathbf{r},t) = S(\mathbf{r},t)$$

concenctration field c subject to calculation, volume fraction α and velocity **u** taken from recurrence database

Discrete: Non-interacting tracer particles

$$d\mathbf{r}_i = \mathbf{u}^{(\mathrm{rec})}(\mathbf{r}_i,t)dt + d\mathbf{r}_{\mathrm{rnd}}$$

$$\frac{d}{dt}Cm_iT_i = \dot{q}_{\text{p-f}} + \dot{q}_{\text{p-p}}$$

tracers follow particle velocity field; random fluctuations, **no contact detection**!

heat transfer from/to surrounding fluid; chemistry

Application case

rCFD for a turbulent double jet

Bubble transport in a submerged double jet

- toy model for continuous casting of steel
- Argon bubbles injected with jet
- characteristic pattern: turbulent eddies
- long-term bubble distribution important

$$v_{\text{bubble}} = v_{\text{liquid}}^{(\text{rec})} + v_{\text{drift}}$$

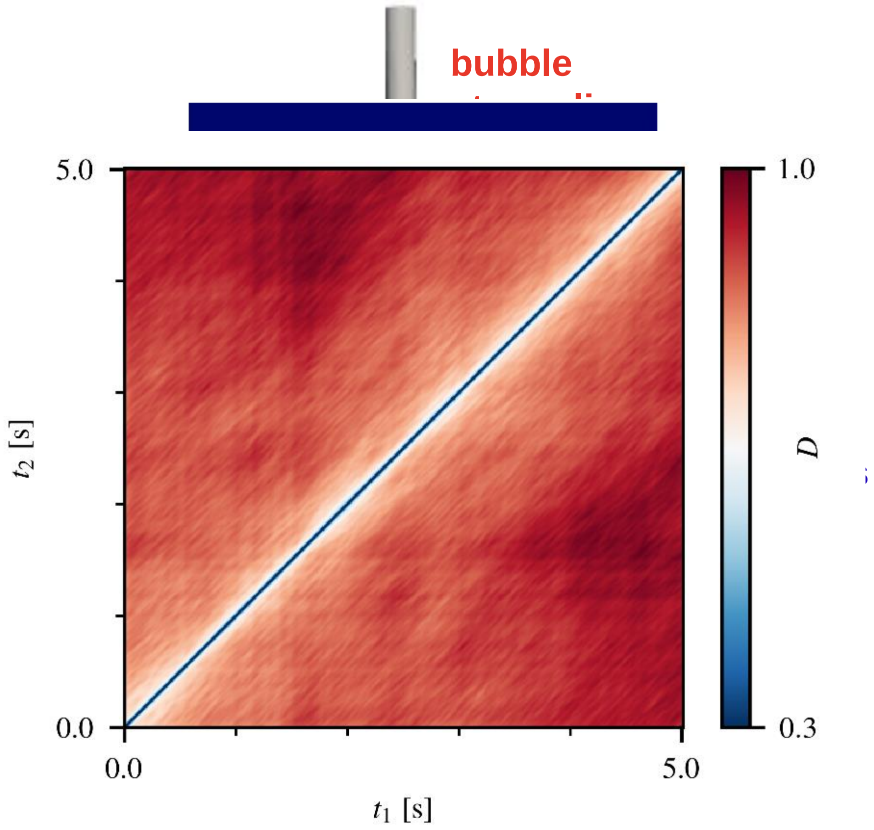
Turbulent fluctuations hide recurrences!

➔ Is rCFD doomed to fail?

rec. process
on LES data

buoyancy

Javurek and Wincor, Steel Res. Int. 91 (2020)



TL, Abbasi, Pirker, Chem. Eng. Sci. 259 (2022)

