Turbulence-scalar interactions in flows featuring significant density variations

Arnaud MURA
(arnaud.mura@ensma.fr)
Institut P', UPR3346 du CNRS
ISAE-ENSMA et Université de Poitiers

Turbulence-scalar interactions in flows featuring significant density variations

From premixed flames to compressible or multiphase flows

Arnaud MURA
(arnaud.mura@ensma.fr)
Institut P', UPR3346 du CNRS
ISAE-ENSMA et Université de Poitiers

Outlines of the presentation

1. **Context**: **scalar mixing** and **variable density** fluid turbulence, scalar dissipation rate, **turbulence scalar interaction**, scalar gradient orientation, velocity gradient invariants, etc.

2. **Analysis**: **passive scalar** in homogeneous **turbulence** interacting with a planar **shock wave**, **vaporizing two-phase flows** in homogeneous isotropic turbulence, fully **premixed flame** kernel development in homogeneous isotropic turbulence

3. **Discussion, comments, questions**

Some among the various contributions of Fabien in this field of research

Scalar mixing and **variable density turbulence**

Seminal papers with some of them focused on the link between fluctuations of a passive scalar and its dissipation rate (see below), an important problem for **turbulent flow modelling** both **with and without chemical reactions**

F. Anselmet, R.A. Antonia, Joint statistics between temperature and its dissipation in a turbulent jet, ***The Physics of Fluids***, vol. 28, pp. 1048-1054 (1985)

F. Anselmet, H. Djeridi, L. Fulachier, Joint statistics of a passive scalar and its dissipation in turbulent flows, ***Journal of Fluid Mechanics***, vol. 280(10), pp. 173-197 (1994)

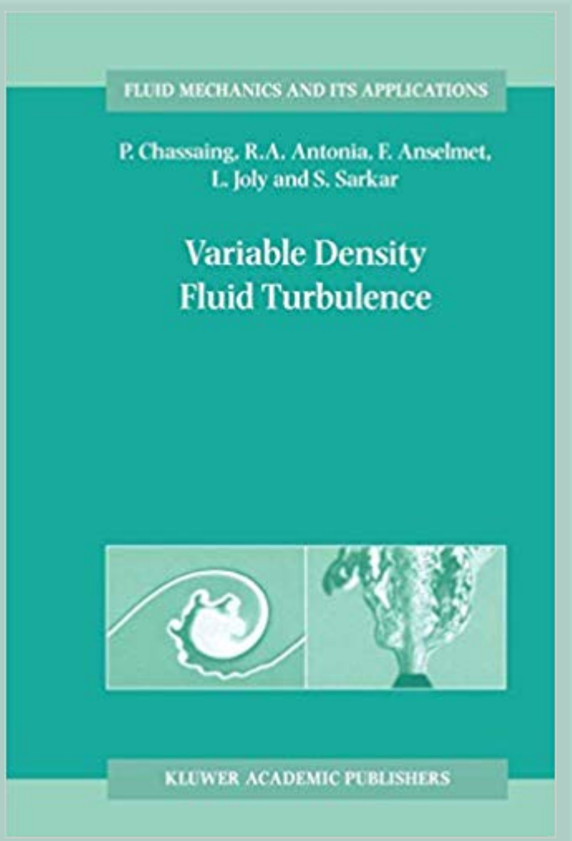
J. Mi, R.A. Antonia, F. Anselmet, Joint statistics between temperature and its dissipation rate components in a round ***Physics of Fluids***, vol. 7(7), pp. 1665-1673 (1995)

Some among the various contributions of Fabien in this field of research

Scalar mixing and **variable density turbulence**

Seminal papers with some of them focused on the link between fluctuations of a passive scalar and its dissipation rate (see below), an important problem for turbulent flow modelling both with and without chemical reactions

… and a **reference book** in the field



FLUID MECHANICS AND ITS APPLICATIONS

P. Chassaing, R.A. Antonia, F. Anselmet,
L. Joly and S. Sarkar

Variable Density
Fluid Turbulence

KLUWER ACADEMIC PUBLISHERS

F. Anselmet, R.A. Antonia, Joint statistics between temperature and its dissipation in a turbulent jet, ***The Physics of Fluids***, vol. 28, pp. 1048-1054 (1985)

F. Anselmet, H. Djeridi, L. Fulachier, Joint statistics of a passive scalar and its dissipation in turbulent flows, ***Journal of Fluid Mechanics***, vol. 280(10), pp. 173-197 (1994)

J. Mi, R.A. Antonia, F. Anselmet, Joint statistics between temperature and its dissipation rate components in a round ***Physics of Fluids***, vol. 7(7), pp. 1665-1673 (1995)

1- Scalar mixing and variable density turbulence

Small-scale scalar mixing : the **scalar dissipation rate** (SDR)

$$N_\xi = D \frac{\partial \xi}{\partial x_k}\frac{\partial \xi}{\partial x_k}$$

product of the **diffusivity** and **squared scalar gradient**

- positive-defined quantity
- measures the (local) mixing rate
- related to a characteristic mixing time (mixing frequency)

Its **transport equation** reads

$$\mathrm{L}\left(\rho N_\xi\right) = \rho \frac{D N_\xi}{Dt} - \frac{\partial}{\partial x_k}\left(\rho D \frac{\partial N_\xi}{\partial x_k}\right)$$

$$\mathrm{L}\left(\overline{\rho N_\xi}\right) = \frac{\partial}{\partial t}\left(\overline{\rho N_\xi}\right) + \frac{\partial}{\partial x_k}\left(\overline{\rho u_k N_\xi}\right) - \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial N_\xi}{\partial x_k}}\right)$$

$$= \mathrm{TSI} + 2\overline{\rho D^2 \frac{\partial^2 \xi}{\partial x_i \partial x_j}\frac{\partial^2 \xi}{\partial x_i \partial x_j}} + \mathrm{OT}$$

with OT for others terms (including reaction, vaporization, etc.)

Turbulence-scalar interaction (TSI): one of the leading-order term

$$\mathrm{TSI} = -2\overline{\rho D \frac{\partial \xi}{\partial x_i}\frac{\partial u_i}{\partial x_j}\frac{\partial \xi}{\partial x_j}}$$

SDR tensor $D \frac{\partial \xi}{\partial x_i}\frac{\partial \xi}{\partial x_j}$ and velocity gradient tensor (VGT) $\frac{\partial u_i}{\partial x_j}$

1- Scalar mixing and variable density turbulence

Turbulence-scalar interaction (TSI)

$$\mathrm{TSI} = -2\overline{\rho D \frac{\partial \xi}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial \xi}{\partial x_j}}$$

The **velocity gradient tensor** (VGT)

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + W_{ij}$$

Characteristic equation of the **velocity gradient tensor** (or traceless counterpart $\boldsymbol{A}^*$)

$$\lambda^3 + P_A \lambda^2 + Q_A \lambda + R_A = 0$$

with the three **invariants** P_A, Q_A, and R_A defined by the following expressions

$$P_A = -S_{ii}$$

$$Q_A = \frac{1}{2}\left(P_A - S_{ij} S_{ji} - W_{ij} W_{ji}\right)$$

$$R_A = \frac{1}{3}\left(-P_A^3 + 3 P_A Q_A - S_{ij} S_{jk} S_{ki} - W_{ij} W_{jk} W_{ki}\right)$$

1- Scalar mixing and variable density turbulence

Turbulence-scalar interaction (TSI)

$$\mathrm{TSI} = -2\overline{\rho D \frac{\partial \xi}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial \xi}{\partial x_j}}$$

The **velocity gradient tensor**

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + W_{ij}$$

Anti-symmetric (skew-symmetric) part W_{ij} : modifies the **orientation** of the scalar gradient but not (at least directly) the norm of the scalar gradient (dissipation rate)

$$-2\rho D \frac{\partial \xi}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial \xi}{\partial x_j} = -2\rho D \frac{\partial \xi}{\partial x_i} S_{ij} \frac{\partial \xi}{\partial x_j} = -2\rho N_\xi \left(\boldsymbol{n}_\xi^T \cdot \boldsymbol{S} \cdot \boldsymbol{n}_\xi\right) \quad \text{with} \quad \boldsymbol{n}_\xi = \boldsymbol{\nabla}\xi / \|\boldsymbol{\nabla}\xi\|$$

Symmetric part S_{ij} : can be made **diagonal** (eigenvalues λ_i and eigenvectors $\boldsymbol{e}_i$)

Once written **in the strain-rate tensor eigen-frame**

$$\mathrm{TSI} = -2\rho N_\xi \sum_{i=1}^{i=3} \lambda_i \cos^2\left(\boldsymbol{n}_\xi, \boldsymbol{e}_i\right)$$

Scalar dissipation rate (SDR)

$$N_\xi = D \frac{\partial \xi}{\partial x_k} \frac{\partial \xi}{\partial x_k}$$

Turbulence-scalar interaction (TSI)

$$\mathrm{TSI} = -2\rho D \frac{\partial \xi}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial \xi}{\partial x_j}$$

Velocity gradient tensor

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + W_{ij}$$

Scalar gradient orientation in the strain-rate tensor eigen-frame

$$\hat{n}_i = \boldsymbol{n}_\xi \cdot \boldsymbol{e}_i = \cos\left(\boldsymbol{n}_\xi, \boldsymbol{e}_i\right) = \boldsymbol{R}^T \cdot \boldsymbol{n}_\xi \quad \text{avec} \quad \boldsymbol{R} = [\boldsymbol{e}_1 | \boldsymbol{e}_2 | \boldsymbol{e}_3]$$

1- Scalar mixing and variable density turbulence

Scalar dissipation rate (SDR)

$$N_\xi = D \frac{\partial \xi}{\partial x_k} \frac{\partial \xi}{\partial x_k}$$

Turbulence-scalar interaction (TSI)

$$\mathrm{TSI} = -2\rho D \frac{\partial \xi}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial \xi}{\partial x_j}$$

Velocity gradient tensor

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + W_{ij}$$

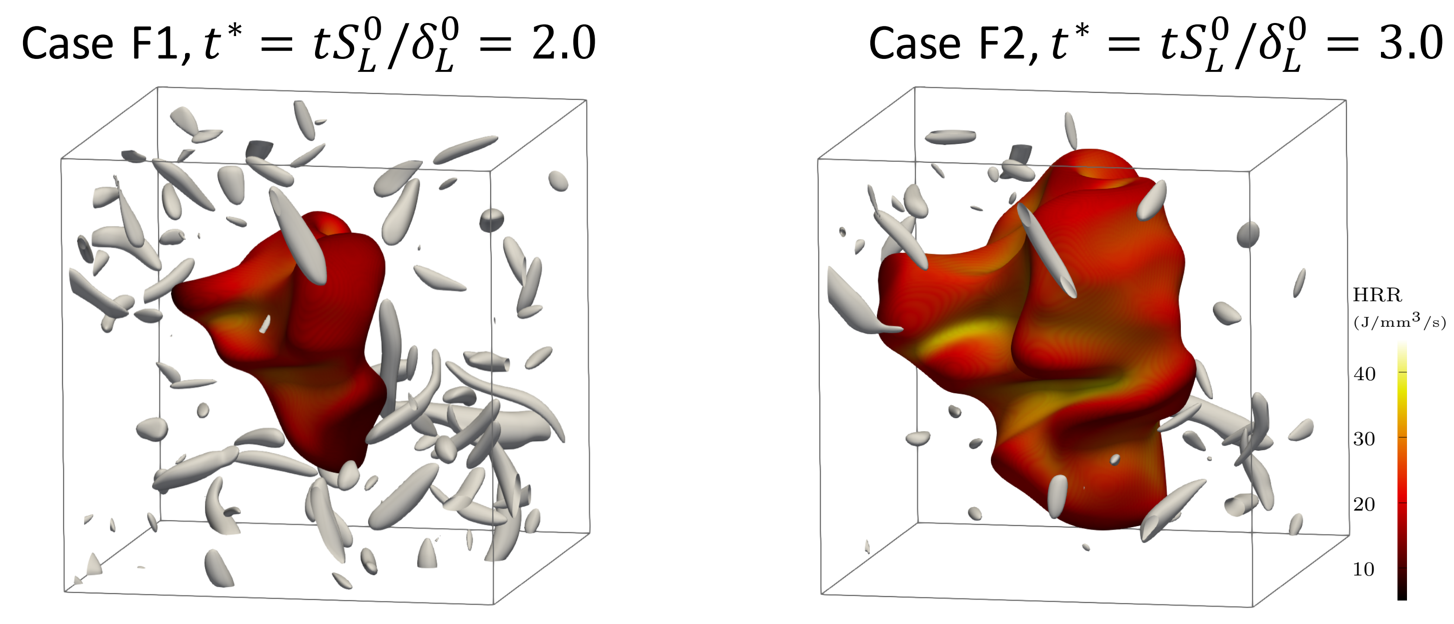
Scalar gradient orientation in the strain-rate tensor eigen-frame

$$\hat{n}_i = \boldsymbol{n}_\xi \cdot \boldsymbol{e}_i = \cos\left(\boldsymbol{n}_\xi, \boldsymbol{e}_i\right) = \boldsymbol{R}^T \cdot \boldsymbol{n}_\xi \quad \text{avec} \quad \boldsymbol{R} = [\boldsymbol{e}_1 | \boldsymbol{e}_2 | \boldsymbol{e}_3]$$

Let us take a closer look at these quantities in non-standard turbulent flow conditions

2- Flame kernel development in homogeneous turbulence

Weakly turbulent premixed flame databases



Case F1, $t^* = tS_L^0/\delta_L^0 = 2.0$

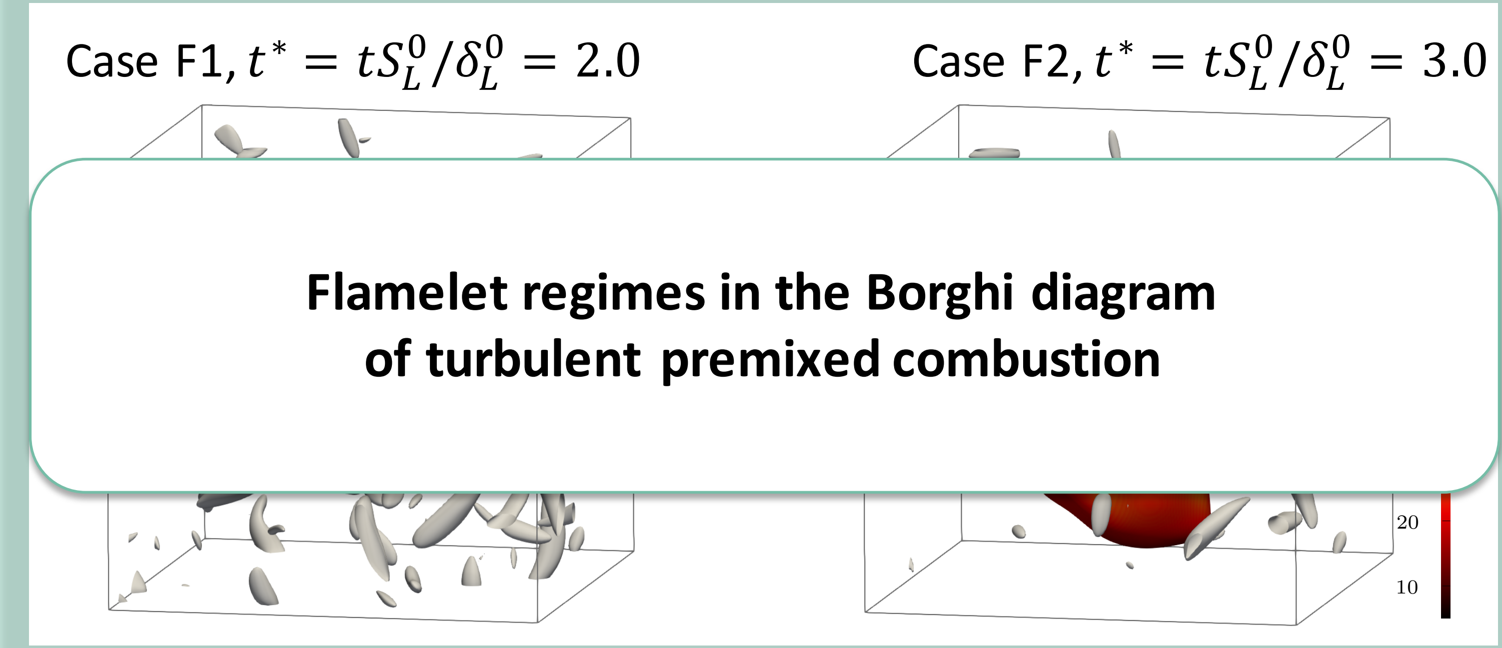
Case F2, $t^* = tS_L^0/\delta_L^0 = 3.0$

