Scale-Sensitive Analysis of Turbulent Mixing with Differential Diffusion

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Differential diffusion

- The turbulent mixing of **two or more scalars** is encountered in a variety of engineering and environmental applications
- When the **molecular diffusivity of the scalars is different**, the scalars evolve differently even if they are initially perfectly correlated

→ This process is known as **differential diffusion**

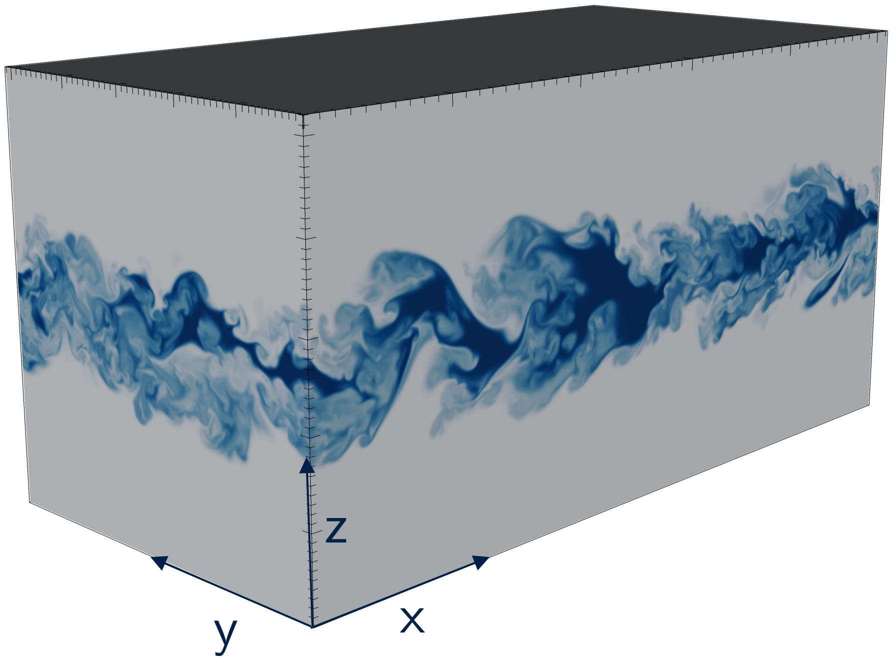
Differential diffusion is analyzed in the context of

1) Jet flows → turbulent/non-turbulent interface
2) Homogeneous forced turbulence → inter-scale transfer

DNS of turbulent jet flow

- Direct numerical simulation of **temporally evolving plane jet flow**
- Periodic in *x* and *y* directions
- 6^{th} order implicit finite difference scheme for spatial derivatives
- 4^{th} order low storage Runge-Kutta scheme for temporal integration
- Pressure treatment: fractional step method with Helmholtz equation for pseudo pressure