outflow

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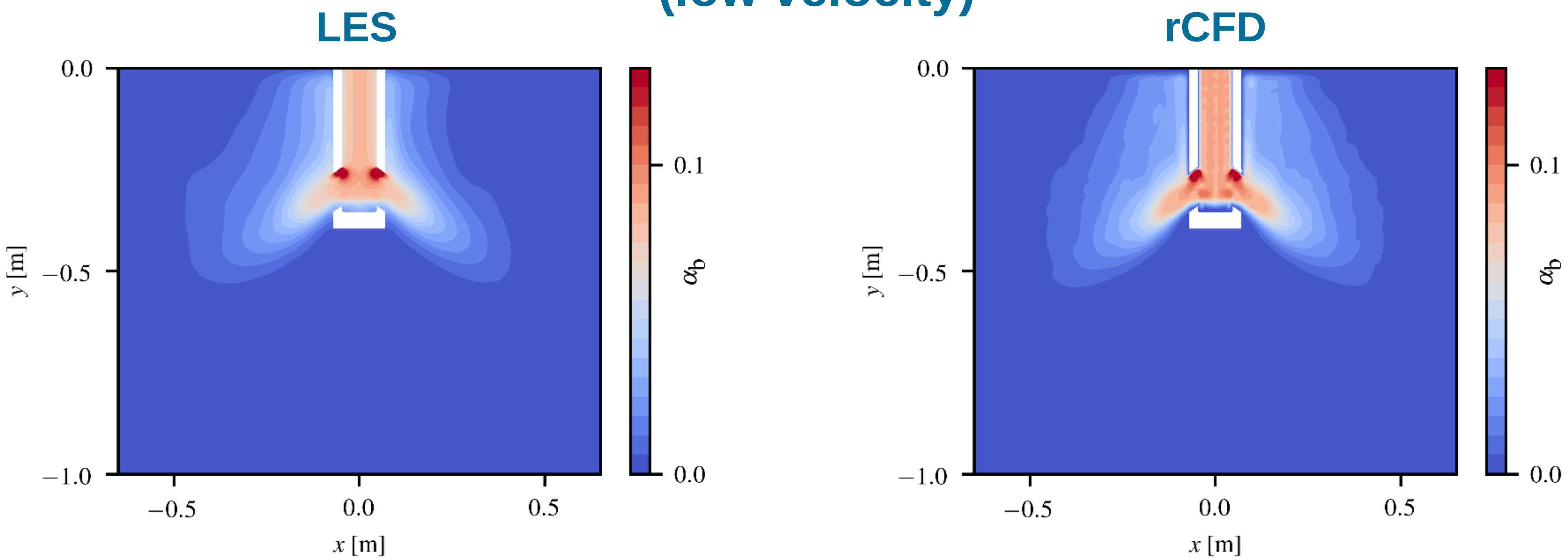
rCFD for a turbulent double jet

Mean bubble concentration (low velocity)



(very) good agreement with reference simulation – **why?**

TL, Abbasi, Pirker, Chem. Eng. Sci. 259 (2022)

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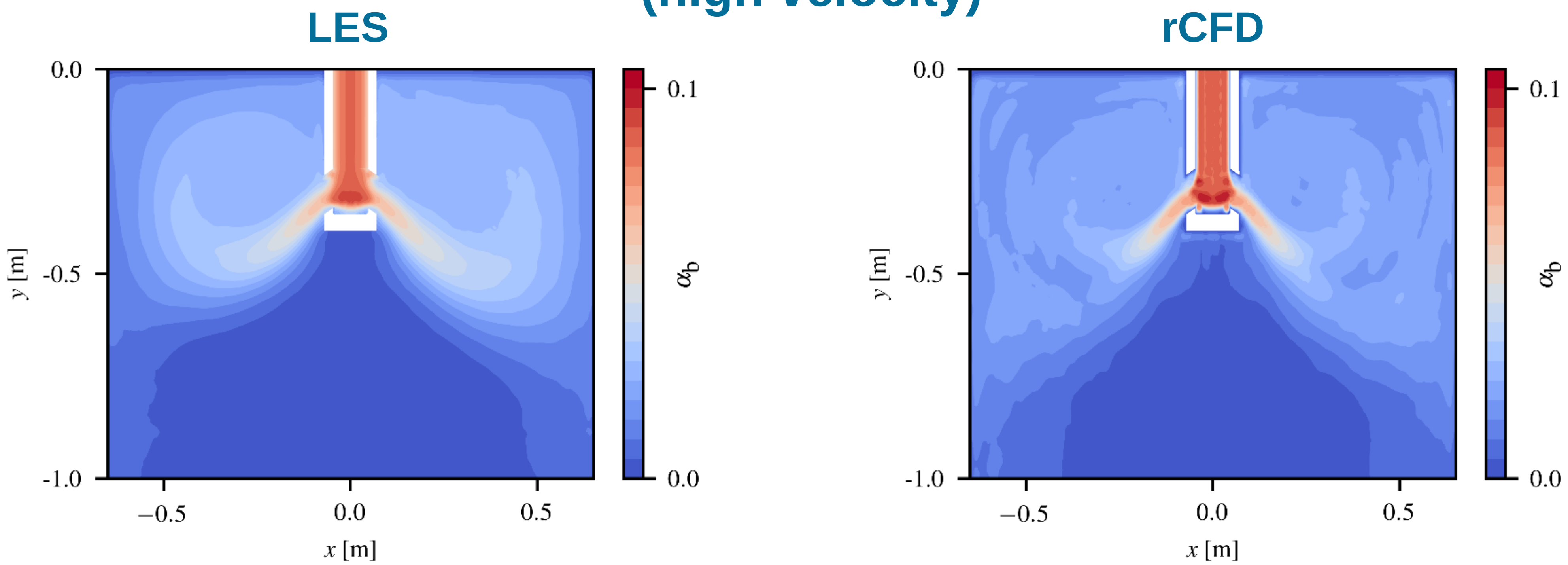
Particulate Flow Modelling