Simulation	l_t/δ_L^0	u_{RMS}/S_L^0	Da	Ka	N_B
F1	33	0.7	55	0.11	1.65
F2	22	1.4	15	0.37	0.83

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Weakly turbulent premixed flame databases



Case F1, $t^* = tS_L^0/\delta_L^0 = 2.0$

Case F2, $t^* = tS_L^0/\delta_L^0 = 3.0$

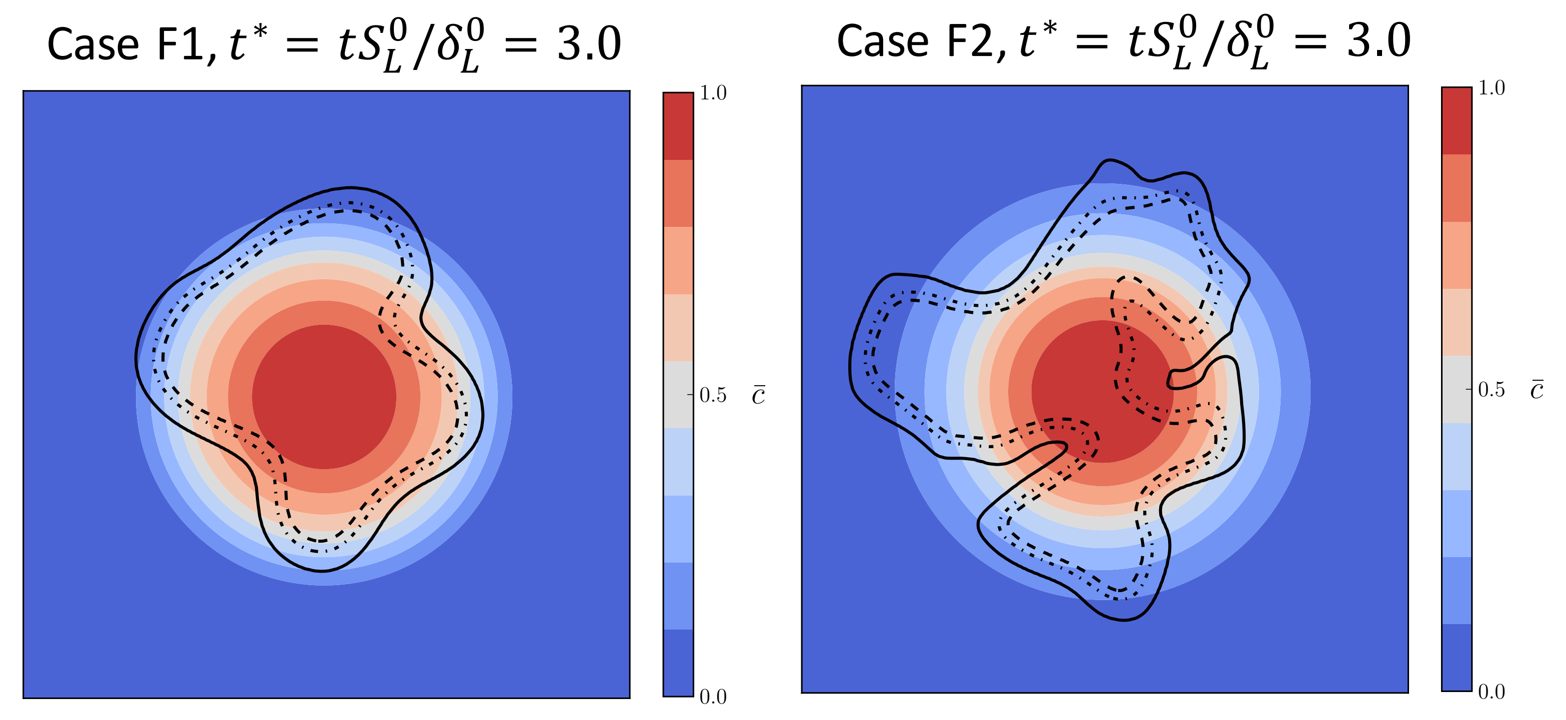
Flamelet regimes in the Borghi diagram of turbulent premixed combustion

Simulation	l_t/δ_L^0	u_{RMS}/S_L^0	Da	Ka	N_B
F1	33	0.7	55	0.11	1.65
F2	22	1.4	15	0.37	0.83

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Field of the **averaged progress variable** together with **three instantaneous progress variable iso-lines** issued from a cut-plane of the computational domain

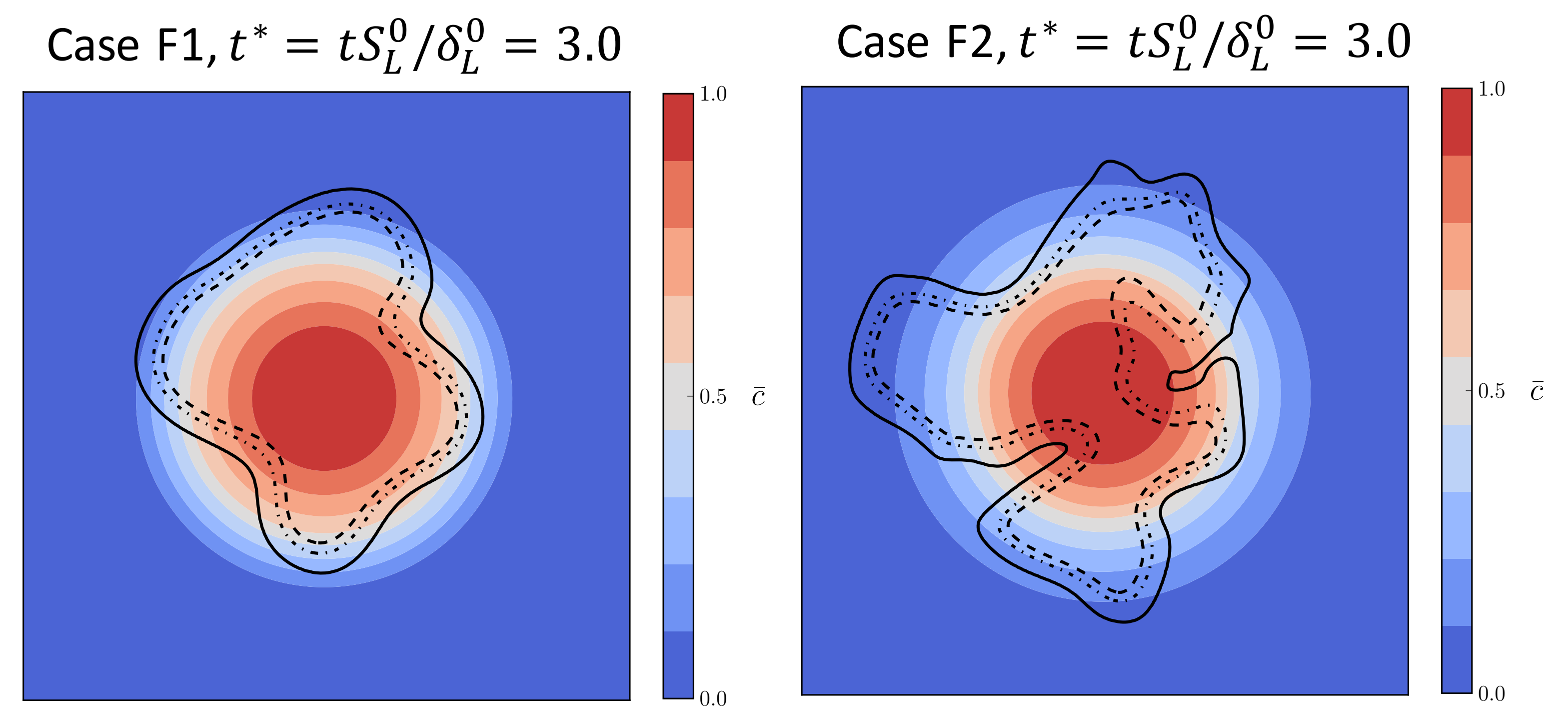


Case F1, $t^* = tS_L^0/\delta_L^0 = 3.0$

Case F2, $t^* = tS_L^0/\delta_L^0 = 3.0$

2- Flame kernel development in homogeneous turbulence

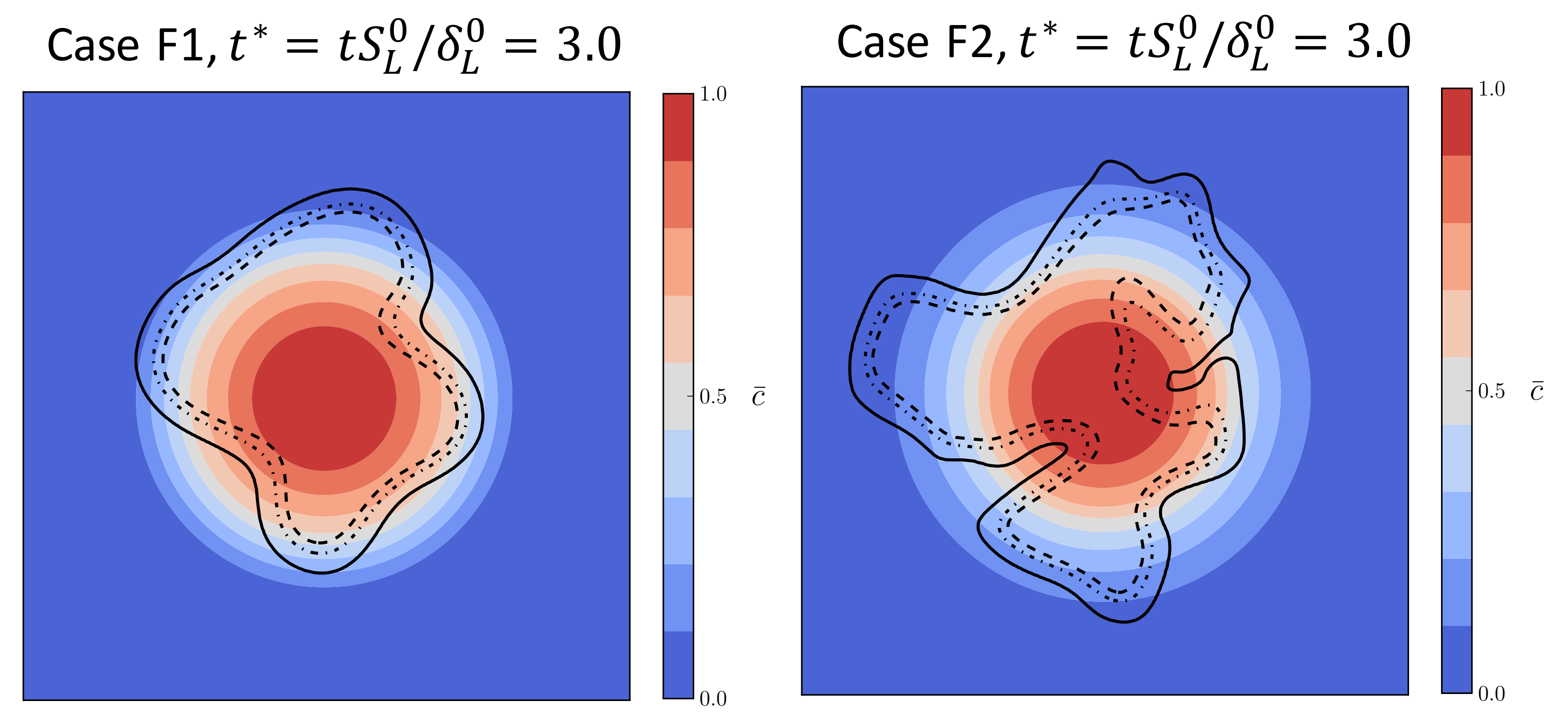
Field of the **averaged progress variable** together with **three instantaneous progress variable iso-lines** issued from a cut-plane of the computational domain



A. Mura, F. Galzin, R. Borghi, A unified PDF-flamelet model for turbulent premixed combustion, ***Combustion Science and Technology***, vol. 175, pp. 1573-1609 (2003)

2- Flame kernel development in homogeneous turbulence

Field of the **averaged progress variable** together with **three instantaneous progress variable iso-lines** issued from a cut-plane of the computational domain

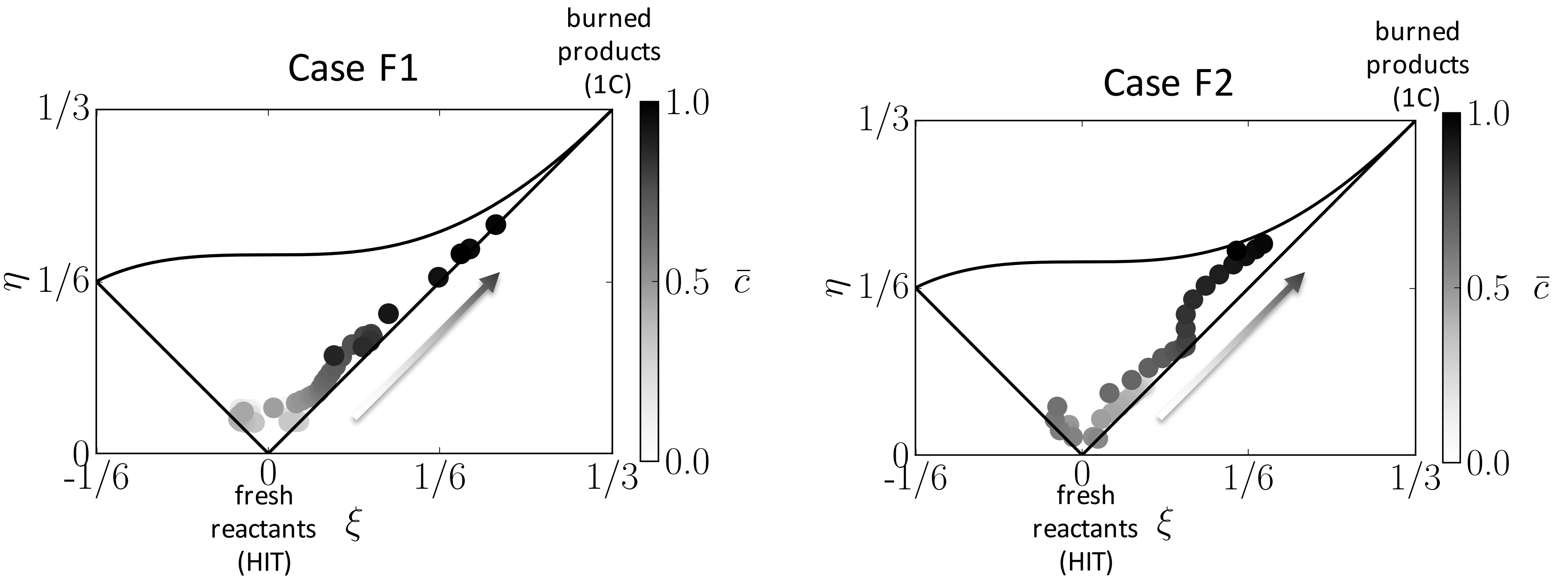


A. Mura, F. Galzin, R. Borghi, A unified PDF-flamelet model for turbulent premixed combustion, ***Combustion Science and Technology***, vol. 175, pp. 1573-1609 (2003)

K.Q.N. Kha, V. Robin, A. Mura, M. Champion, Implications of laminar flame finite thickness on the structure of turbulent premixed flames, ***Journal of Fluid Mechanics***, vol. 787, pp. 116-147 (2016)

2- Flame kernel development in homogeneous turbulence

Reynolds stress **anisotropy** for increasing values of the **mean progress variable**