$$\frac{\partial^2 \hat{p}}{\partial x_3^2} - (k_1^2 + k_2^2)\hat{p} = \hat{R}$$

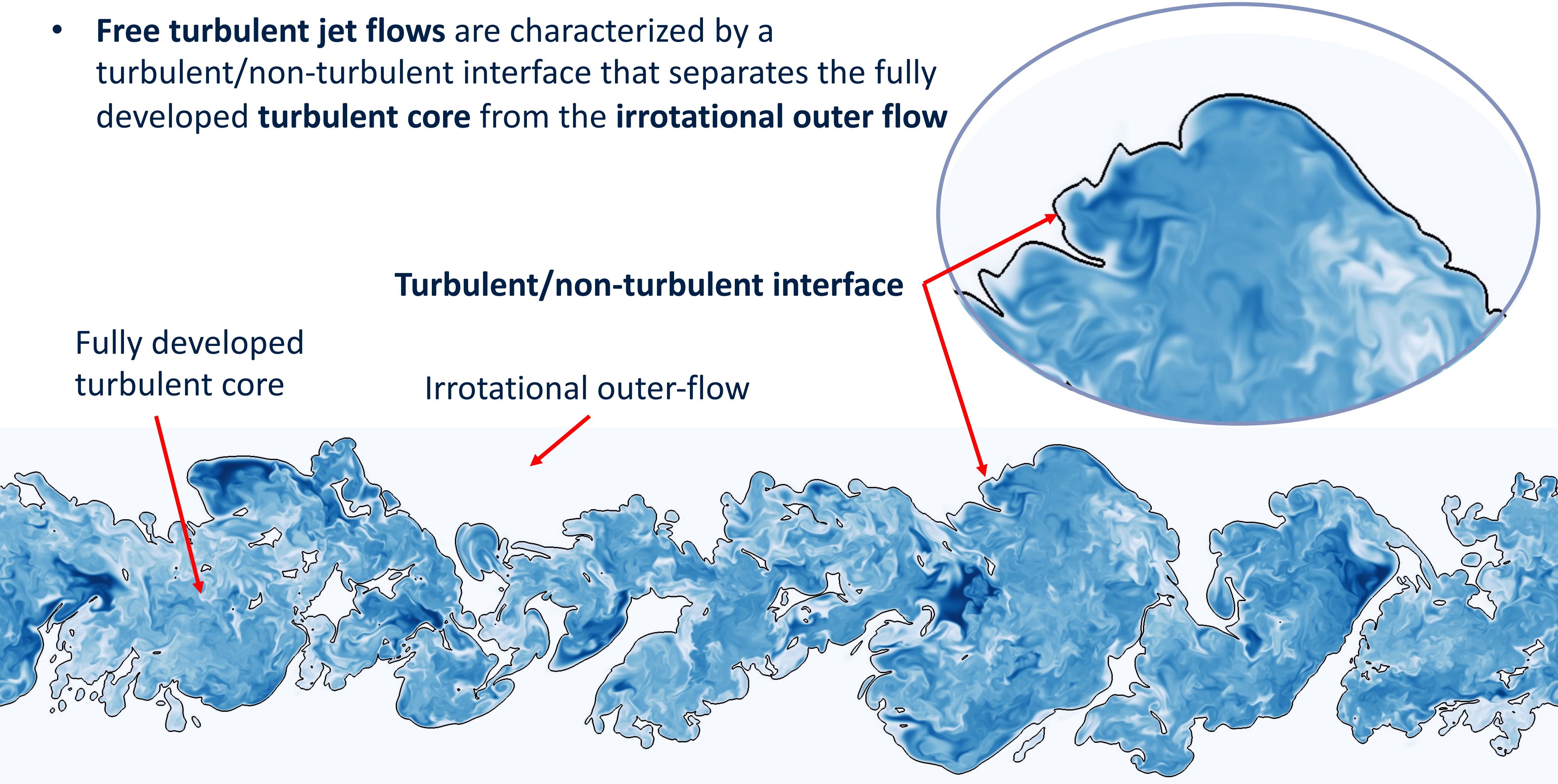


- Grid size is 2816 x 2816 x 1500
- Initial jet Reynolds number is 9000

- **Two passive scalars** with
  - Sc=1 and
  - Sc=0.25

Turbulent jet flow: turbulent/non-turbulent interface

- **Free turbulent jet flows** are characterized by a turbulent/non-turbulent interface that separates the fully developed **turbulent core** from the **irrotational outer flow**