rCFD for a turbulent double jet

Mean bubble concentration (high velocity)



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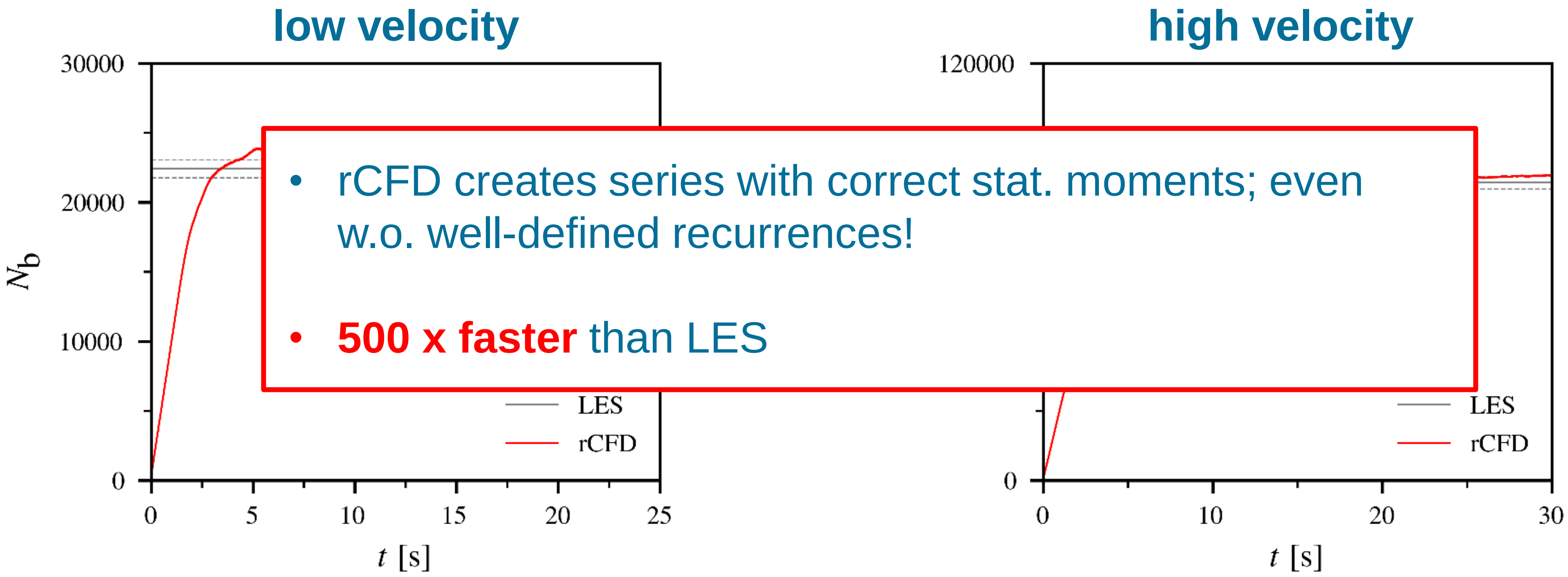
rCFD for a turbulent double jet

Bubbles in domain



- rCFD creates series with correct stat. moments; even w.o. well-defined recurrences!
- **500 x faster** than LES

(very) good agreement with reference simulation – **why?**

TL, Abbasi, Pirker, Chem. Eng. Sci. 259 (2022)