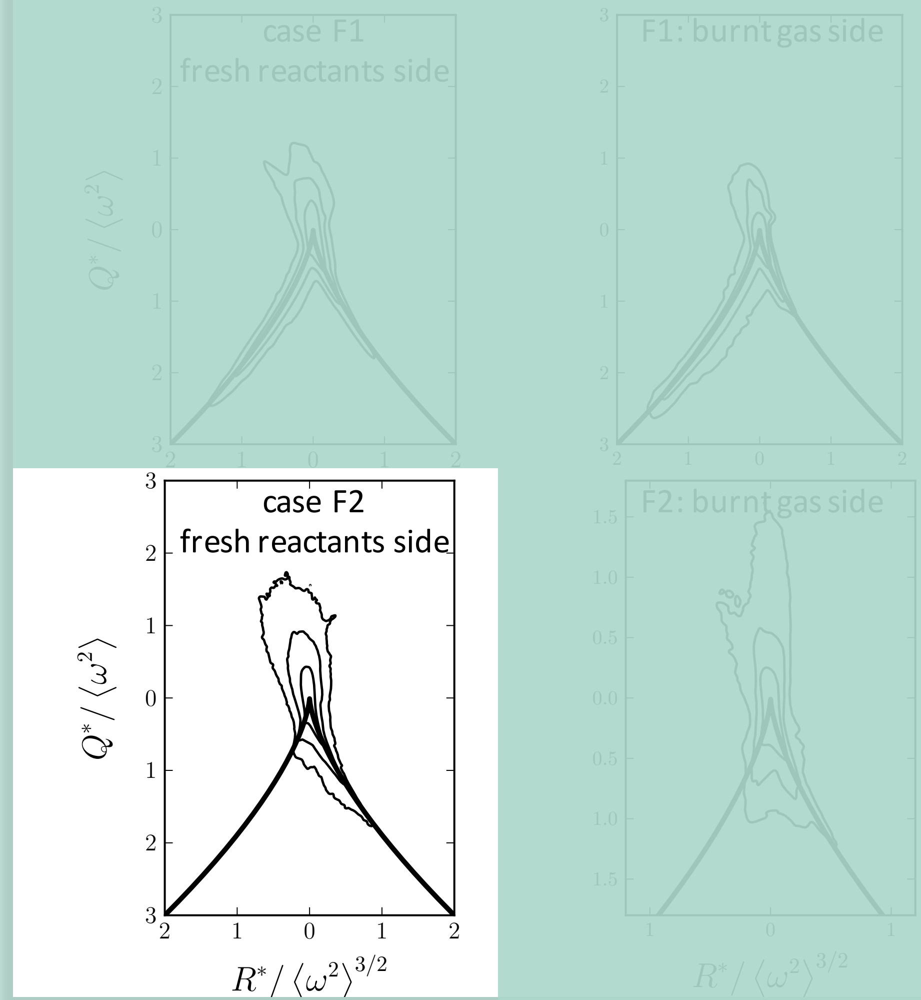


From **3D isotropic turbulence** (fresh reactants) towards **one-component turbulence** (burned products)

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

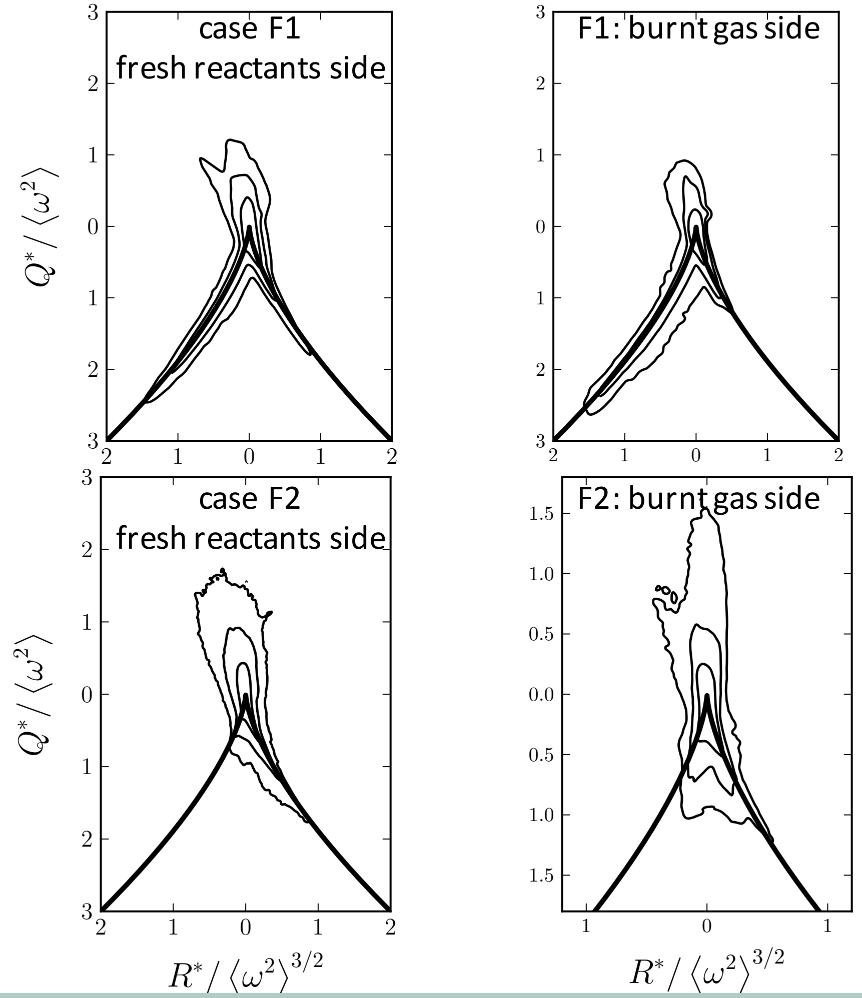
2- Flame kernel development in homogeneous turbulence

Weakly turbulent premixed flame databases



S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

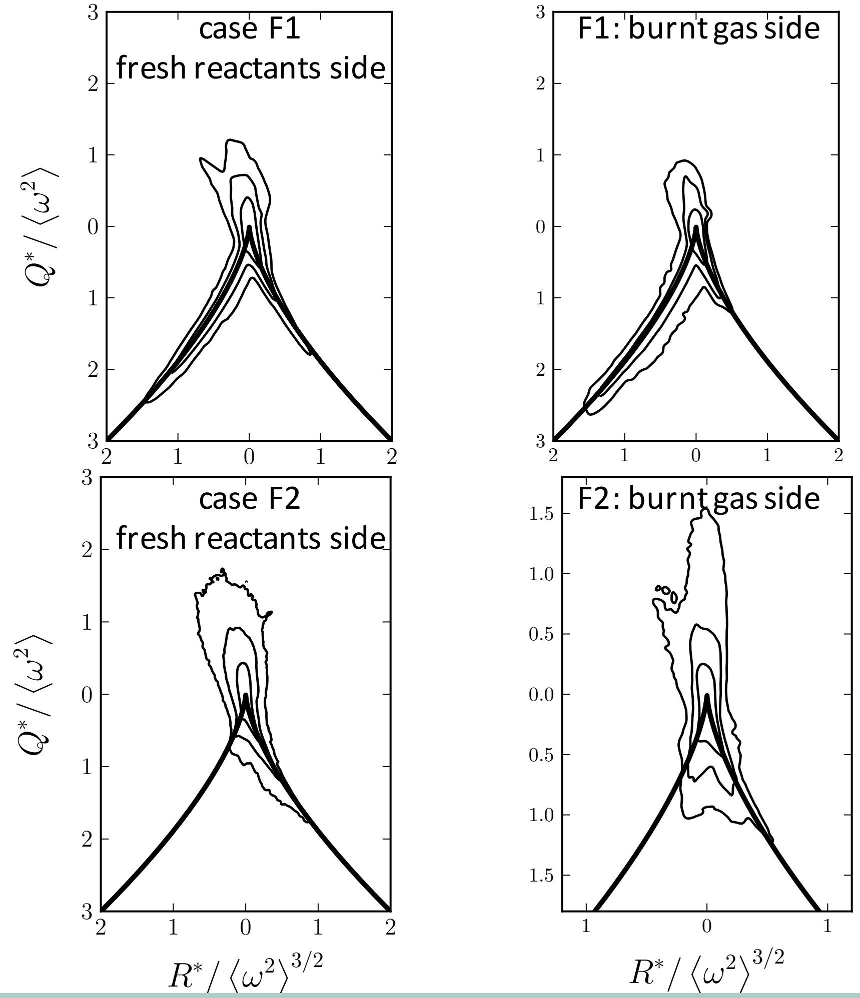
Weakly turbulent premixed flame databases



S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Weakly turbulent premixed flame databases

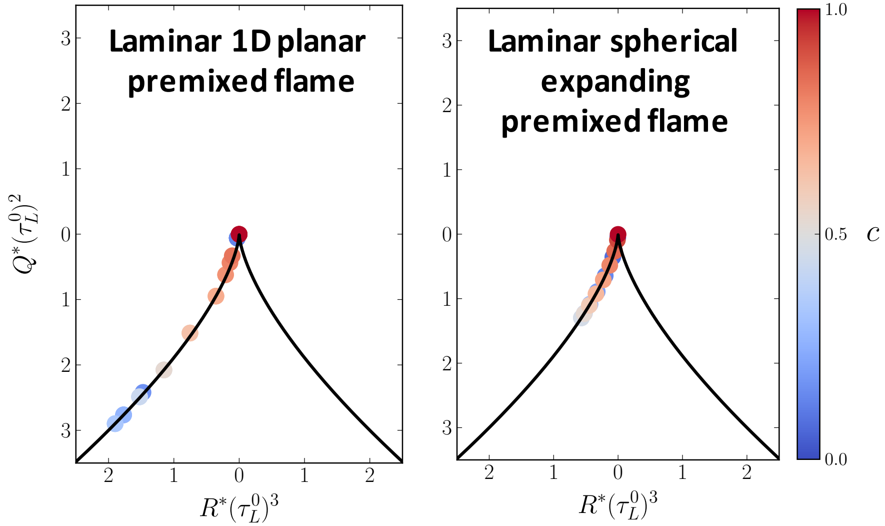


VGT across a one-dimensional flame: $A = \begin{bmatrix} E_f & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

with $E_f = \tau S_L^0/\delta_L^0$

Traceless VGT:: $A^* = \begin{bmatrix} 2E_f/3 & 0 & 0 \\ 0 & -E_f/3 & 0 \\ 0 & 0 & -E_f/3 \end{bmatrix}$

which verifies the left branch of the zero discriminant



S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Evolution of the **reactive scalar gradient orientation** vector

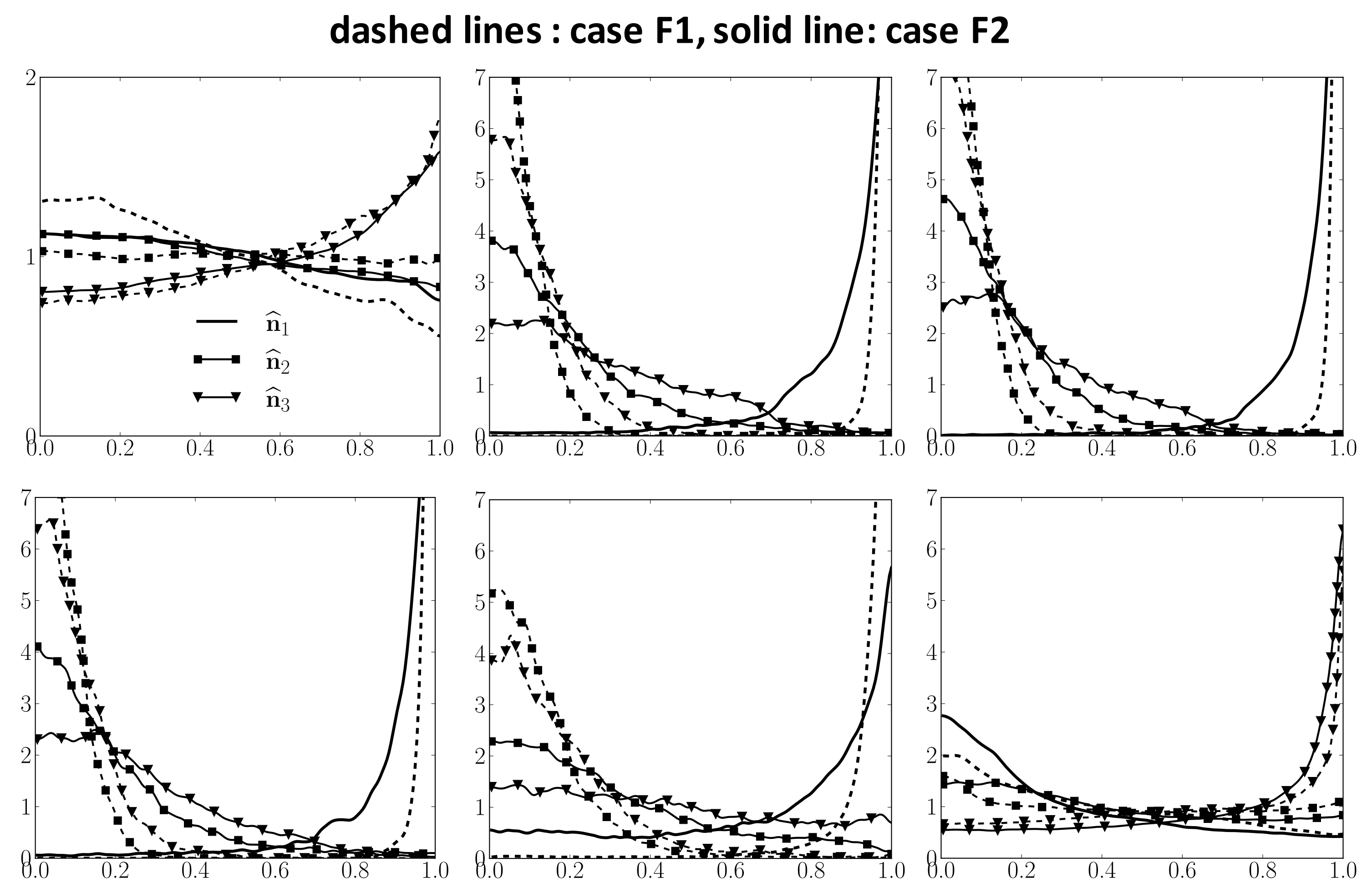
$$\hat{\boldsymbol{n}} = \begin{pmatrix} \hat{n}_1 \\ \hat{n}_2 \\ \hat{n}_3 \end{pmatrix} = \begin{pmatrix} \boldsymbol{n}_c \cdot \boldsymbol{e}_1 \\ \boldsymbol{n}_c \cdot \boldsymbol{e}_2 \\ \boldsymbol{n}_c \cdot \boldsymbol{e}_3 \end{pmatrix} = \begin{pmatrix} \cos(\boldsymbol{n}_c, \boldsymbol{e}_1) \\ \cos(\boldsymbol{n}_c, \boldsymbol{e}_2) \\ \cos(\boldsymbol{n}_c, \boldsymbol{e}_3) \end{pmatrix} = \boldsymbol{R}^T \cdot \boldsymbol{n}_c \qquad \boldsymbol{n_c} = \boldsymbol{\nabla} c / \|\boldsymbol{\nabla} c\|$$

with $c \in [0; 1]$ a progress variable (normalized temperature or mass fraction)