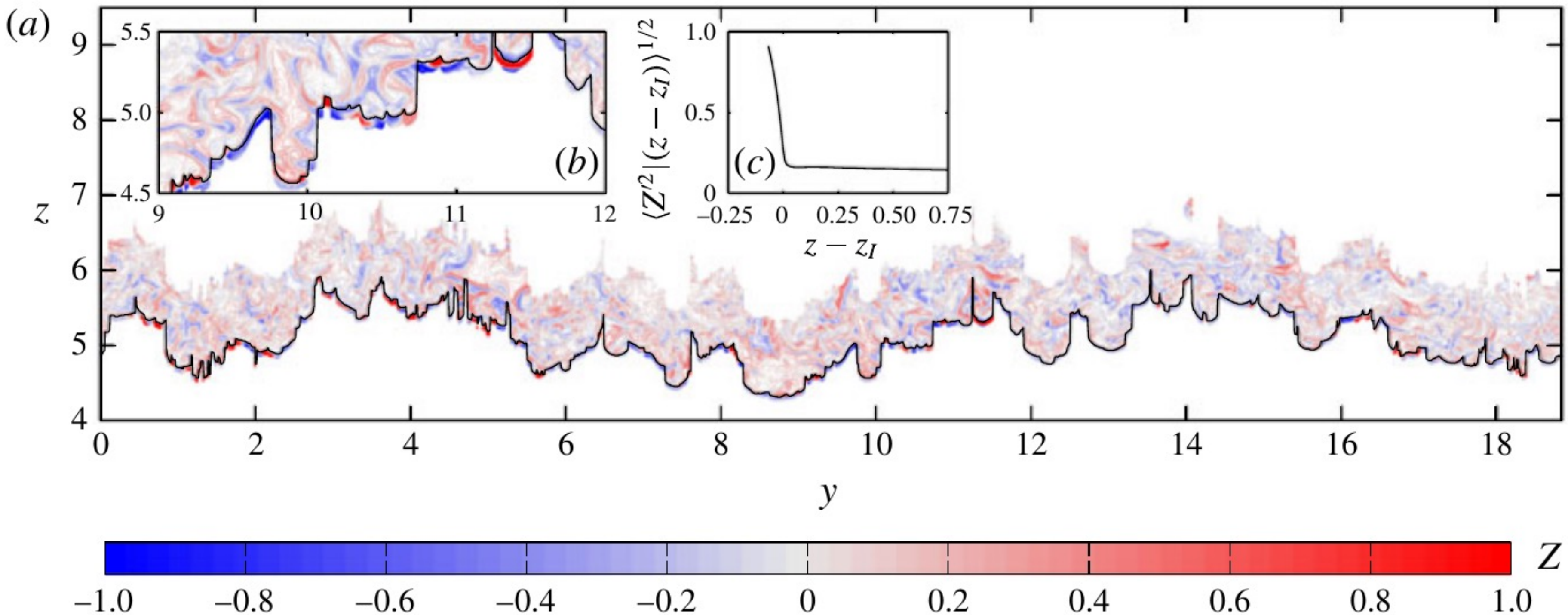


→ Large local gradients across the TNTI: Diffusive effects become important

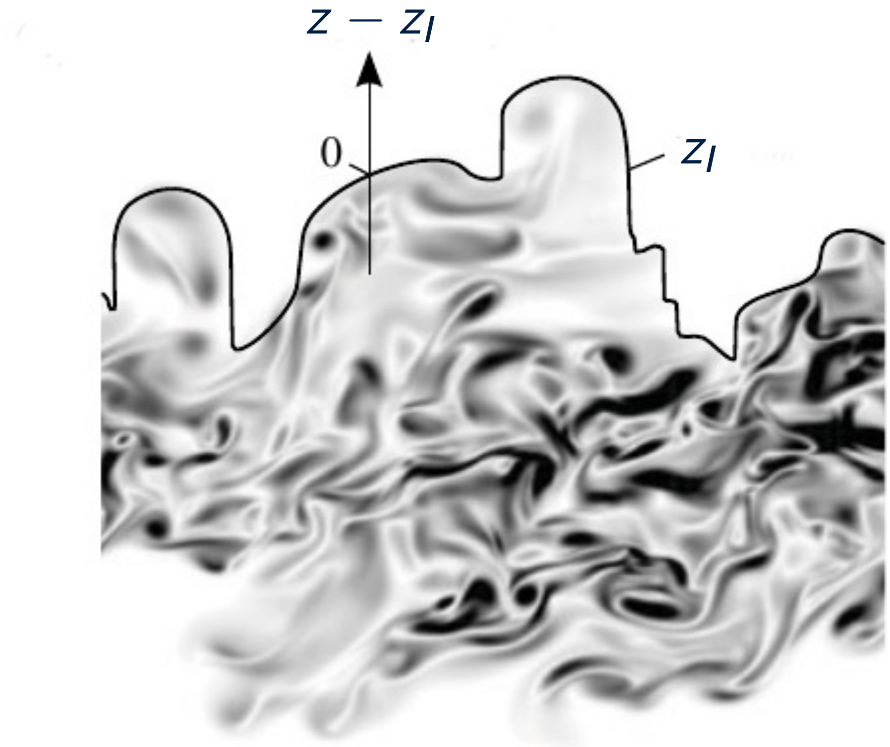
Differential diffusion parameter

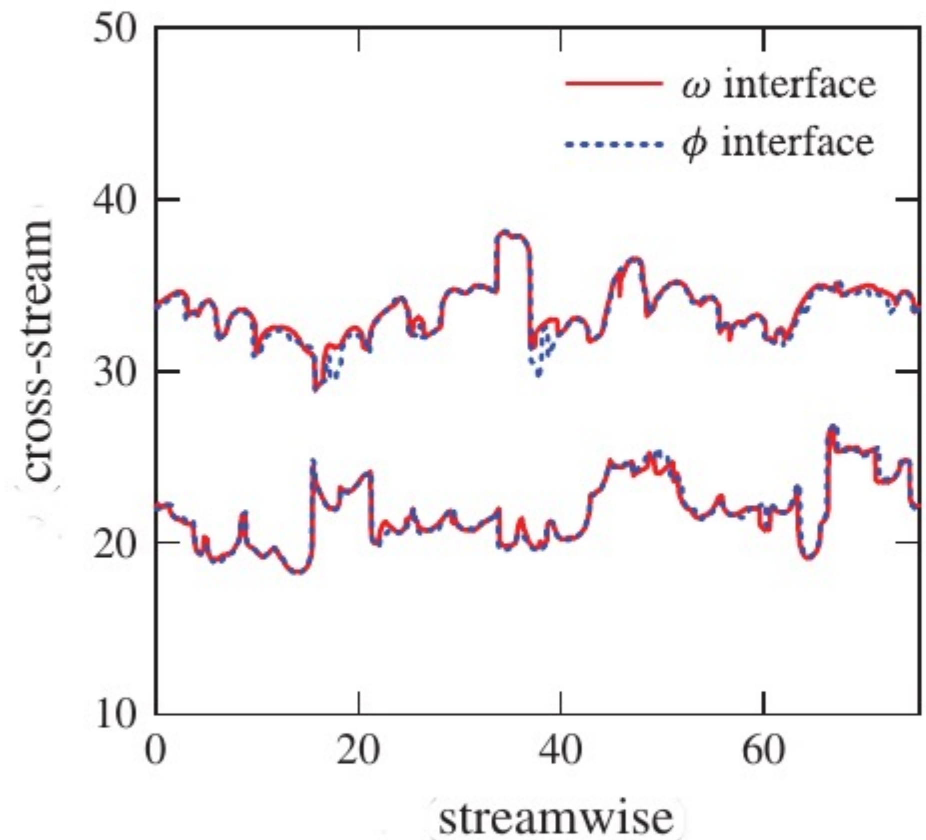
- The **mixture field** of two initially correlated passive scalars **depart from each** other when the Schmidt number is different
- Differential diffusion parameter *Z* is introduced for quantification

$$Z = \frac{\phi_1}{\langle \phi_1 \rangle} - \frac{\phi_2}{\langle \phi_2 \rangle}$$