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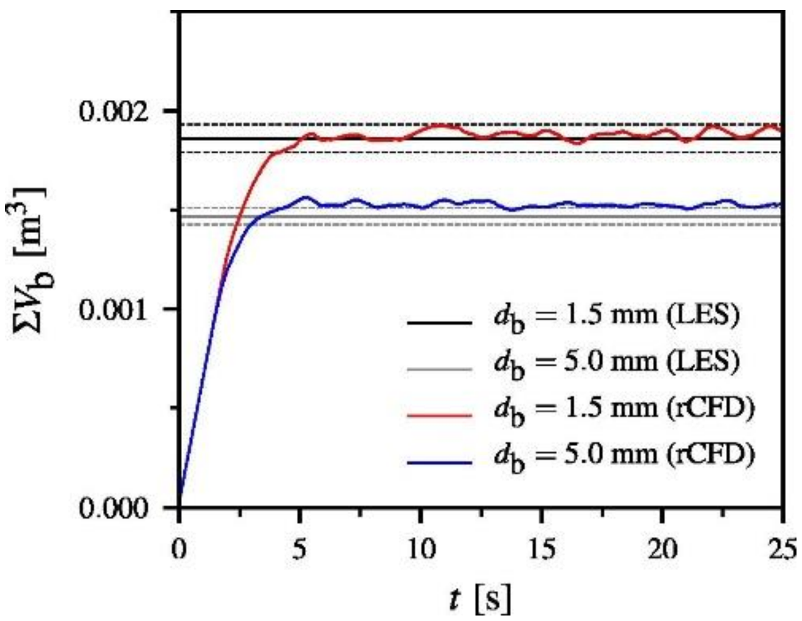
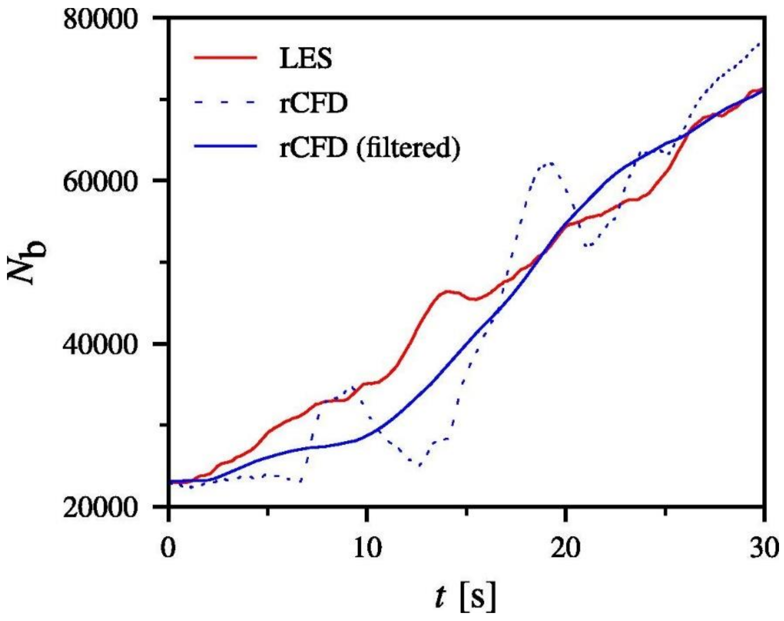
rCFD for a turbulent double jet

Generalization to off-database conditions? Sometimes, somehow ...

bubble diameter



increasing inlet velocity



TL, Abbasi, Pirker, Chem. Eng. Sci. 259 (2022)

rCFD for a turbulent double jet

LES too slow for long-term simulations of mold flow

- speed up 500 by rCFD
- next steps: real-time capability

rCFD can capture turbulent transport despite chaotic dynamics

- worked better than expected
- BUT: bound to database, only limited generalizability