2- Flame kernel development in homogeneous turbulence

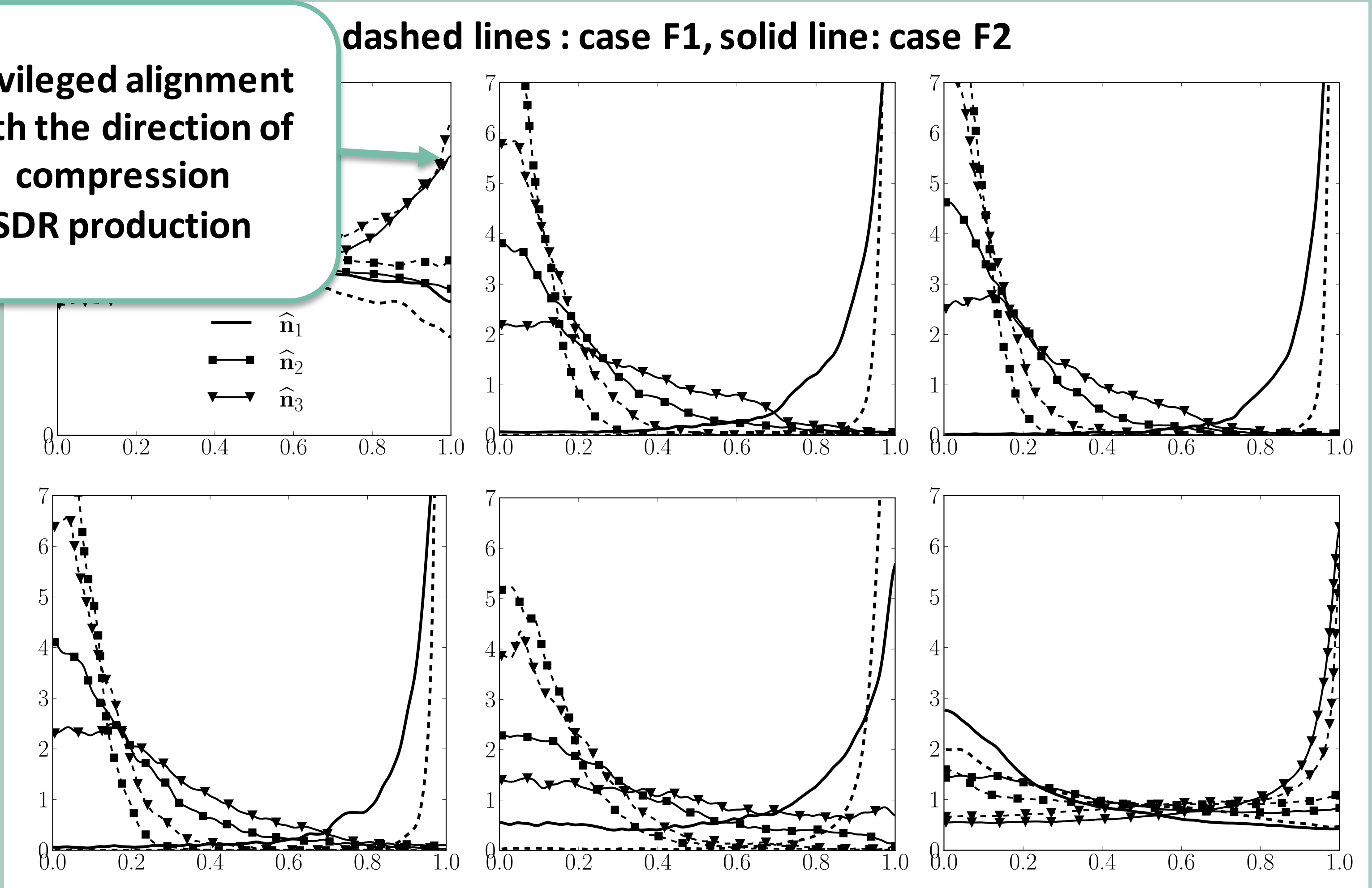
Evolution of the reactive scalar gradient orientation vector

dashed lines : case F1, solid line: case F2



S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

Evolution of the **reactive scalar gradient orientation** vector



Privileged alignment with the direction of compression SDR production

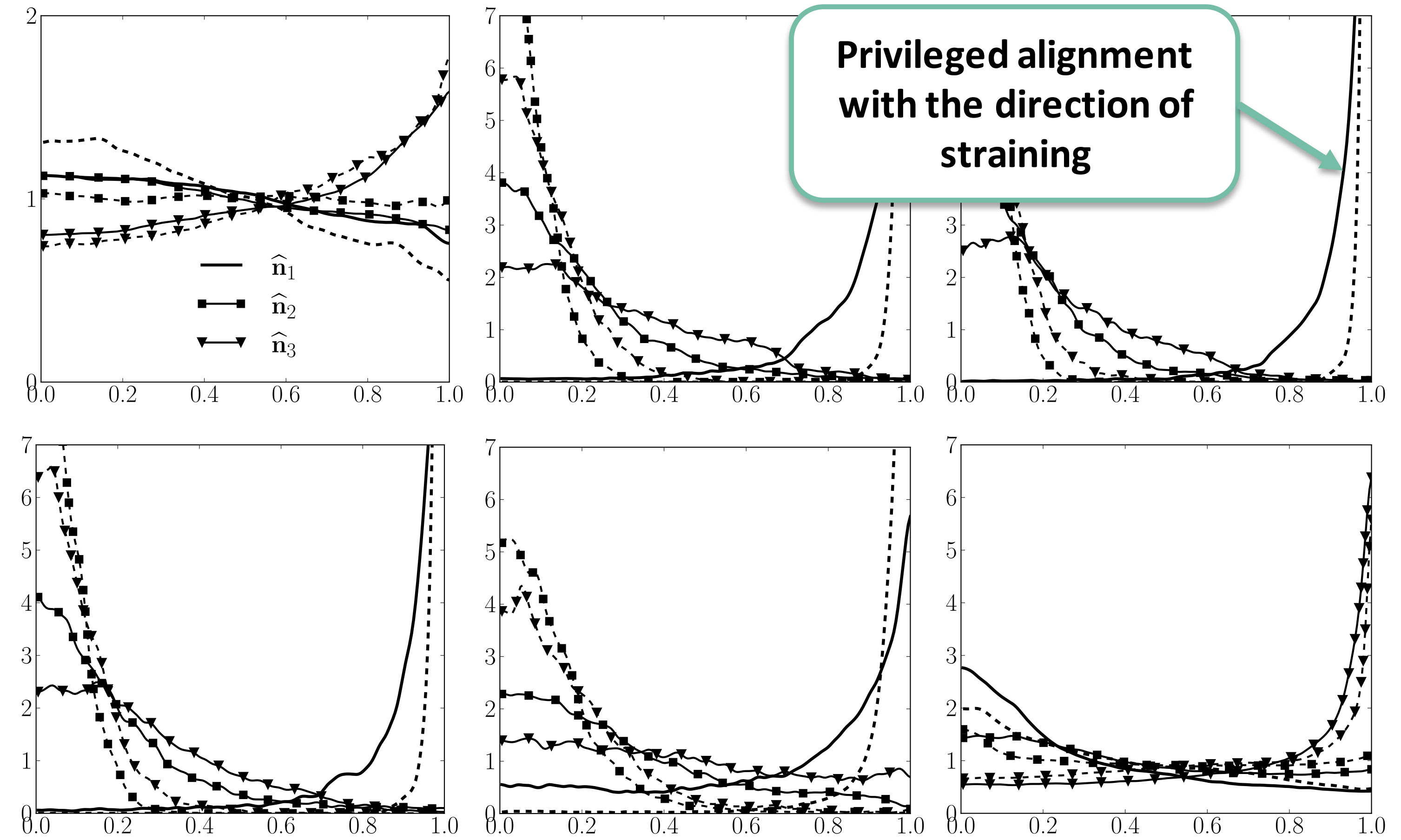
dashed lines : case F1, solid line: case F2

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Evolution of the **reactive scalar gradient orientation** vector

dashed lines : case F1, solid line: case F2



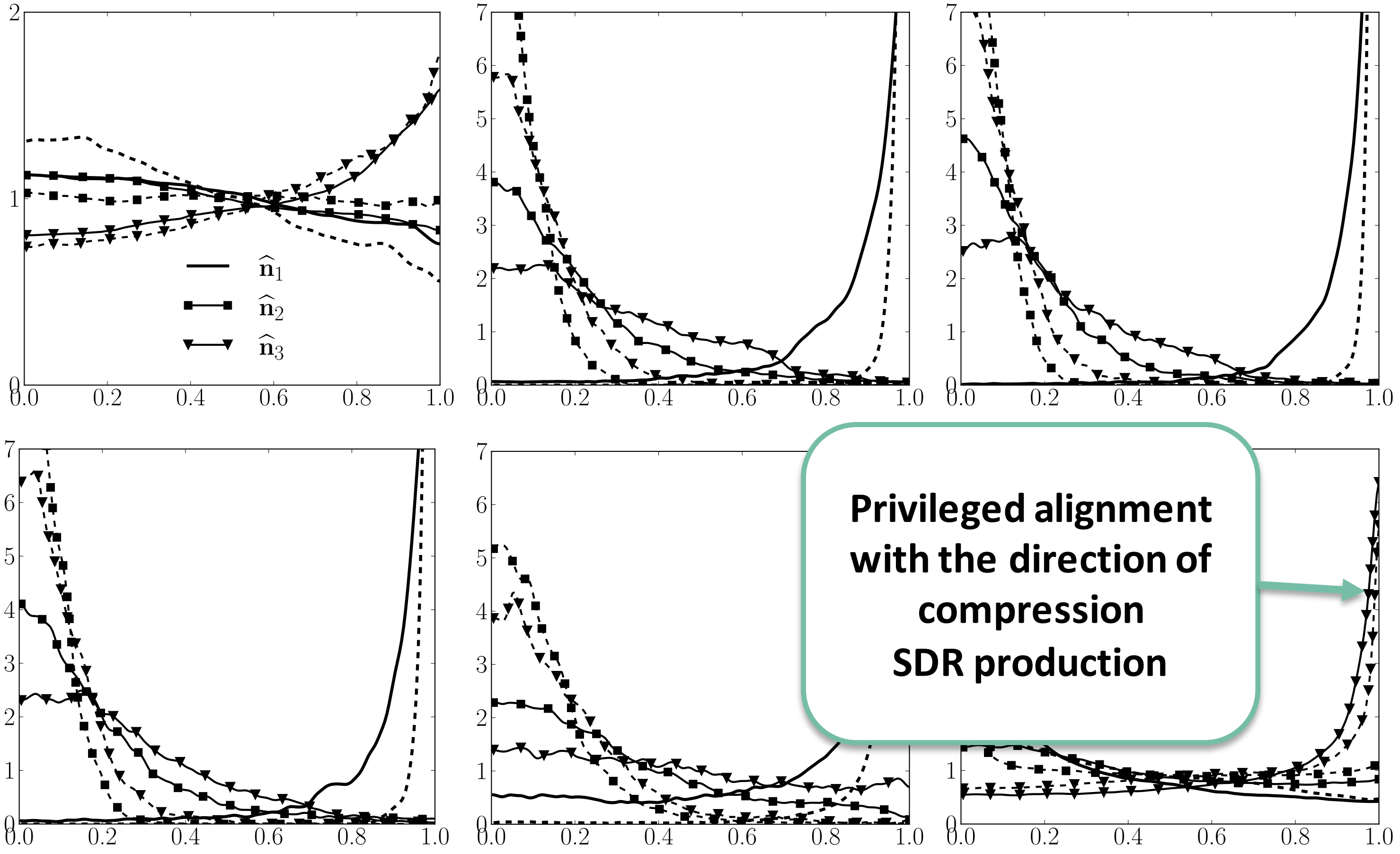
Privileged alignment with the direction of straining

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Evolution of the **reactive scalar gradient orientation** vector

dashed lines : case F1, solid line: case F2

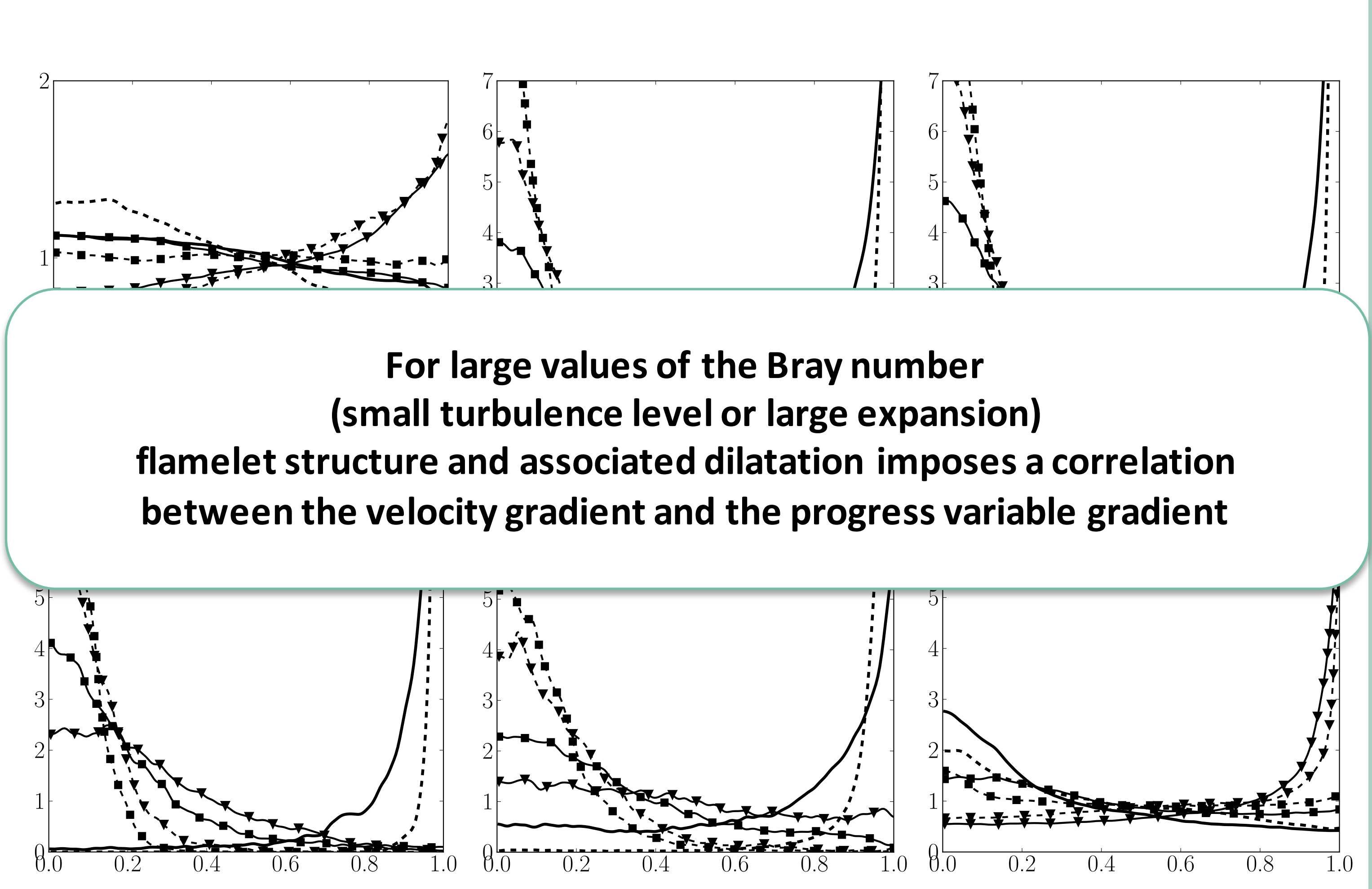


Privileged alignment with the direction of compression
SDR production

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Evolution of the **reactive scalar gradient orientation** vector



For large values of the Bray number
(small turbulence level or large expansion)
flamelet structure and associated dilatation imposes a correlation
between the velocity gradient and the progress variable gradient

A. Mura, K. Tsuboi, T. Hasegawa, Modelling of the correlation between velocity and reactive scalar gradients in turbulent premixed flames based on DNS data, ***Combustion Theory and Modelling,*** vol. 12, pp. 671-698 (2008)

2- Flame kernel development in homogeneous turbulence

Evolution of the **reactive scalar gradient orientation** vector

$$\hat{\boldsymbol{n}} = \begin{pmatrix} \hat{n}_1 \\ \hat{n}_2 \\ \hat{n}_3 \end{pmatrix} = \begin{pmatrix} \boldsymbol{n}_c \cdot \boldsymbol{e}_1 \\ \boldsymbol{n}_c \cdot \boldsymbol{e}_2 \\ \boldsymbol{n}_c \cdot \boldsymbol{e}_3 \end{pmatrix} = \begin{pmatrix} \cos(\boldsymbol{n}_c, \boldsymbol{e}_1) \\ \cos(\boldsymbol{n}_c, \boldsymbol{e}_2) \\ \cos(\boldsymbol{n}_c, \boldsymbol{e}_3) \end{pmatrix} = \boldsymbol{R}^T \cdot \boldsymbol{n}_c \qquad \boldsymbol{n}_c = \boldsymbol{\nabla} c / \|\boldsymbol{\nabla} c\|$$

with $c \in [0; 1]$ a progress variable (normalized temperature or mass fraction)

Lagrangian evolution of the orientation vector: $\frac{D\hat{\boldsymbol{n}}}{Dt} = \mathbf{GR} + \mathbf{TS} + \mathbf{TW} + \mathbf{WN}$