Turbulent/non-turbulent interface

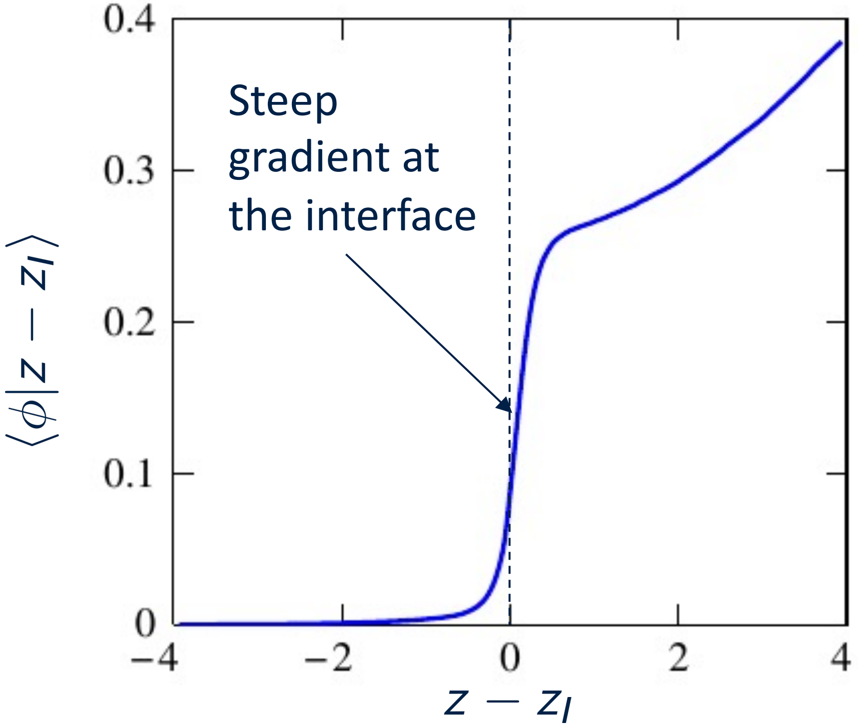


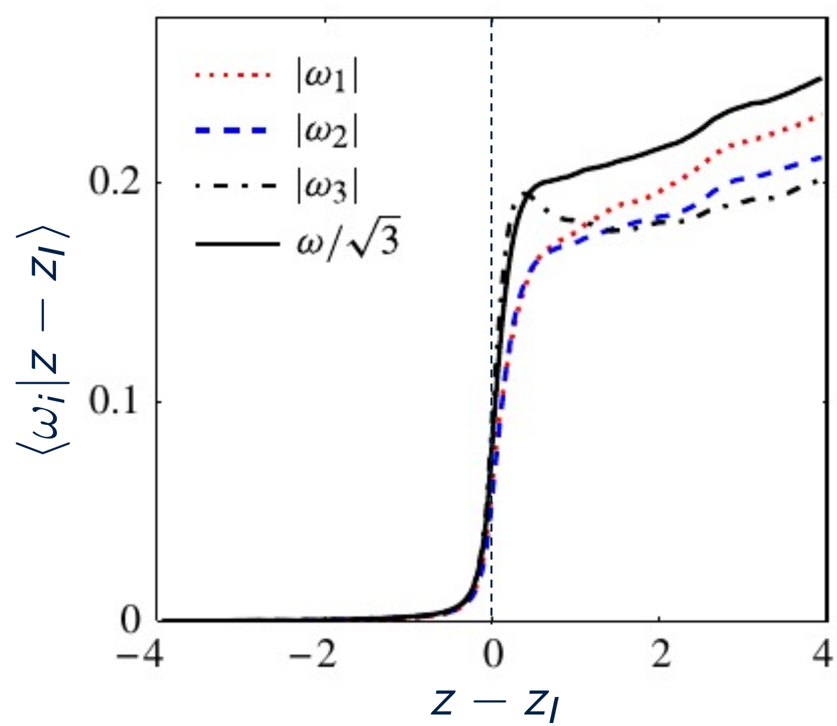


- Introduce new interface dependent coordinate:
- Define interface based on threshold of vorticity ω or scalar ϕ
- The interface defined by both criteria is virtually the same

M. Gampert et al., J. Fluid Mech. (2014)

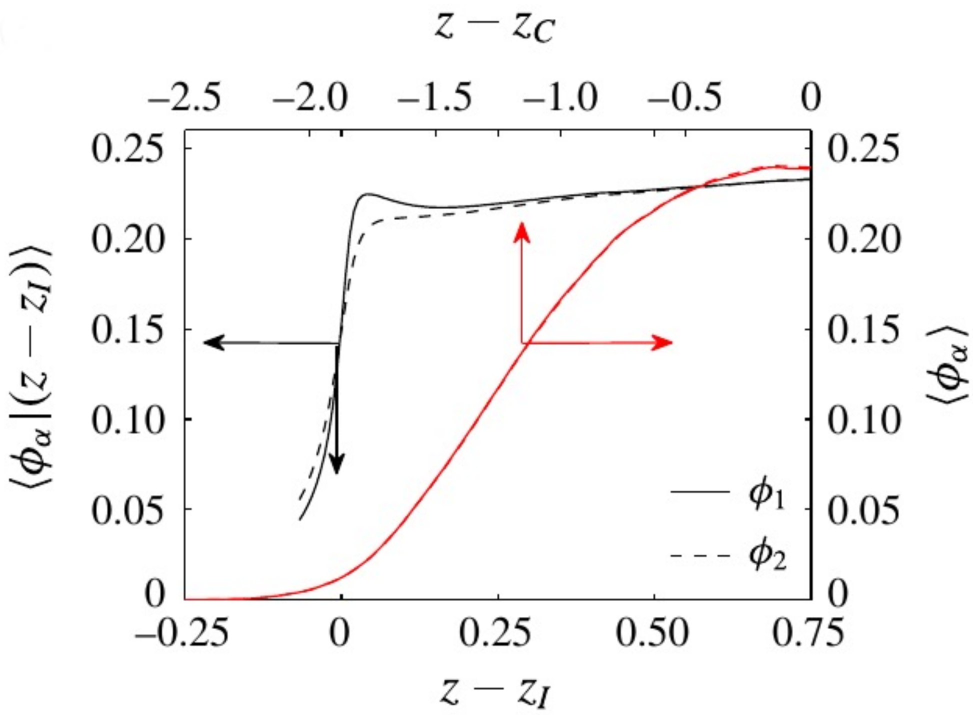
Detection of the turbulent/non-turbulent interface