structureless distance plot =!= purely stochastic process

- strong temporal correlations, cannot just use stochastic process

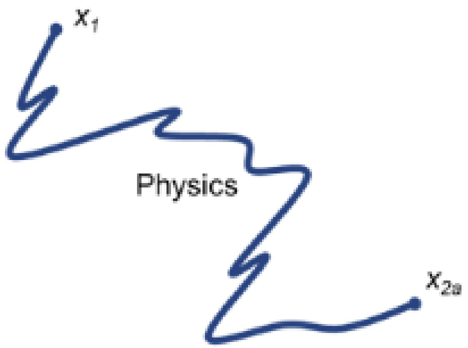
Current activities

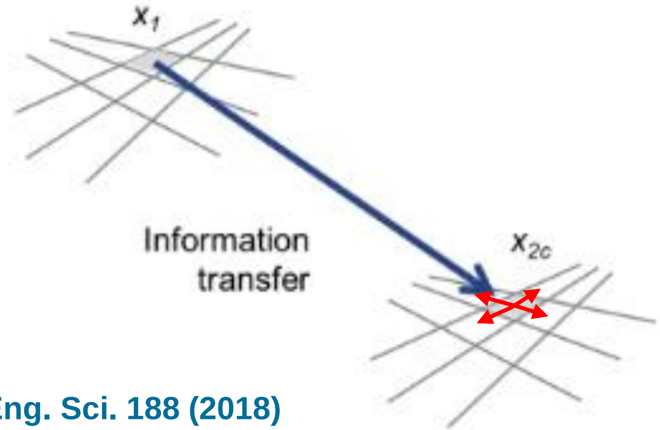
Recurrence CFD and its flavors (2)

“Transport-based“ rCFD: a propagator approach to transport processes

$$\frac{\partial}{\partial t}c(\boldsymbol{r},t)+\nabla\cdot c(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t)=\nabla\cdot D(\boldsymbol{r},t)\nabla c(\boldsymbol{r},t) \quad \textit{implies} \quad c(\boldsymbol{r},t)=\int K_{\mathrm{cc}}(\boldsymbol{r},\boldsymbol{r'};t,t')c(\boldsymbol{r'},t')\mathrm{d}^3r'$$

- K_{cc} propagator of the passive transport equation
- simplest approximation: cell-to-cell map + diffusion
- time-ext ... ator instead of ve



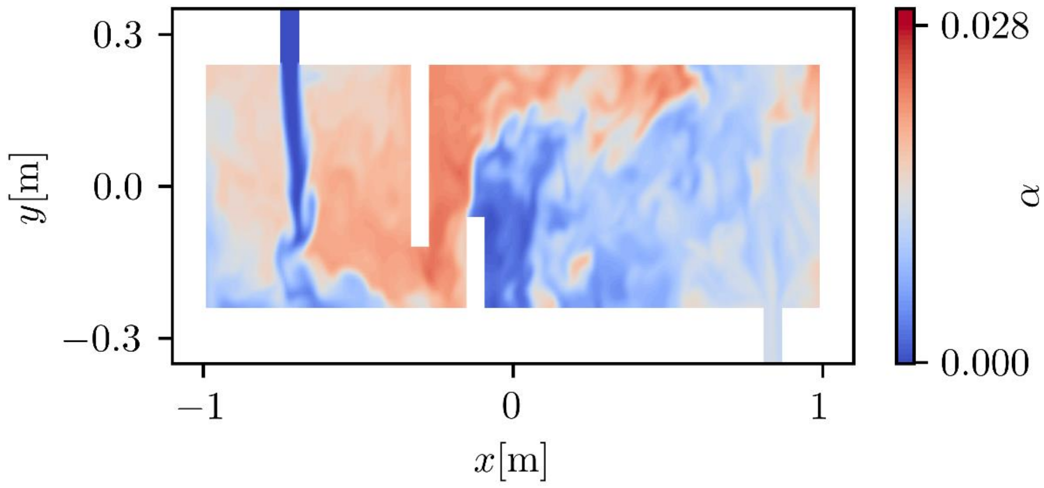


Pirker and TL, Chem. Eng. Sci. 188 (2018)
Lumetzberger, Pirker, TL, Chem. Eng. Sci. 311 (2025)

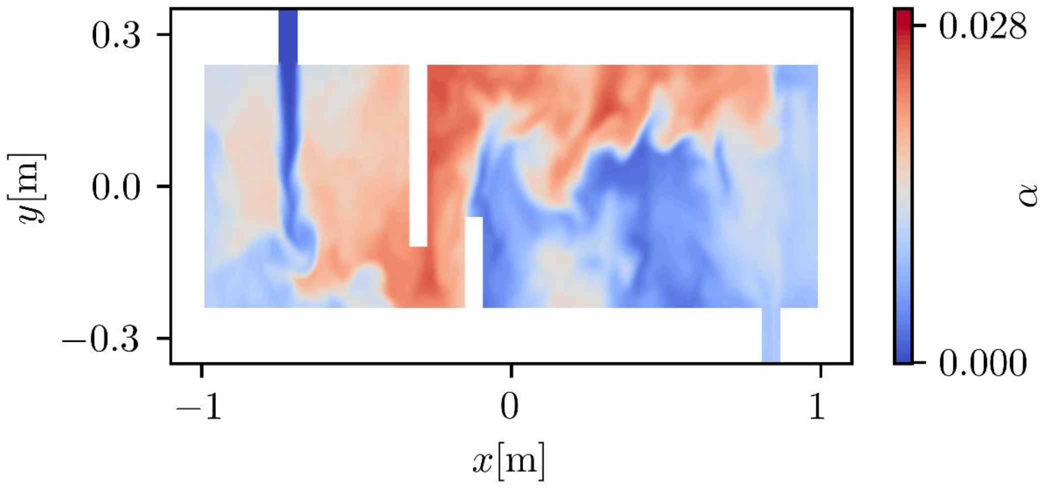
Demo case: species transport in a tundish