GR: reactive scalar transport

TS: direct effect of strain rate

TW: vorticity effects

WN: rotation of the eigenframe

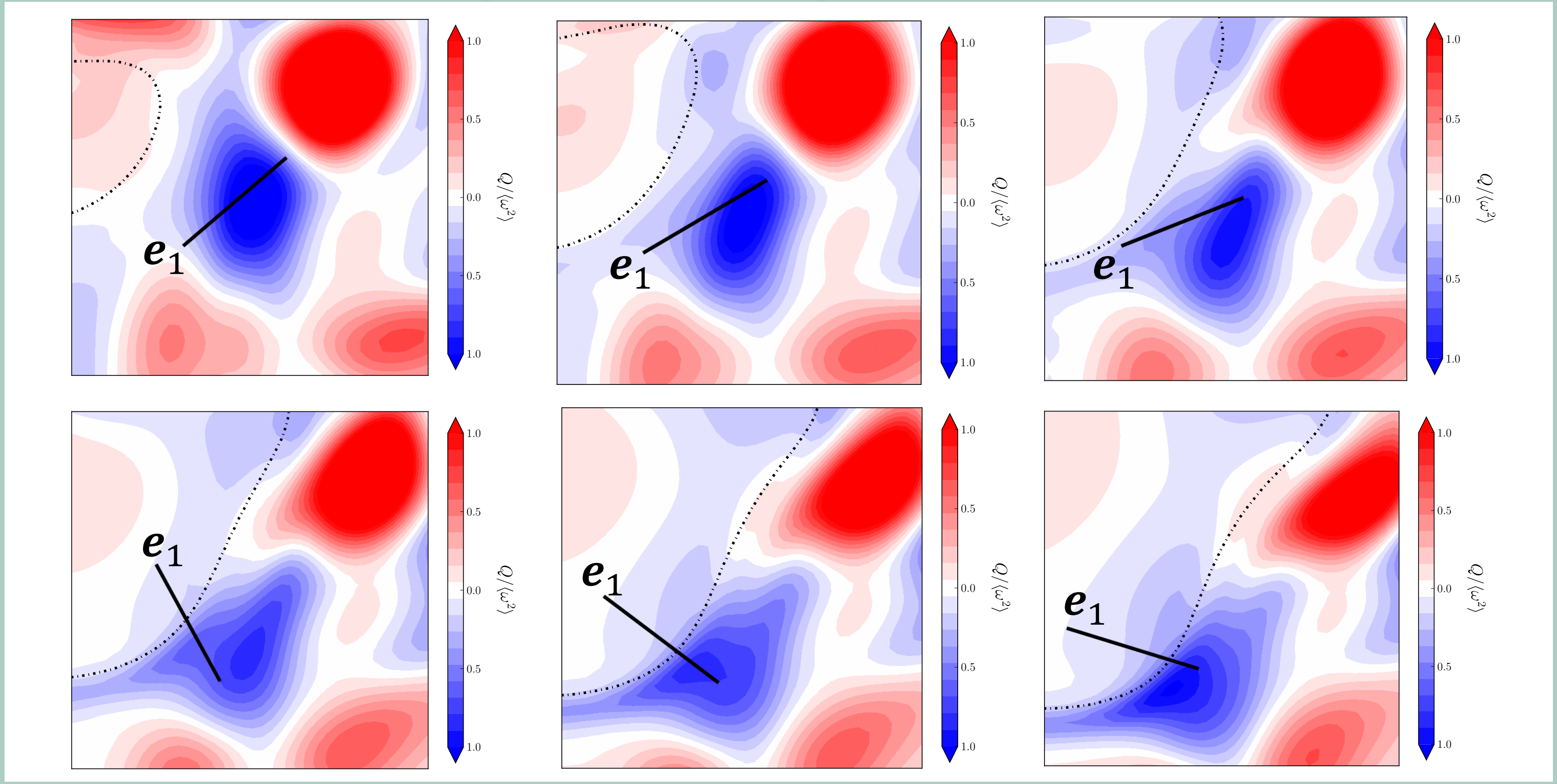
$$\mathrm{TSI} = -2\mathrm{N}_c(\boldsymbol{n}_c^T \cdot \boldsymbol{S} \cdot \boldsymbol{n}_c) = -2\mathrm{N}_c \sum_{i=1}^{i=3} \lambda_i \,\hat{\boldsymbol{n}}_i^{\,2} \quad \text{where} \quad N_c = D\,\frac{\partial c}{\partial x_i}\,\frac{\partial c}{\partial x_i}$$

K.K. Nomura, G.K. Post, The structure and dynamics of vorticity and rate of strain in incompressible homogeneous turbulence, ***Journal of Fluid Mechanics***, vol. 377, 65–97 (1998)

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Unsteady (Lagrangian) evolution of the direction of the **most extensive strain-rate** eigenvector at one location (minimum value)



M. Gonzalez, P. Parathoën, Effects of variable mass density on the kinematics of scalar gradient, ***Physics of Fluids***, *vol.* 23 pp. 075107 (2011)

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

2- Flame kernel development in homogeneous turbulence

Evolution of the **scalar gradient orientation** vector

Evolution is piloted by the term $\mathbf{WN}$, i.e., **rotation of the eigen-frame,**

$\mathbf{WN} = \frac{D\boldsymbol{R}^T}{Dt} \cdot \boldsymbol{n}_c = \frac{D\boldsymbol{R}^T}{Dt} \cdot \boldsymbol{R} \cdot \widehat{\boldsymbol{n}} = \boldsymbol{\mathcal{W}} \cdot \widehat{\boldsymbol{n}}$ with $\boldsymbol{\mathcal{W}}$ the **rate of rotation of the principal axes** of the strain-rate tensor $\boldsymbol{S}$

$\mathbf{WN}$ contains the terms that influence the velocity gradient but written in the the eigen-vector basis, e.g., the pressure Hessian $\Pi = \boldsymbol{\nabla}(\boldsymbol{\nabla} p)$ written in the following form: $\boldsymbol{R}^{\boldsymbol{T}} \cdot \Pi \cdot \boldsymbol{R}$

A detailed inspection shows that the leading contribution is related to this **pressure Hessian** term

Non-localness, no scaling law available from the laminar premixed flame of reference, …

not good news for modellers

S. Zhao, A. Er-raiy, Z. Bouali, A. Mura, Dynamics and kinematics of the reactive scalar gradient in weakly turbulent premixed flames, ***Combustion and Flame***, 198, 436-454 (2018)

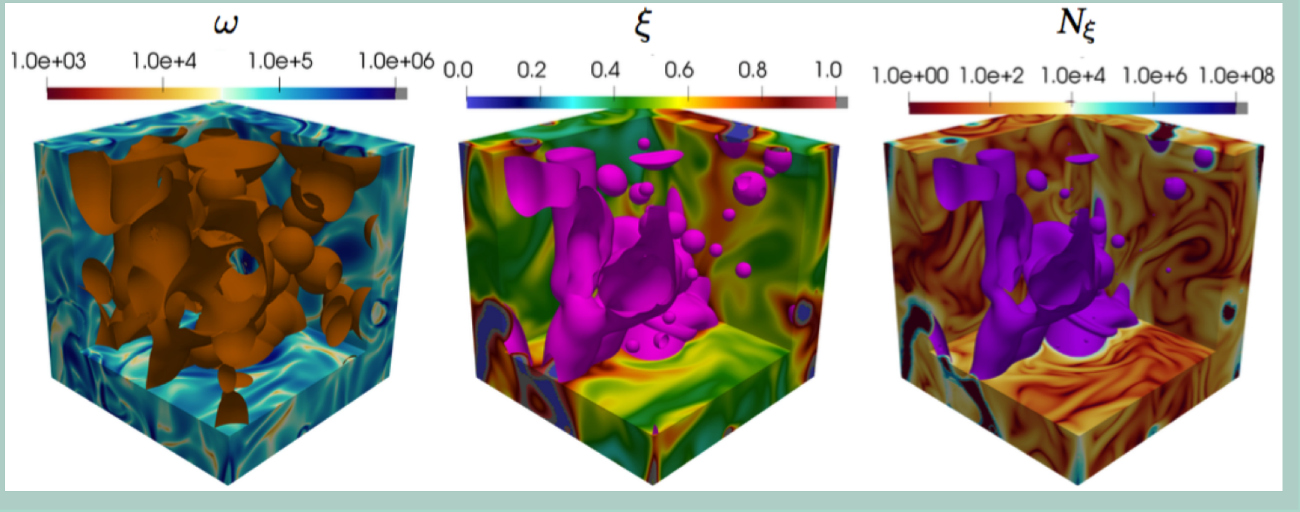
2- Vaporizing two-phase flows in homogeneous isotropic turbulence

Direct numerical simulation solver **ARCHER**

- **Spatial discretization**
  - WENO5 for convective terms
  - Central finite difference (FD) for molecular terms
- **Time discretization**
  - Third-order low storage Runge-Kutta
- **Two-phase flow description**
  - Coupled level-set / volume of fluid (CLSVOF) method interface tracking
  - Ghost-fluid method to handle jump conditions at the interface

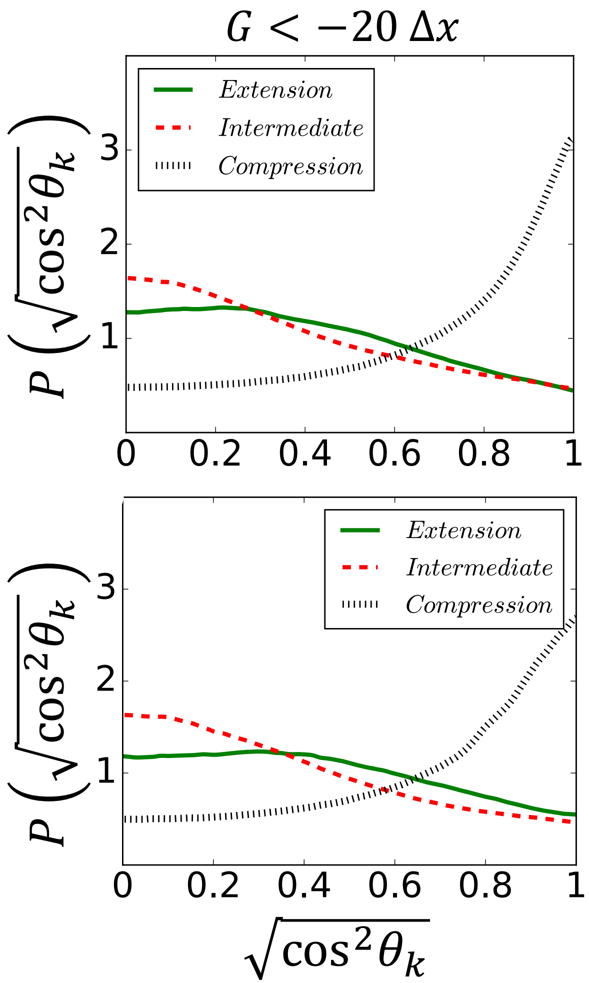
Computational setup

- Two-phase flow in HIT
- Two values of the liquid volume fraction (5% and 10%)



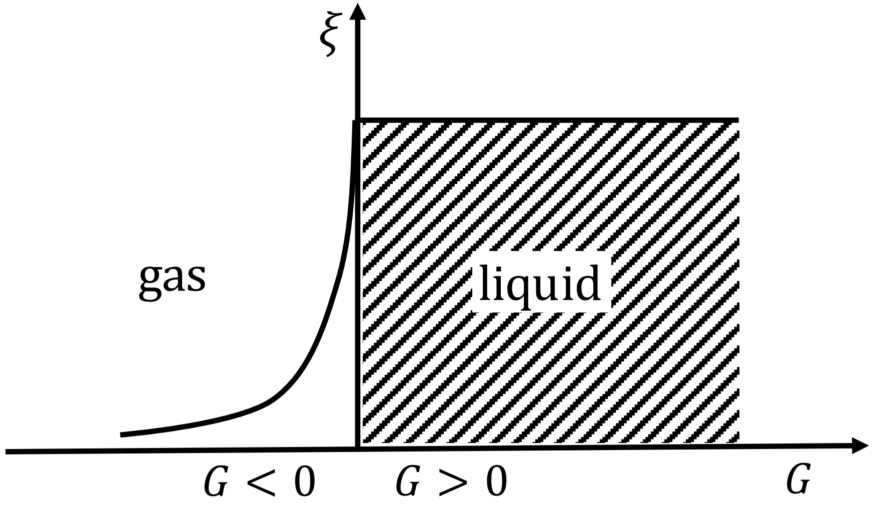
2- Vaporizing two-phase flows in homogeneous isotropic turbulence

Orientations statistics of the scalar gradient in the strain-rate eigen-frame



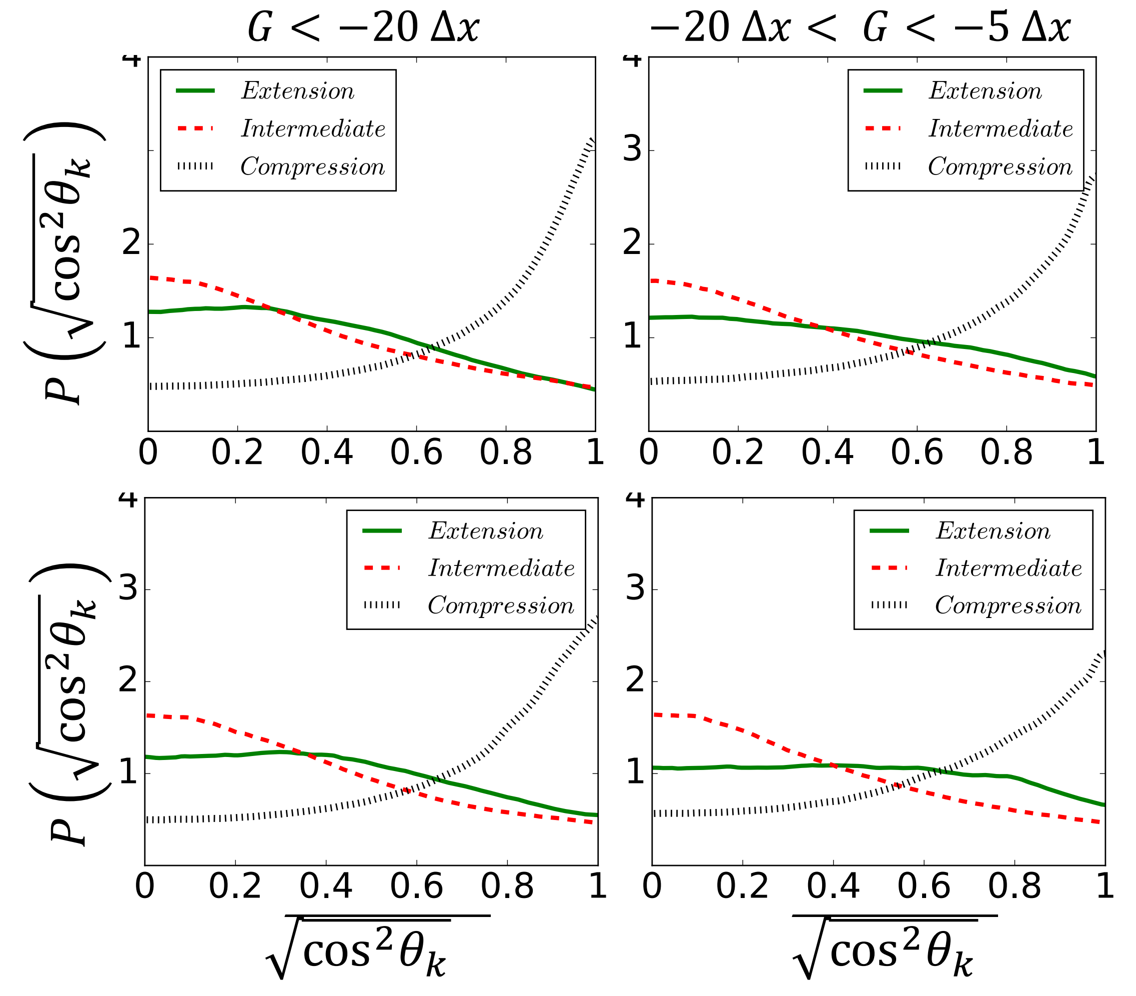
$$\theta_k = (\boldsymbol{n}_\xi, \boldsymbol{e}_k)$$

$\xi = (Y_v / Y_{v,s}) \in [0; 1]$ with $Y_{v,s}$ the saturation level of the vapour mass fraction



Z. Bouali, B. Duret, F.X. Demoulin, A. Mura, DNS analysis of small-scale turbulence-scalar interactions in evaporating two-phase flows, ***International Journal of Multiphase Flow***, vol. 85, pp. 326-335 (2018)