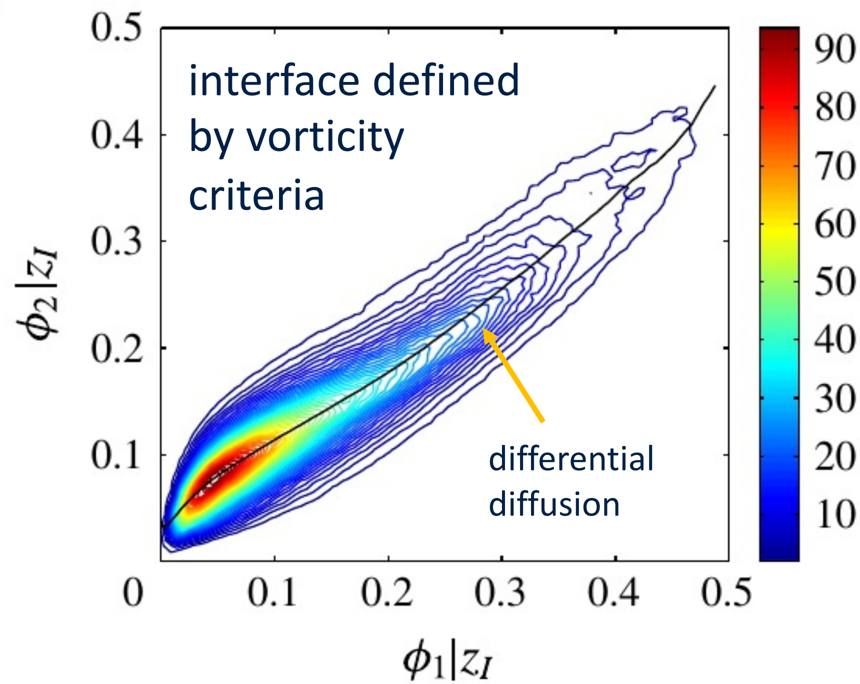




- Conditional average reveals steep gradient at the turbulent/non-turbulent interface
- -> Interface position is **not sensitive** with respect to the threshold

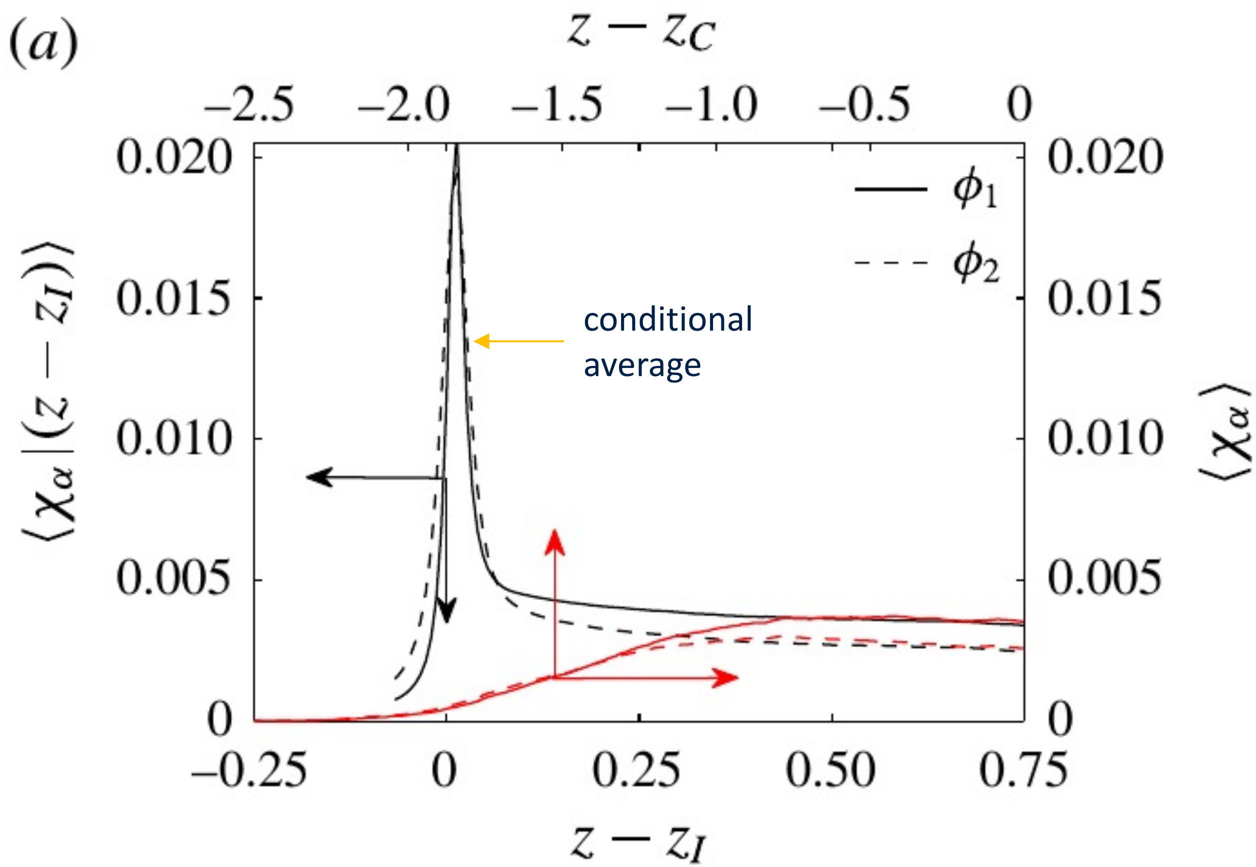
Differential diffusion: decorrelation at the interface