Residence time: pulse of ‘impurity-laden‘ steel (red)

LES



rCFD



Lumetzberger, Pirker, TL, Chem. Eng. Sci. 311 (2025)

K1MET project: Advancement of simulation acceleration for process applications

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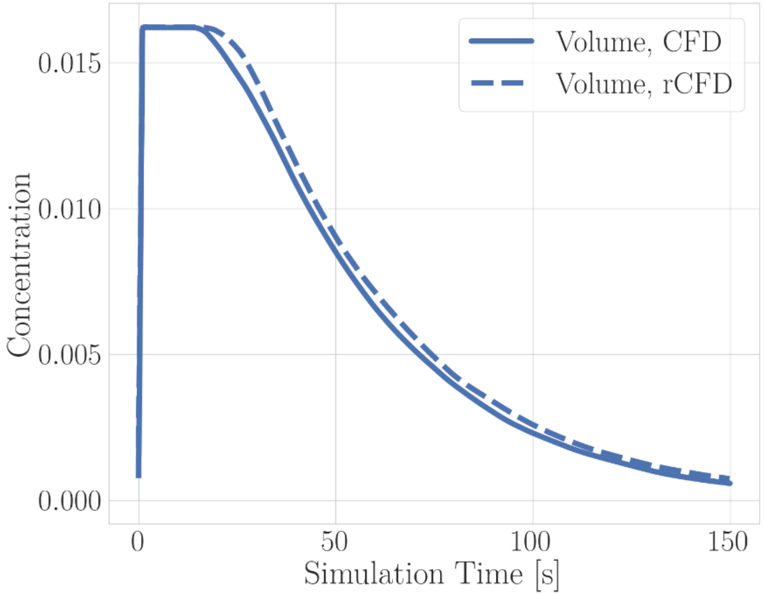
Particulate Flow Modelling

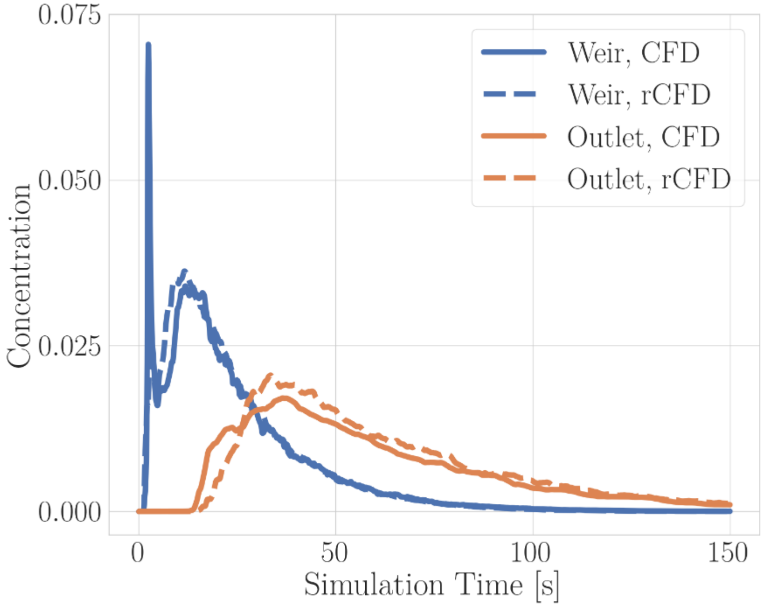
Demo case: species transport in a tundish

Residence time: pulse of ‘impurity-laden‘ steel (red)

total



local



Lumetzberger, Pirker, TL, Chem. Eng. Sci. 311 (2025)

K1MET project: Advancement of simulation acceleration for process applications

Demo case: species transport in a tundish

We have the means for *accurate*, faster-than-real-time simulations!