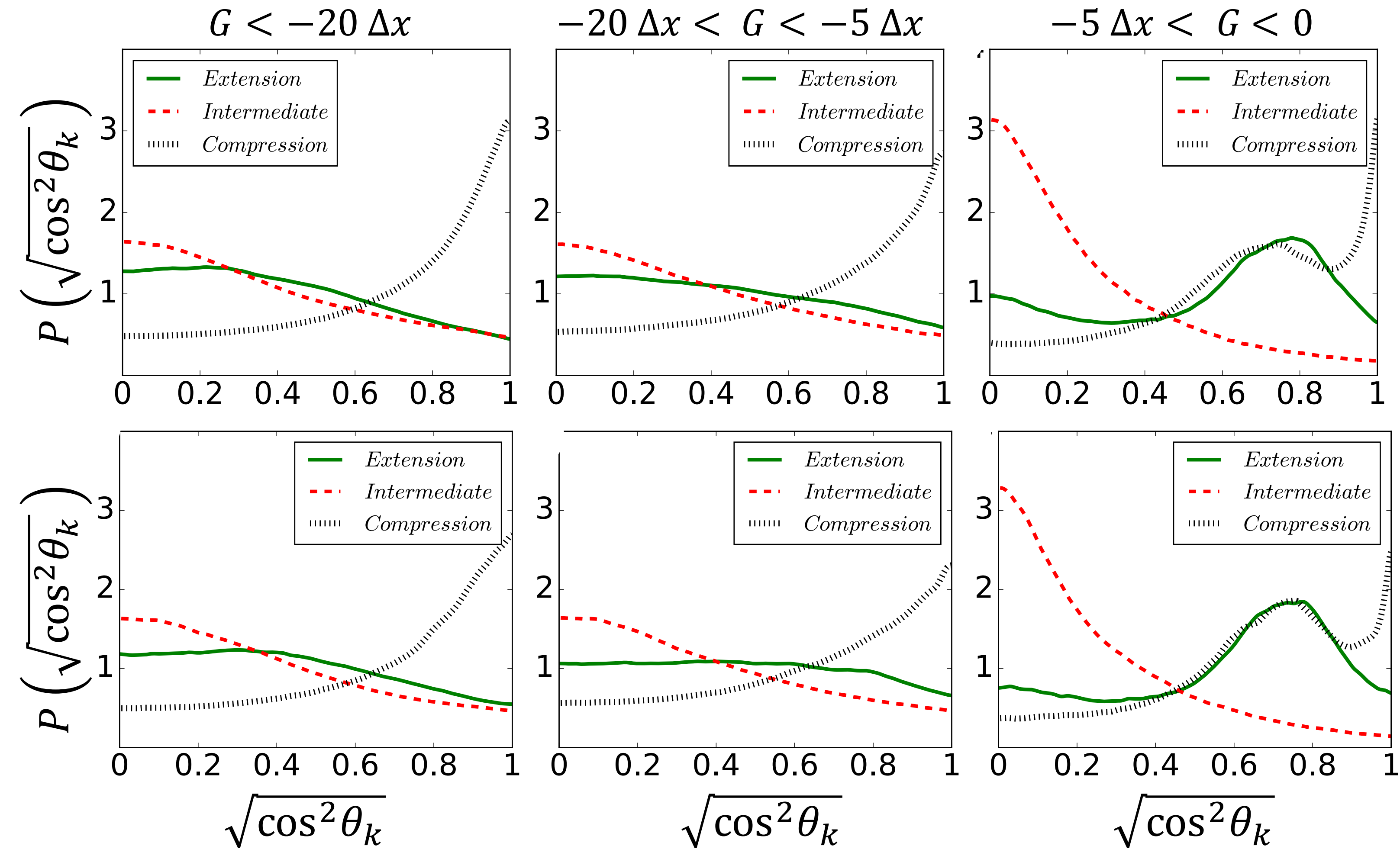
Orientations statistics of the scalar gradient in the strain-rate eigen-frame



Z. Bouali, B. Duret, F.X. Demoulin, A. Mura, DNS analysis of small-scale turbulence-scalar interactions in evaporating two-phase flows, ***International Journal of Multiphase Flow***, vol. 85, pp. 326-335 (2018)

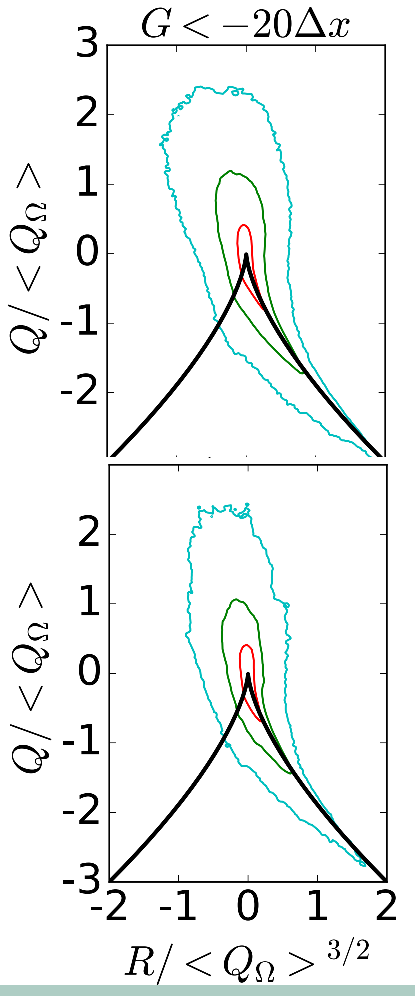
2- Vaporizing two-phase flows in homogeneous isotropic turbulence

Orientations statistics of the scalar gradient in the strain-rate eigen-frame



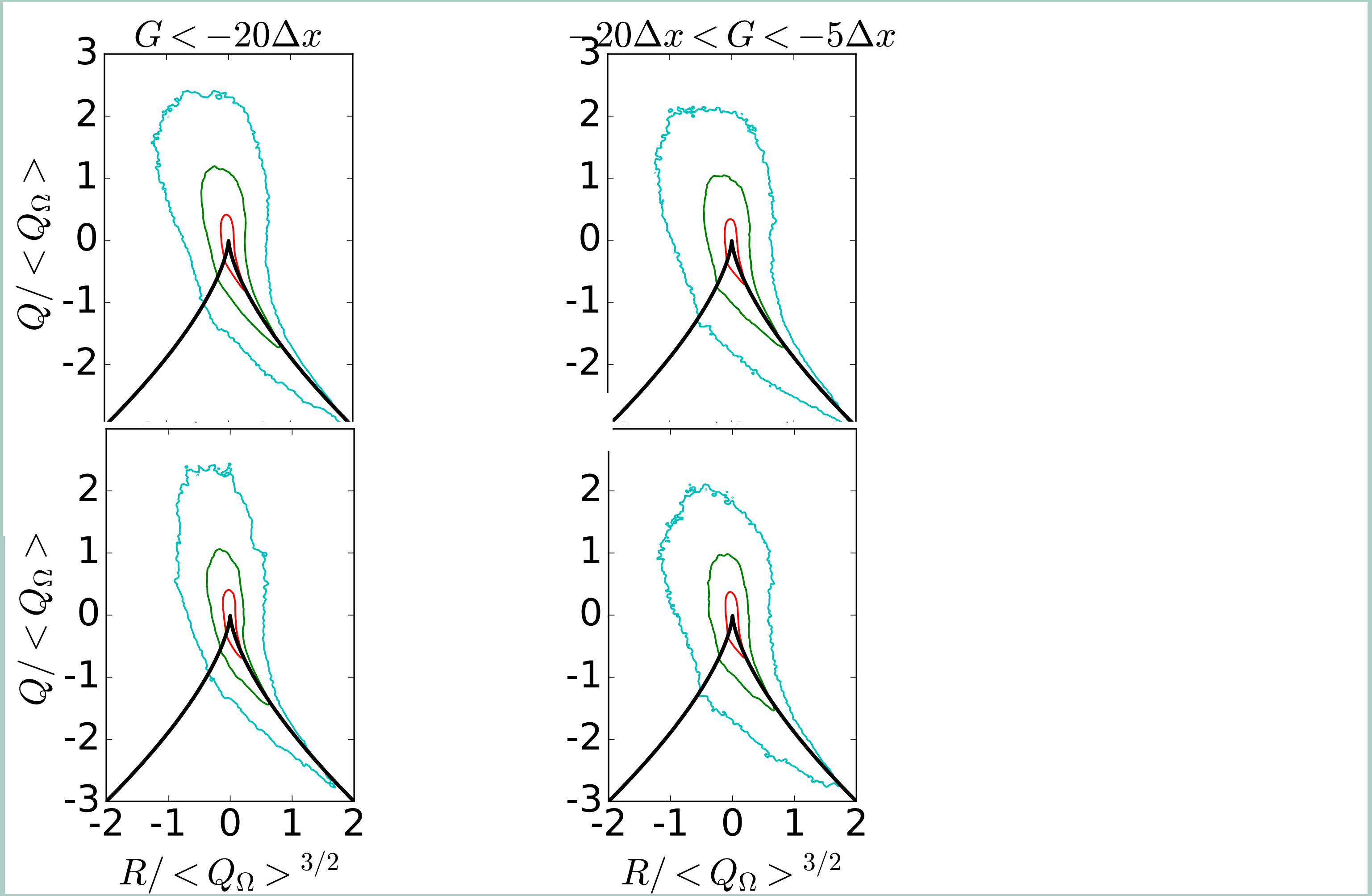
Z. Bouali, B. Duret, F.X. Demoulin, A. Mura, DNS analysis of small-scale turbulence-scalar interactions in evaporating two-phase flows, ***International Journal of Multiphase Flow***, vol. 85, pp. 326-335 (2018)

JPDF of the second and third invariants of the VGT



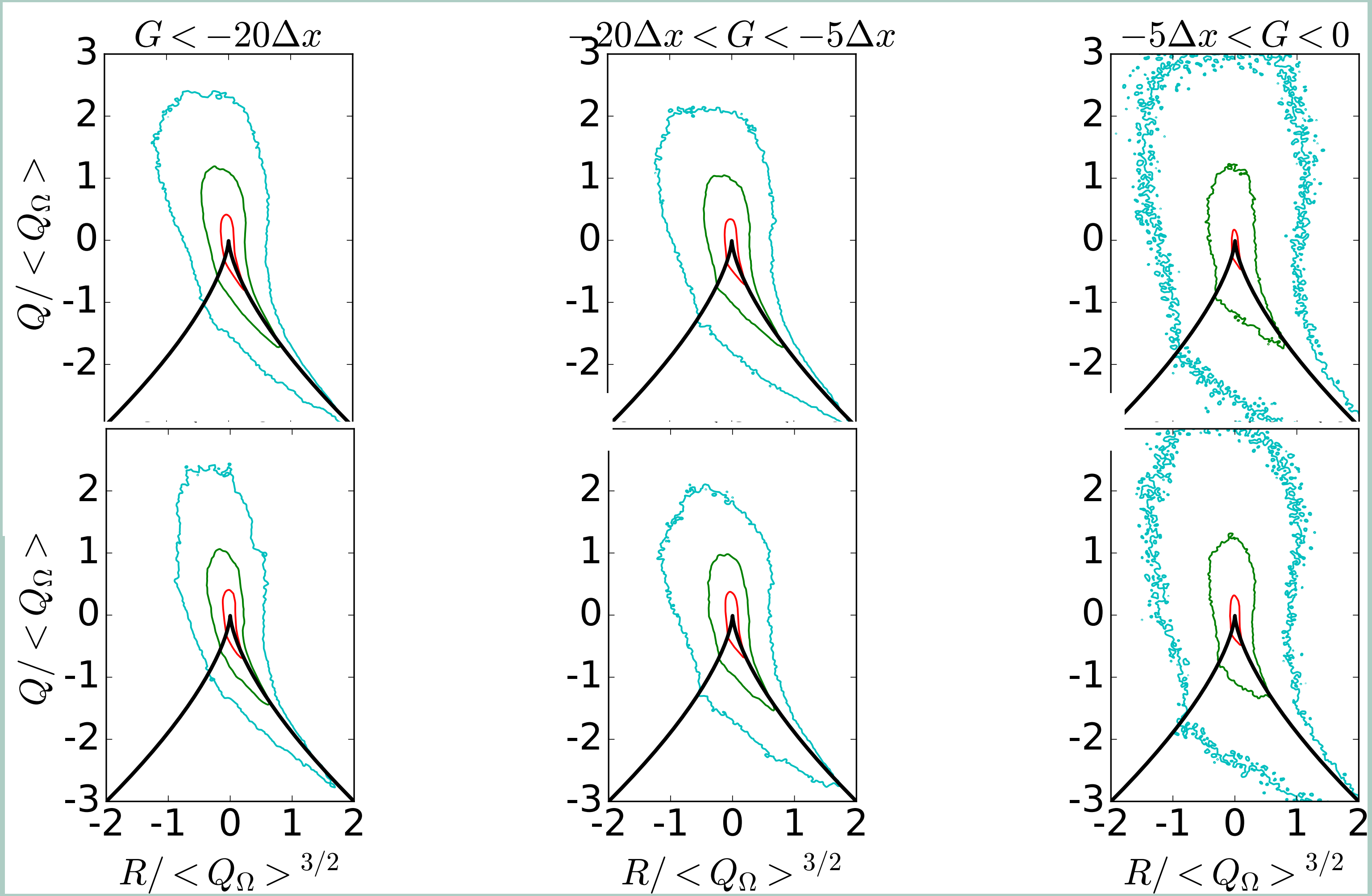
M. Onofre, S. Zhao, Z. Bouali, A. Mura, On some scalar and velocity statistics in two-phase flow turbulence with evaporation, ***Proceedings of the Eleventh Mediterranean Symposium on Combustion*** (2019)

JPDF of the second and third invariants of the VGT



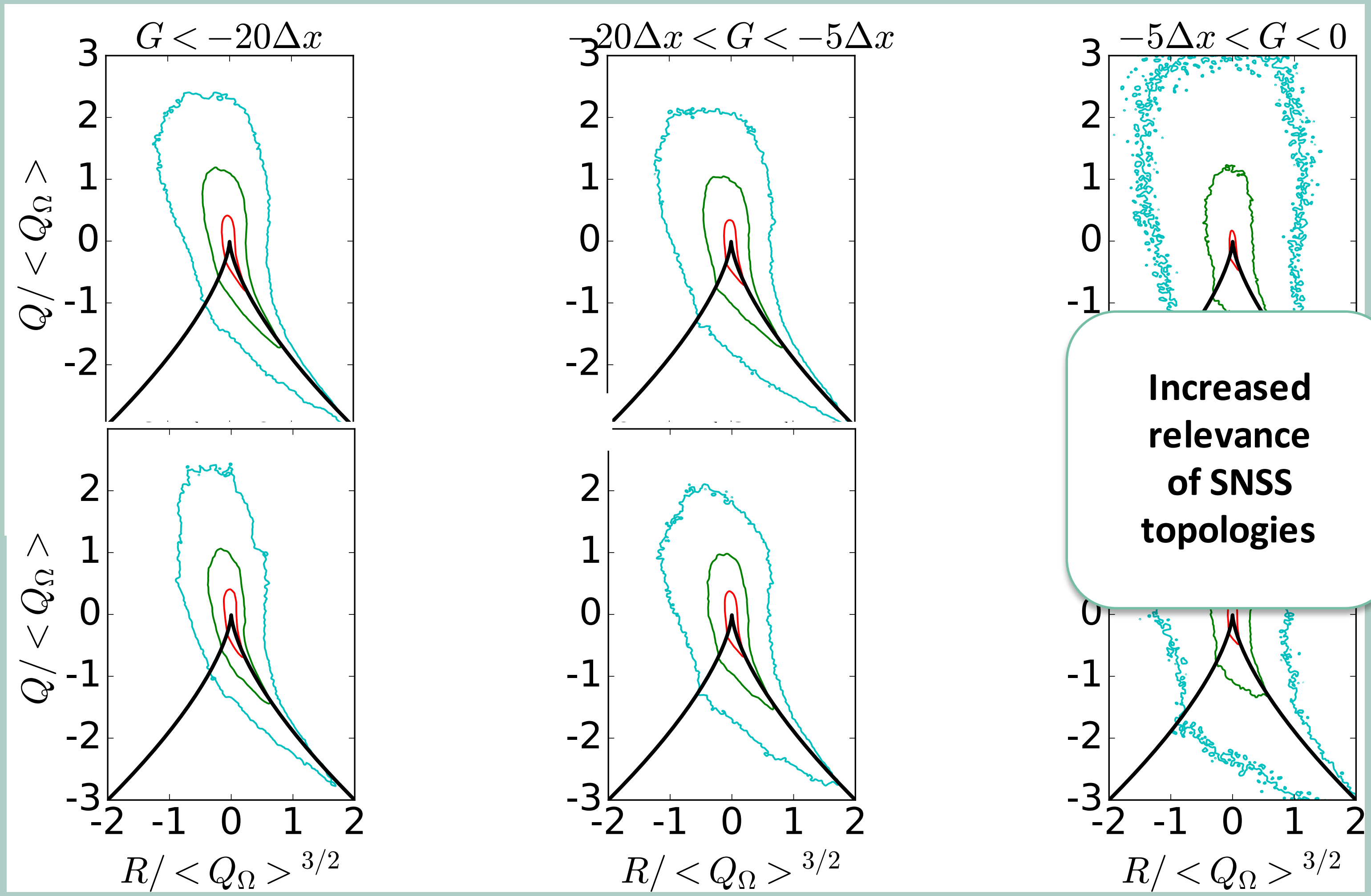
M. Onofre, S. Zhao, Z. Bouali, A. Mura, On some scalar and velocity statistics in two-phase flow turbulence with evaporation, ***Proceedings of the Eleventh Mediterranean Symposium on Combustion*** (2019)

JPDF of the second and third invariants of the VGT



M. Onofre, S. Zhao, Z. Bouali, A. Mura, On some scalar and velocity statistics in two-phase flow turbulence with evaporation, ***Proceedings of the Eleventh Mediterranean Symposium on Combustion*** (2019)