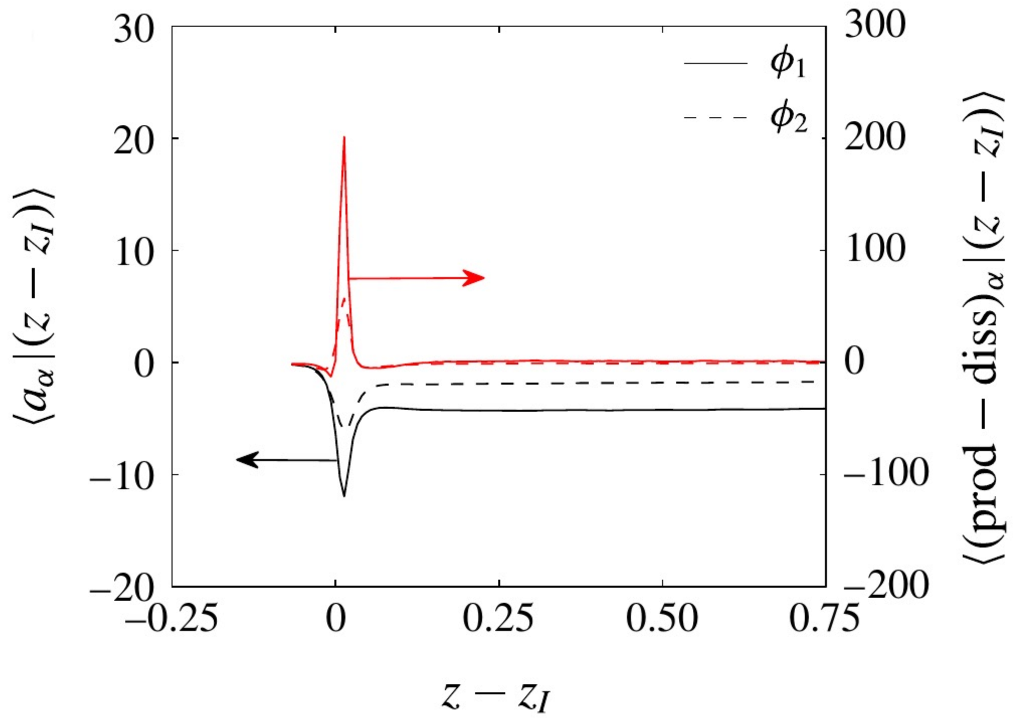
- Conditional average reveals steep gradient at the interface
- Joint pdf $P(\phi_1, \phi_2; z_I)$ shows decorrelation of the two scalars at the interface

Differential diffusion: scalar dissipation



- Conditional scalar dissipation reveals peak in the vicinity of the interface, which is not seen by conventional averaging

Differential diffusion: gradient production at the interface



- Transport equation for square of scalar gradient $g_\alpha^2 \propto \chi / D$

$$\frac{\partial g_\alpha^2}{\partial t} + u_i \frac{\partial g_\alpha^2}{\partial x_i} = \boxed{-2 g_{\alpha,j} s_{i,j} g_{\alpha,i}} - \boxed{\frac{2}{Pe_{0,\alpha}} \left(\frac{\partial g_{\alpha,i}}{\partial x_j} \right)^2} + \frac{1}{Pe_{0,\alpha}} \frac{\partial^2 g_\alpha^2}{\partial x_i^2}$$

Production

Dissipation

Direct numerical simulations in a periodic box

- Three-dimensional **incompressible Navier-Stokes equations** with large-scale stochastic forcing
- **Pseudo-spectral method** in triply periodic box

external stochastic force

$$\frac{\partial u_j}{\partial t} + \frac{\partial}{\partial x_i}(u_i u_j) = -\frac{\partial p}{\partial x_j} + \nu \frac{\partial^2 u_j}{\partial x_i^2} + \boxed{f_j} \quad \text{and} \quad \frac{\partial u_i}{\partial x_i} = 0$$

- In spectral space: $\frac{\partial \hat{u}_j}{\partial t} + \nu \kappa^2 \hat{u}_j = -i\kappa_j \hat{p} - \hat{G}_j$ with $\hat{G}_j(\boldsymbol{\kappa}, t) = \mathcal{F}_\kappa \left[\frac{\partial}{\partial x_k}(u_j u_k) \right] + \hat{f}_j$
- Using the Poisson equation: $-i\kappa_j \hat{p} = \frac{\kappa_j \kappa_k}{\kappa^2} \hat{G}_k$
- Gives: $\frac{\partial \hat{u}_j}{\partial t} + \nu \kappa^2 \hat{u}_j = -\boxed{\left(\delta_{jk} - \frac{\kappa_j \kappa_k}{\kappa^2} \right)} \hat{G}_k = -P_{jk} \hat{G}_k$