1 sec process time → CFD: 2700 sec

1 sec process time → rCFD: 0.75 sec

Lumetzberger, Pirker, TL, Chem. Eng. Sci. 311 (2025)

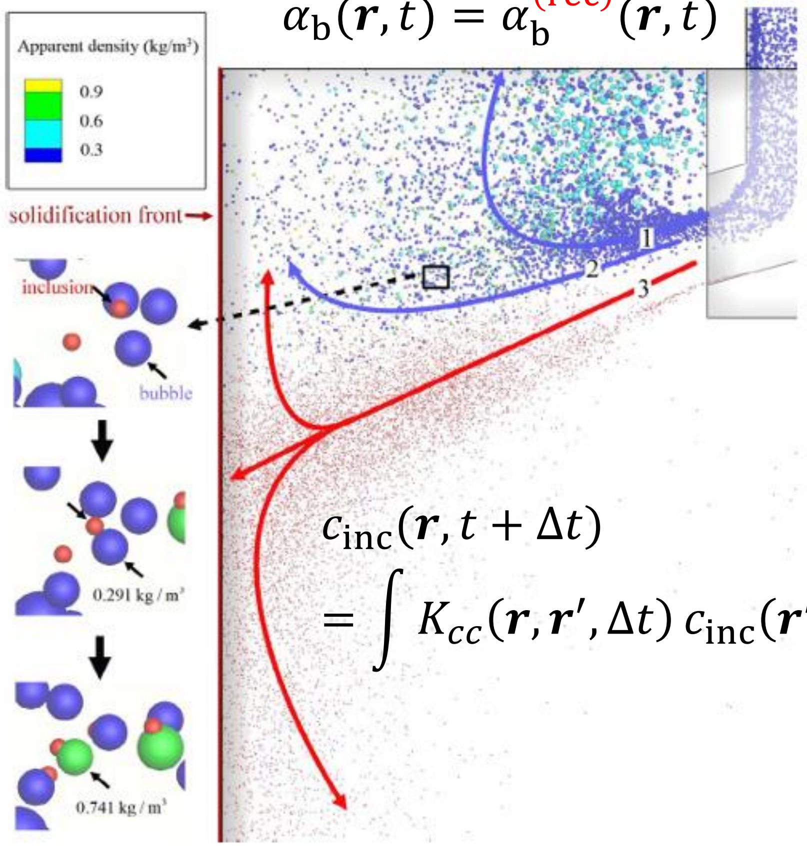
K1MET project: Advancement of simulation acceleration for process applications

Application to full-scale SEN flow

Strategy to simulate impurity removal

- time-extrapolate bubble distribution
- simulate impurity transport via propagator approach
- empirical capturing efficiency of impurities at bubbles

$$\alpha_{\mathrm{b}}(\boldsymbol{r},t) = \alpha_{\mathrm{b}}^{(\mathrm{rec})}(\boldsymbol{r},t)$$



$$c_{\mathrm{inc}}(\boldsymbol{r},t+\Delta t) = \int K_{cc}(\boldsymbol{r},\boldsymbol{r}',\Delta t)\, c_{\mathrm{inc}}(\boldsymbol{r}',t) d^3r'$$

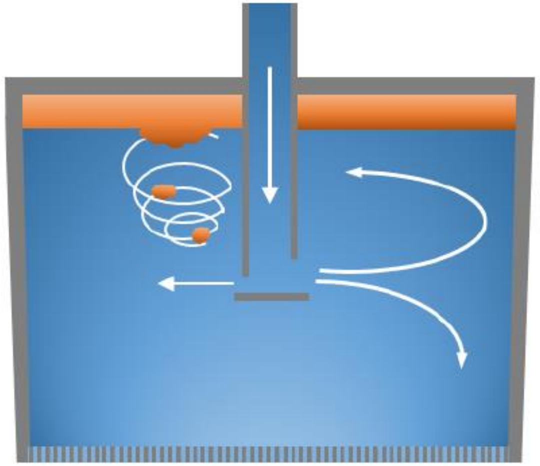
Lai et al., ISIJ Int. 58 (2018)

Future perspectives

Submerged, turbulent jets

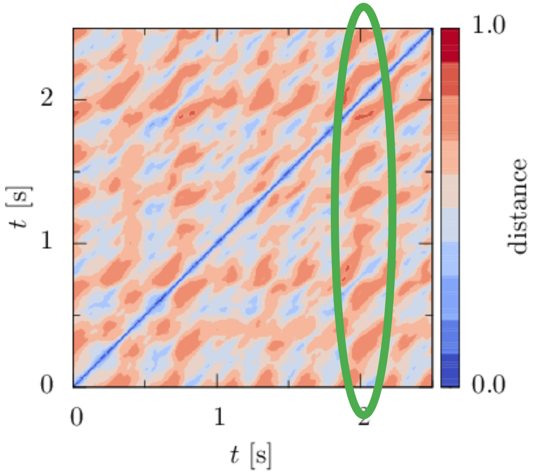
Goal and challenges

- predictions about undesired behavior (e.g. entrainment)
- rare events: difficult for both classical and data-driven simulations