JPDF of the second and third invariants of the VGT

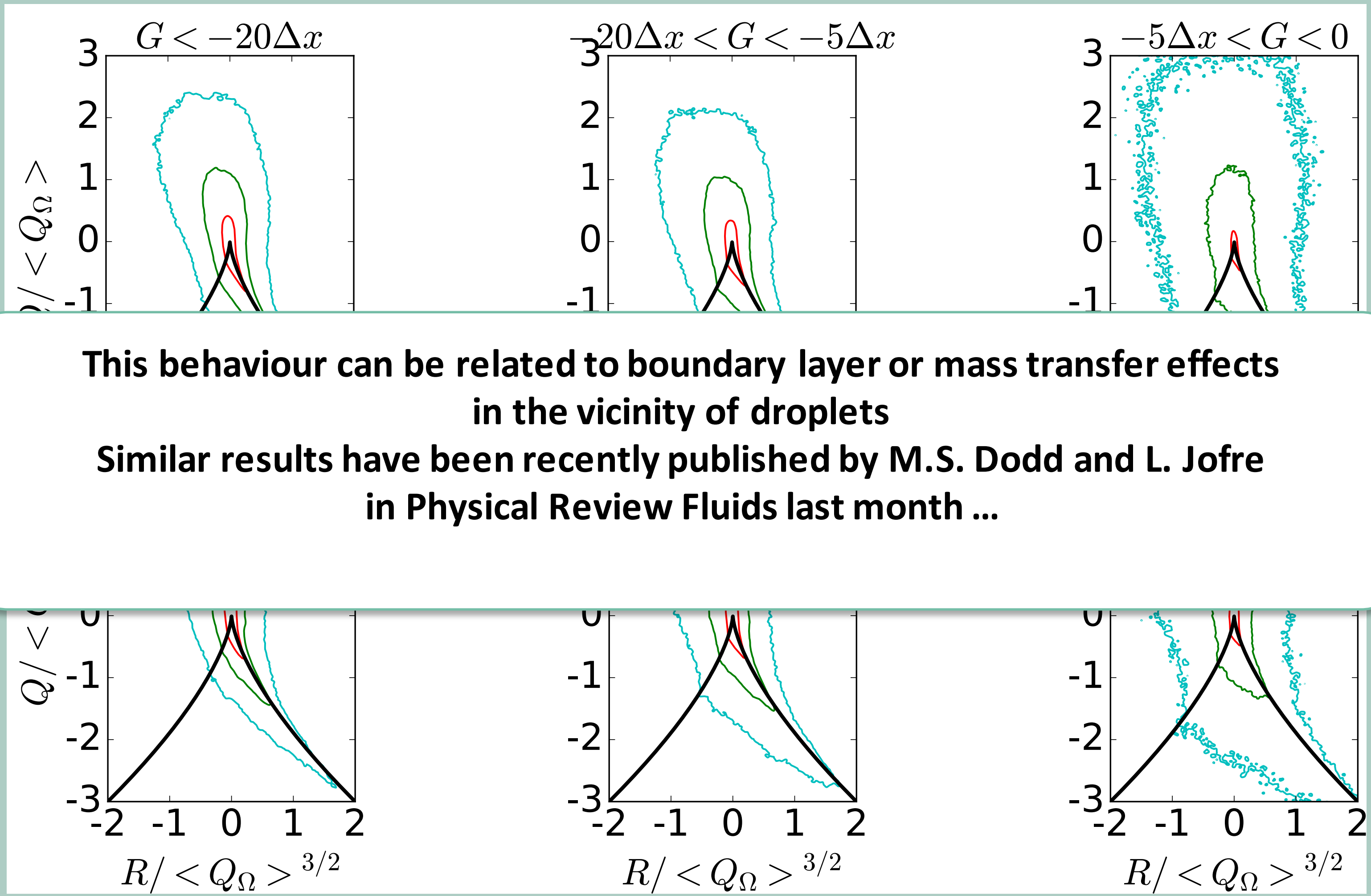


Increased relevance of SNSS topologies

M. Onofre, S. Zhao, Z. Bouali, A. Mura, On some scalar and velocity statistics in two-phase flow turbulence with evaporation, ***Proceedings of the Eleventh Mediterranean Symposium on Combustion*** (2019)

2- Vaporizing two-phase flows in homogeneous isotropic turbulence

JPDF of the second and third invariants of the VGT



This behaviour can be related to boundary layer or mass transfer effects in the vicinity of droplets

Similar results have been recently published by M.S. Dodd and L. Jofre in Physical Review Fluids last month …

M. Onofre, S. Zhao, Z. Bouali, A. Mura, On some scalar and velocity statistics in two-phase flow turbulence with evaporation, ***Proceedings of the Eleventh Mediterranean Symposium on Combustion*** (2019)

2- Shock-turbulence interactions

CREAMS solver: **C**ompressible **RE**Active **M**ulti-**S**pecies solver: cartesian, coupled to an **immersed boundary method** (IBM), compressible formulation, unsteady, 3D, multi-component, **massively parallel** (MPI; 10,000 < N < 100,000 cores)

Coupled to the **CVODE library**: processing of stiff systems of ODE

Coupled to the **EGlib library**: detailed description of molecular transport

Spatial discretization scheme

- **convective fluxes** (non-viscous) combines a non-linear weighting procedure **(WENO7)** with high-precision **finite difference scheme** (extended Adams & Shariff shock sensor)
- **diffusive or viscous fluxes:** high-precision finite difference scheme **(CDS8)**

Temporal discretization scheme **TVD RK3** (non-reactive contribution) and **CVODE** (reactive contribution), Strang’s « splitting »

P. N. Brown, G. D. Byrne and A. C. Hindmarsh, VODE, a variable-coefficient ODE solver, ***SIAM Journal on Scientific & Statistical Computing***, vol. 10, pp. 1038–1051 (1989)

A. Ern and V Giovangigli, Fast and accurate multicomponent transport property evaluation, ***Journal of Computational Physics,*** vol. 120, pp. 105-116 (1995)

N.A. Adams and K. Shariff, A high-resolution hybrid compact-ENO scheme for shock-turbulence interaction problems,, ***Journal of Computational Physics***, vol. 127, pp. 27-51 (1996)

J.C. Strikwerda, Finite difference schemes and partial differential equations. Wadsworth, Belmont (1989)

2- Shock-turbulence interactions

CREAMS solver: **C**ompressible **RE**Active **M**ulti-**S**pecies solver: cartesian, coupled to an **immersed boundary method** (IBM), compressible formulation, unsteady, 3D, multi-component, **massively parallel** (MPI; 10,000 < N < 100,000 cores)

Coupled to the **CVODE library**: processing of stiff systems of ODE

Coupled to the **EGlib library**: detailed description of molecular transport

Spatial discretization scheme

- **convective fluxes** (non-viscous) combines a non-linear weighting procedure **(WENO7)** with high-precision **finite difference scheme** (extended Adams & Shariff shock sensor)
- **diffusive or viscous fluxes:** high-precision finite difference scheme **(CDS8)**

Temporal discretization scheme **TVD RK3** (non-reactive contribution) and **CVODE** (reactive contribution), Strang's « splitting »

Detailed verification procedure and application to various test-cases

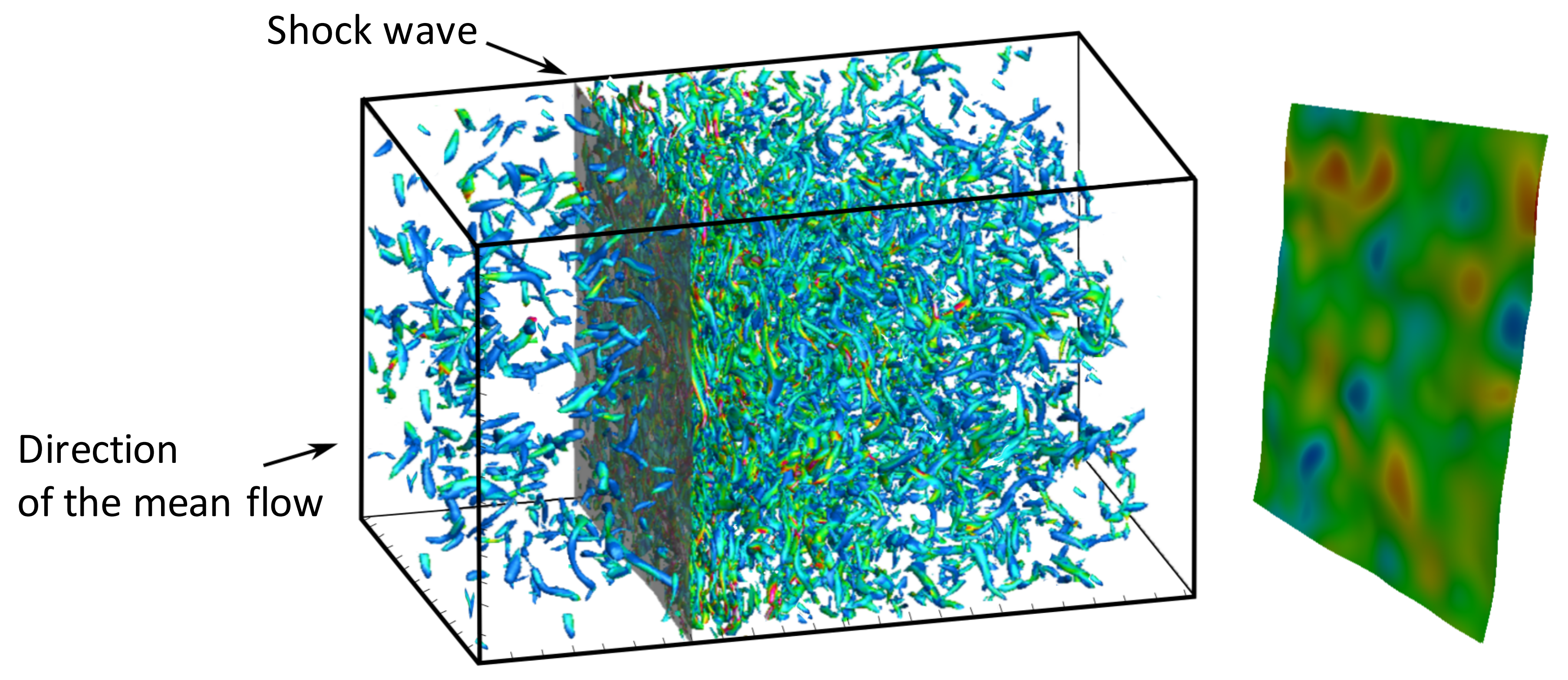
P.J. Martinez Ferrer, R. Buttay, G. Lehnasch, A. Mura, A detailed verification procedure for compressible reactive multi-component Navier-Stokes solvers, ***Computers and Fluids***, vol. 89, pp. 88-110 (2014)

P.J. Martinez Ferrer, G. Lehnasch, A. Mura, Compressibility and heat release effects in high-speed reactive mixing layers, Part I: Growth rates and turbulence characteristics, ***Combustion and Flame***, vol. 180, pp. 284-303 (2017)

R. Boukharfane, F. Ribeiro, Z. Bouali, A. Mura, A combined ghost-point-forcing / direct-forcing immersed boundary method (IBM) for compressible flow simulations, ***Computers and Fluids***, vol. 62, pp. 91-11 (2018)

2- Shock-turbulence interactions

Configuration: interaction of **homogeneous isotropic turbulence** (HIT) with a planar shock-wave (initially)



Iso-value surface of the λ_2 **criterion coloured by the enstrophy**, the shock-wave is visualized by an iso-value (<0) of the dilatation $(\boldsymbol{\nabla} \cdot \boldsymbol{u})$ coloured by **pressure**

2- Shock-turbulence interactions

Simulation conditions

Case	Re	Re_λ	M_s	M_t
1-W/-SW ou 1-W/O-SW	2370	21	1.7	0.17
2-W/-SW ou 1-W/O-SW	2780	21	2.0	0.17
3-W/-SW ou 1-W/O-SW	3200	21	2.3	0.17

Meshes: 750 × 256 × 256, N=50,000,000 computational nodes (inhomogeneous)

Initialisation and injection of **scalar** and **velocity** HIT

- i) Initialisation of **density**, **temperature**, and **velocity fields** with the method of Erlebacher and coworkers (1990)
- ii) Initialisation of density, pressure, and velocity fields with the method of Ristorcelli and Blaisdell (1997)
- Initialisation of a **non-reactive scalar field** (length-scale and PDF) using the method of Reveillon (2005)

2- Shock-turbulence interactions

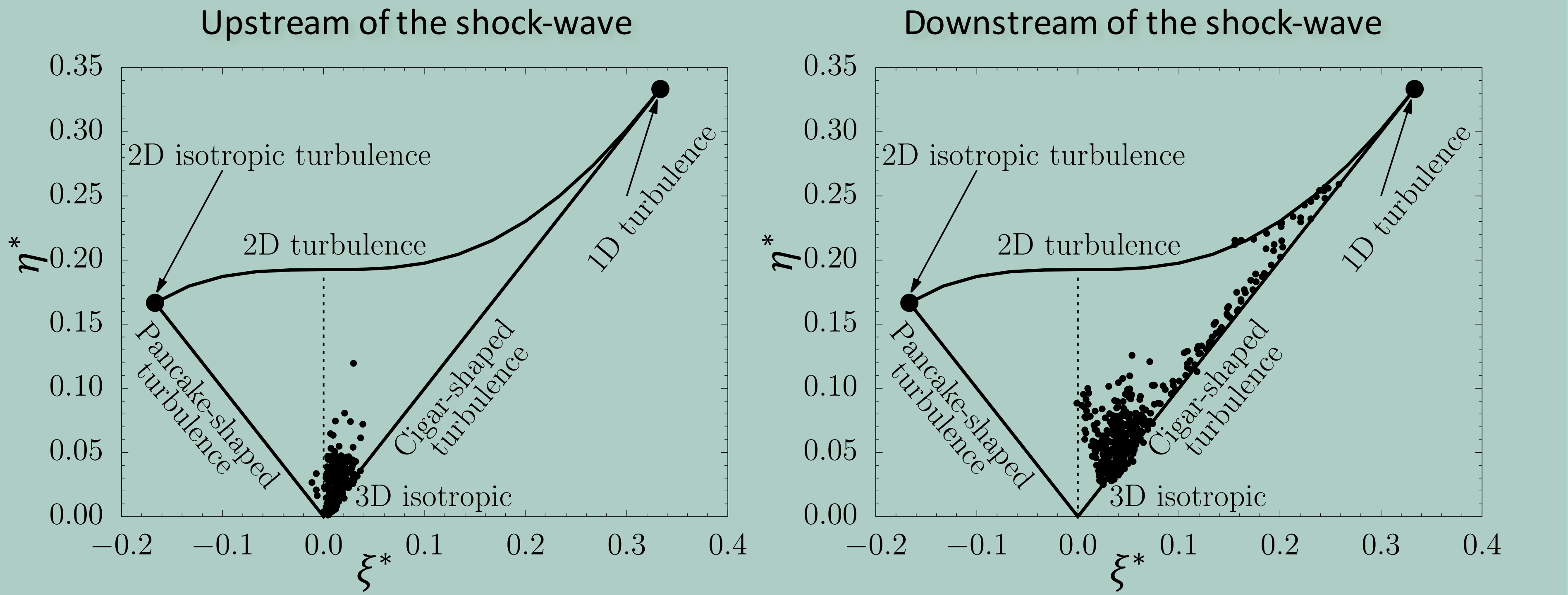
Characteristics of **shocked turbulence**

Lumley triangle

Normalized invariants of the **anisotropy tensor**

$$b_{ij} = \frac{\overline{\rho u_i'' u_j''}}{2\bar{\rho}\tilde{k}} - \delta_{ij}$$

$$\xi^* = -\frac{\Pi_b}{3} = \frac{b_{ii}^2}{6} \, ; \eta^* = \frac{b_{ii}^3}{6}$$