Projection operator

Direct numerical simulations: temporal integration

- Integrating factor approach:

$$\frac{\partial \hat{u}_j}{\partial t} = \mathcal{N}(\hat{u}_j) - \nu\kappa^2 \hat{u}_j \,, \quad \text{with} \quad \mathcal{N}(\hat{u}_j) = -P_{jk}\hat{G}_k$$

- Define new dependent variable:

$$\tilde{u}_j = \hat{u}_j \exp(\nu\kappa^2 t)$$

$$\frac{\partial \tilde{u}_j}{\partial t} = \mathcal{N}(\tilde{u}_j \exp(-\nu\kappa^2 t)) \exp(\nu\kappa^2 t) \qquad (1)$$

- Temporal integration of (1) by third order Runge-Kutta scheme

- **Passive scalar** with **imposed mean gradient in y-direction** and **unity Schmidt number**

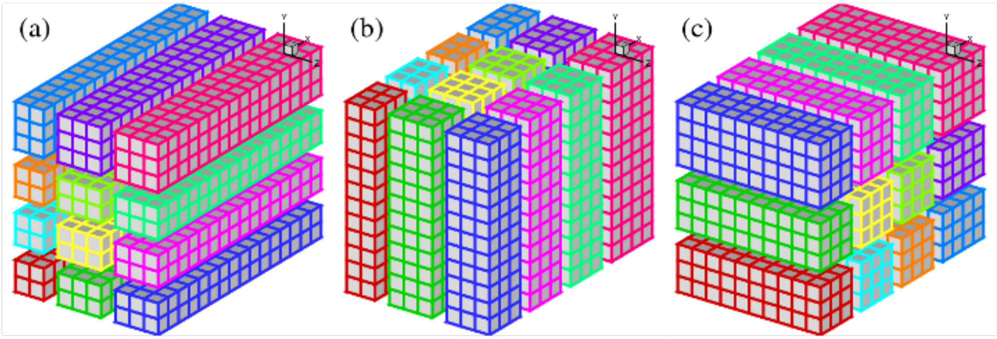
$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = D_\alpha \frac{\partial^2 \phi}{\partial x_i} - u_2 \Gamma \qquad \text{with uniform mean scalar gradient:} \quad \Gamma = \frac{\partial \langle \Phi \rangle}{\partial x_2}$$

Direct numerical simulations: scaling of solver

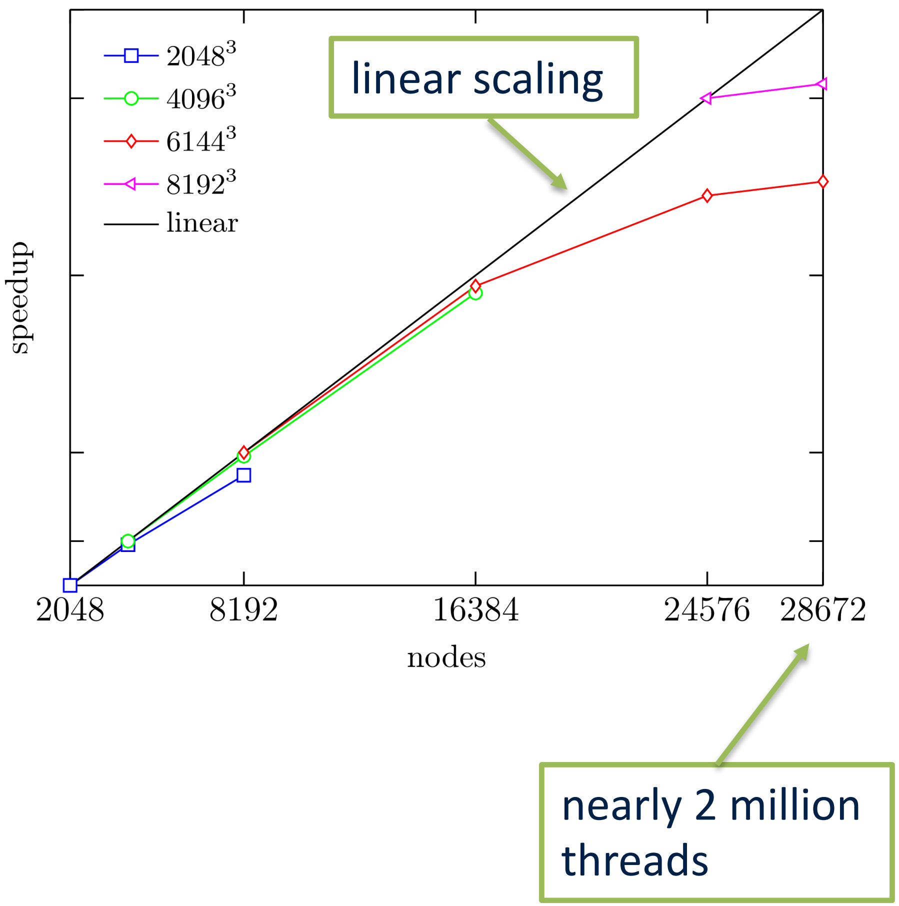
- DNS of turbulent flows is computationally very expensive

$$N^3 \propto Re_\lambda^{9/2}$$

- **Hybrid MPI/OpenMP DNS code** (psOpen[1,2]) with two-dimensional domain decomposition