Rare-event focused data generation

- find ‘rarest’ state in time series and continue with slight perturbation
- iteration: database of rare events



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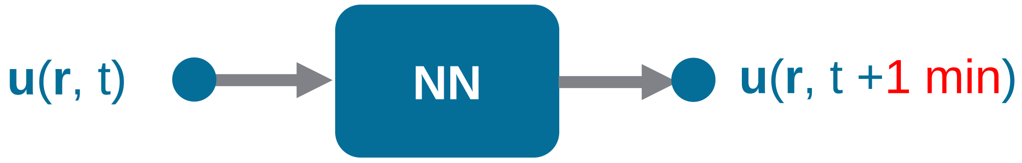
Submerged, turbulent jets

Strategy and planned activities

- let deep NNs learn turbulent dynamics under ‘tame’ conditions



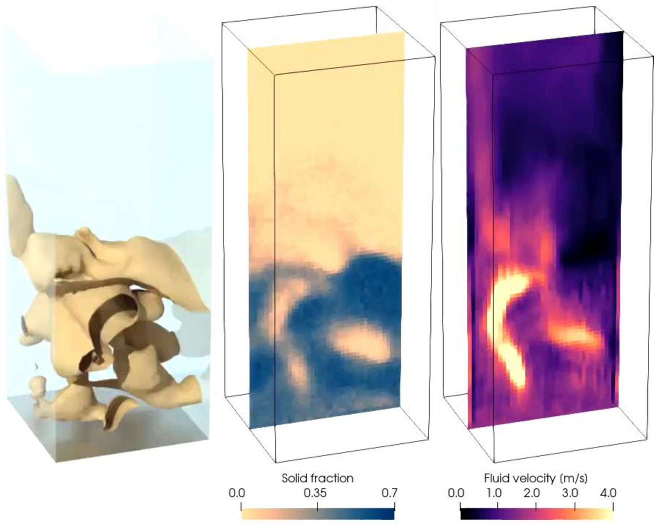
- correlate predictions with sensor measurements (e.g., interface dynamics)

  ➔ trigger rare events

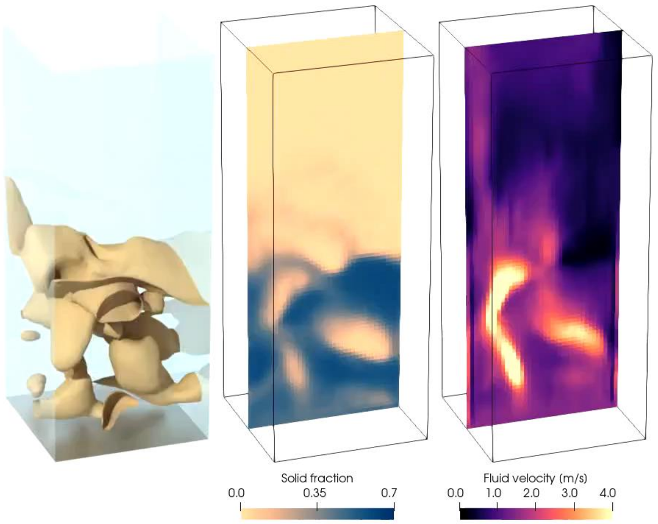
Submerged, turbulent jets

Can we ‘just let a NN learn turbulent dynamics’ ?

- need enough data and appropriate network architecture: universal physics transformers
- proof of concept for fluidized beds



CFD-DEM vs NN:
which is which?



Alkin et al., submitted to Nat. Mach. Intell., arXiv preprint arXiv:2411.09678 (2024)

https://nx-ai.github.io/NeuralDEM/

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Conclusion

Data-assisted simulations will massively improve development, optimization, and control for a *wide range of process types* such as continuous casting of steel.

- real-time capability
- long-term stability and accuracy regarding the *relevant* physics
- flexibility to deal with various types of input data, dynamic regimes etc.

digital process twins

How can we get enough training data?

- physics-informed machine learning
- physics-based augmentation

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