- Runs on IBM BlueGene/Q (JUQUEEN in Germany) on up to **458,752 compute cores**[2]



[1]M. Gauding, Phd thesis (2014)
[2]J.H. Goebbert & M. Gauding, Report FZ-Juelich (2015)

Scale-sensitive framework for differential diffusion

Turbulent mixing of passive scalars with
- different molecular diffusivities and
- imposed mean scalar gradient:

$$\Phi_\alpha = \Gamma x_2 + \phi_\alpha \,. \qquad \frac{\partial \phi_\alpha}{\partial t} + u_i \frac{\partial \phi_\alpha}{\partial x_i} = D_\alpha \frac{\partial^2 \phi_\alpha}{\partial x_i^2} - \Gamma u_2$$

Covariance structure function: $C_{\alpha\beta}(\mathbf{r}, \mathbf{x}) = \langle \Delta\phi_\alpha \Delta\phi_\beta \rangle$

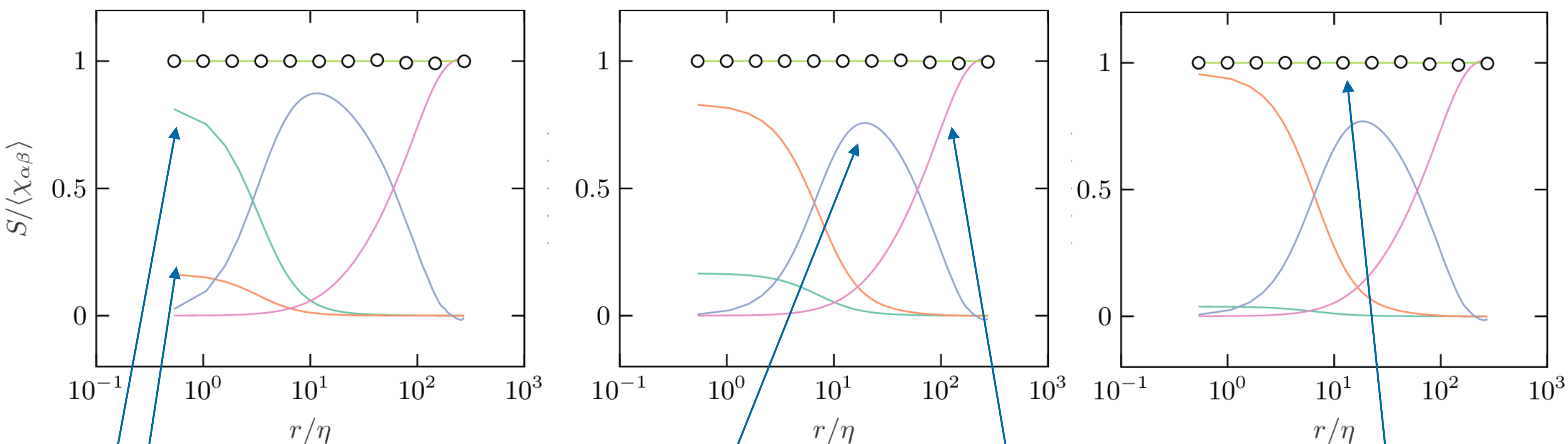
$$\frac{\partial}{\partial t}\langle \Delta\phi_1 \Delta\phi_2 \rangle + \frac{\partial}{\partial r_i}\langle \Delta u_i \Delta\phi_1 \Delta\phi_2 \rangle =$$
$$\frac{\partial}{\partial r_i}\langle D_1 \Delta\phi_2 \left(\frac{\partial \phi_1'}{\partial x_i'} + \frac{\partial \phi_1}{\partial x_i} \right) + D_2 \Delta\phi_1 \left(\frac{\partial \phi_2'}{\partial x_i'} + \frac{\partial \phi_2}{\partial x_i} \right) \rangle -$$
$$2(D_1 + D_2)\langle \frac{\partial \phi_1}{\partial x_i} \frac{\partial \phi_2}{\partial x_i} \rangle - \Gamma \langle \Delta u_2 \left(\Delta\phi_1 + \Delta\phi_2 \right) \rangle$$

Direct numerical simulations
- 3 Schmidt numbers: Sc=1, Sc=5, Sc=1/5
- Taylor-based Reynolds number close to 100
- Pseudo spectral method
- Velocity is forced at the large scales by a stochastic method to maintain steady state

Scale-sensitive budget between transfer, dissipation, diffusion, and production

Scale-by-scale budget

Sc=1 & Sc=1/5 | Sc=1 & Sc=5 | Sc=5 & Sc=1/5



Diffusive transport

Transfer

Production

Budget is satisfied with good accuracy

→ Diffusive transport strongly depends on the combination of Schmidt numbers

Summary & Conclusions

- Differential diffusion dominates at the turbulent/non-turbulent interface
- Conditional statistics based on the interface position can reveal otherwise “hidden features” of turbulence
- Developed a scale-sensitive framework for differential diffusion
- Perspective: Closing the subgrid terms with a spectral closure (M. Oberlack & N. Peters, Apl. Sci. Res. 1993 and M. Gauding et al., JoT 2014)