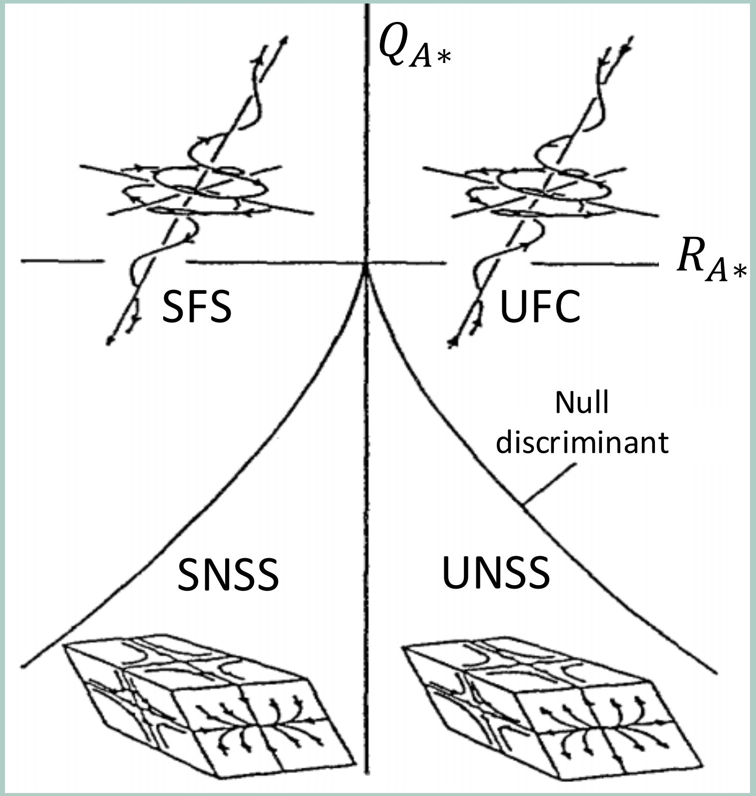

Upstream of the shock-wave

Downstream of the shock-wave

R. Boukharfane, Z. Bouali, A. Mura, Scalar and velocity dynamics evolutions in planar shock-turbulence interaction, ***Shock Waves***, vol. 28(6), pp. 1117–1141 (2018)

Characteristics of **shocked turbulence**

Structure characterized by the velocity gradient tensor $\boldsymbol{A}^*$ (traceless)



$$\boldsymbol{A}^* = \boldsymbol{\nabla u}^{\boldsymbol{T}} - (\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I}/3$$

Characteristic decomposition of the turbulence (Perry and Chong)

Characteristic polynomial of $\boldsymbol{A}^*$

$$\lambda^3 + P_{A*}\lambda^2 + Q_{A*}\lambda + R_{A*} = 0$$

Discriminant : $\Delta = \frac{27}{4} R_{A*}^2 + Q_{A*}^3$

SFS : stable focus / stretching
UFC : unstable focus / compressing
SNSS : stable node / saddle / saddle
UNSS : unstable node / saddle / saddle

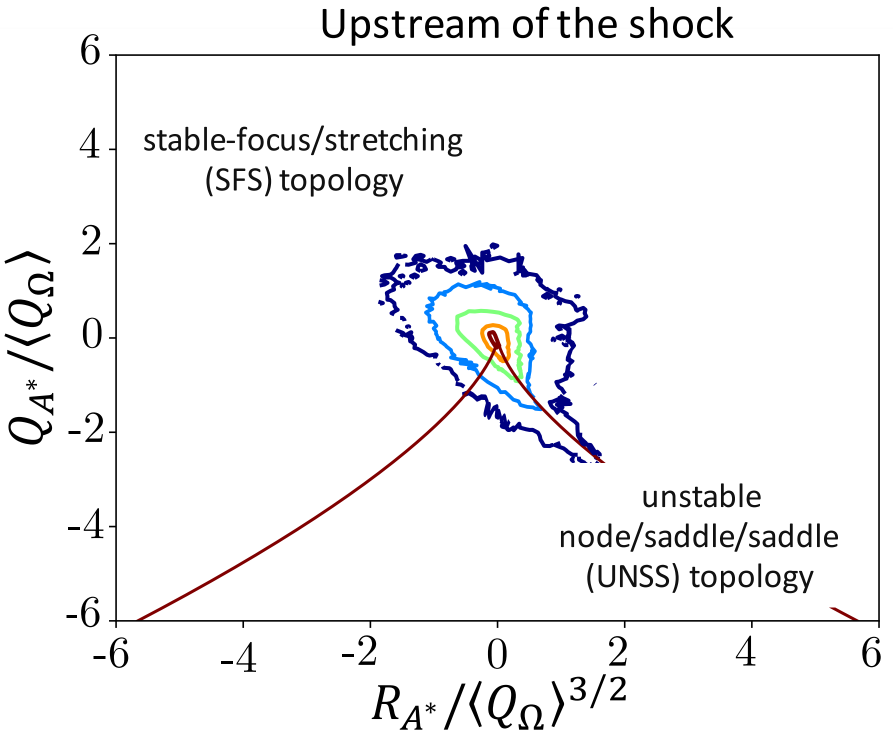
A.E. Perry, M.S. Chong, A description of eddying motions and flow patterns using critical-point concepts, ***Annual Review of Fluid Mechanics***, vol. 19, pp. 125–155 (1987)

M.S. Chong, A.E. Perry, B.J. Cantwell, A general classification of three-dimensional flow fields, ***Physics of Fluids***, vol. 2 pp. 765–777 (1990)

2- Shock-turbulence interactions

Characteristics of **shocked turbulence**

Second- and **third-order invariants** of the tensor $\boldsymbol{A}^*$ $\boldsymbol{A}^* = \boldsymbol{\nabla u}^T - (\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I}/3$



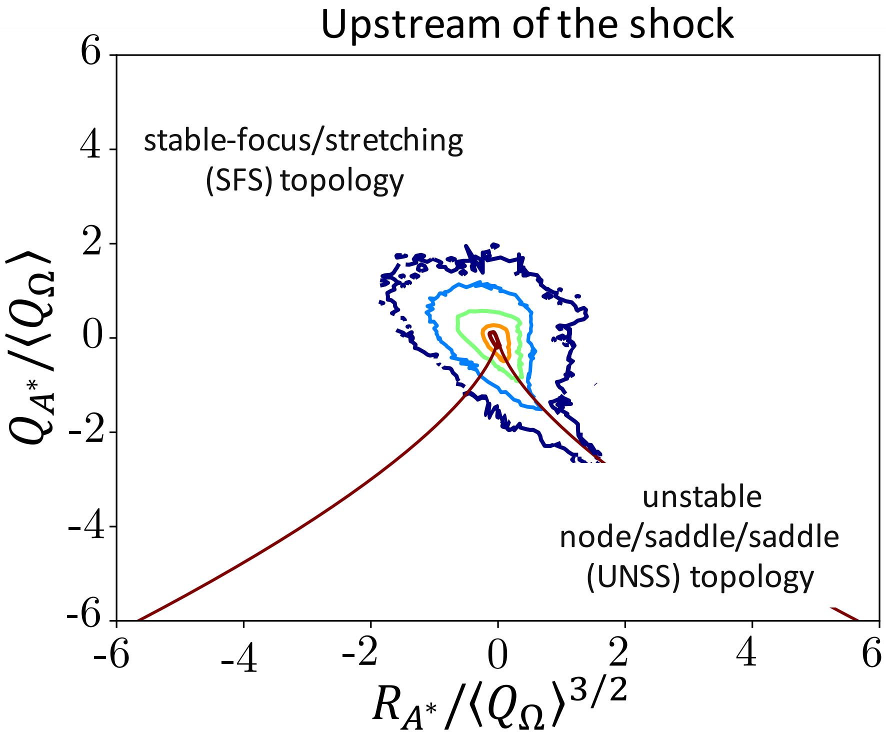
J. Ryu, D. Livescu, Turbulence structure behind the shock in canonical shock–vortical turbulence interaction, ***Journal of Fluid Mechanics***, vol. 756, pp. R1-R13 (2014)

R. Boukharfane, Z. Bouali, A. Mura, Scalar and velocity dynamics evolutions in planar shock-turbulence interaction, ***Shock Waves***, vol. 28(6), pp. 1117–1141 (2018)

2- Shock-turbulence interactions

Characteristics of **shocked turbulence**

Second- and **third-order invariants** of the tensor $\boldsymbol{A}^*$ $\boldsymbol{A}^* = \boldsymbol{\nabla u}^{\boldsymbol{T}} - (\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I}/3$



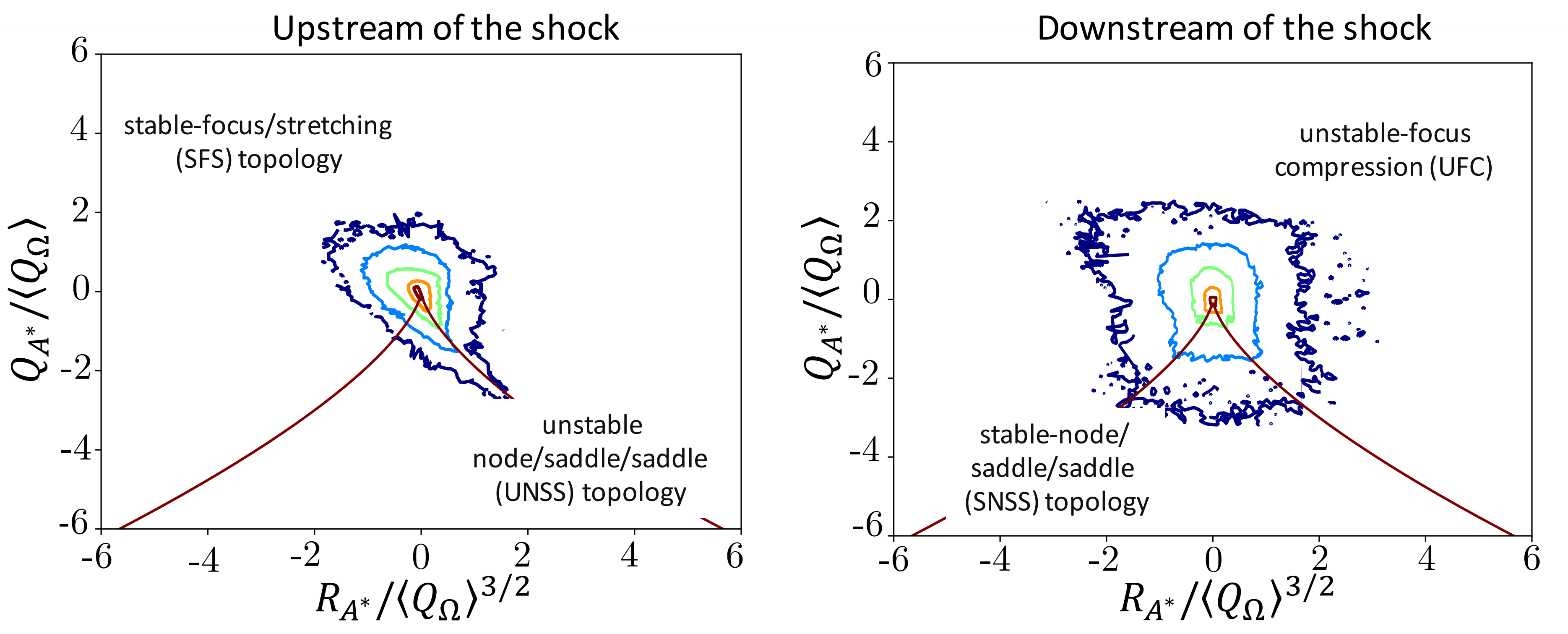
The inclined **teardrop** shape and the **clustering along the Vieillefosse tail** closely resembles the JPDF found in incompressible HIT

J. Ryu, D. Livescu, Turbulence structure behind the shock in canonical shock–vortical turbulence interaction, ***Journal of Fluid Mechanics***, vol. 756, pp. R1-R13 (2014)

R. Boukharfane, Z. Bouali, A. Mura, Scalar and velocity dynamics evolutions in planar shock-turbulence interaction, ***Shock Waves***, vol. 28(6), pp. 1117–1141 (2018)

Characteristics of **shocked turbulence**

Second- and **third-order invariants** of the tensor $\boldsymbol{A}^*$ $\boldsymbol{A}^* = \boldsymbol{\nabla u}^T - (\boldsymbol{\nabla} \cdot \boldsymbol{u})\boldsymbol{I}/3$



Increased relevance of topologies SNSS and UFC

J. Ryu, D. Livescu, Turbulence structure behind the shock in canonical shock–vortical turbulence interaction, ***Journal of Fluid Mechanics***, vol. 756, pp. R1-R13 (2014)

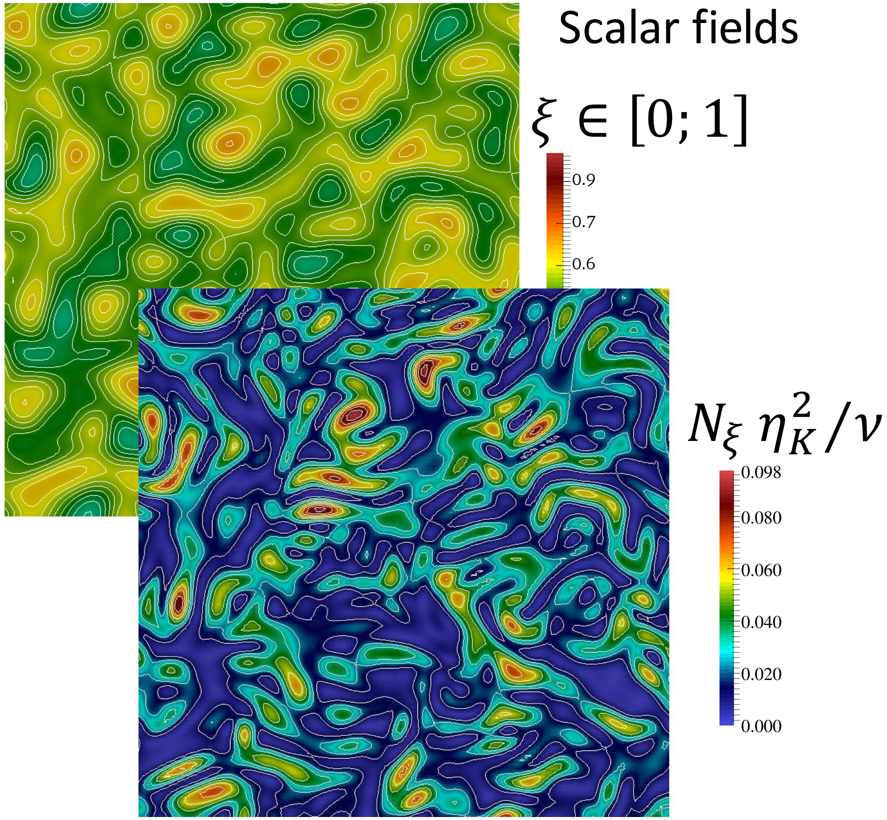
R. Boukharfane, Z. Bouali, A. Mura, Scalar and velocity dynamics evolutions in planar shock-turbulence interaction, ***Shock Waves***, vol. 28(6), pp. 1117–1141 (2018)

2- Shock-turbulence interactions

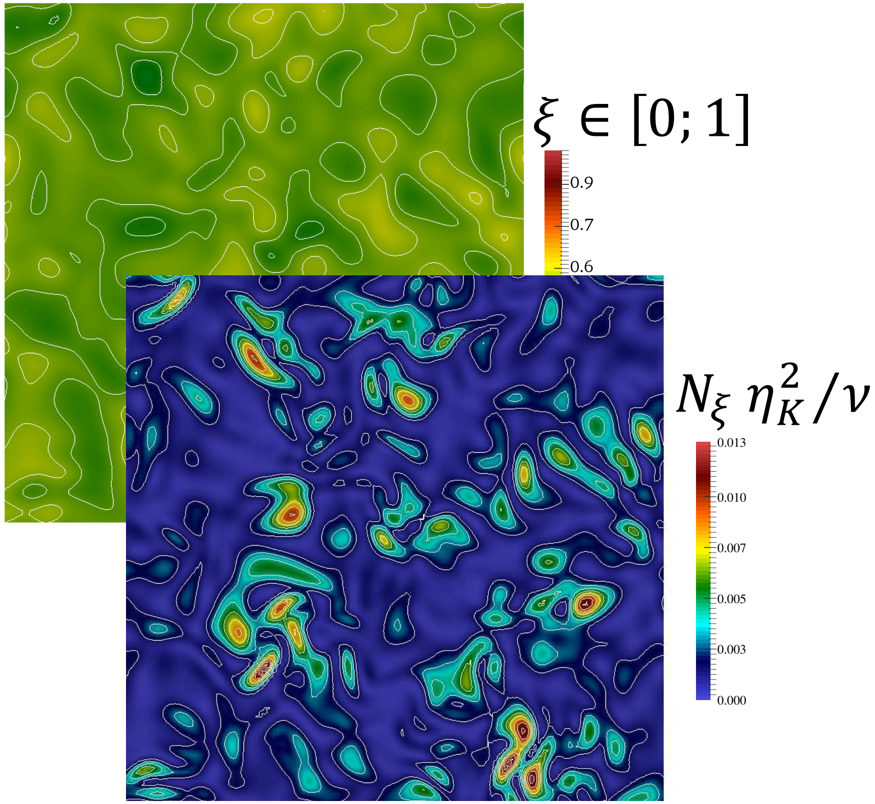
Characteristics of **shocked scalar turbulence**

Downstream of the shock location (case 1-W/O-SW)

Scalar fields



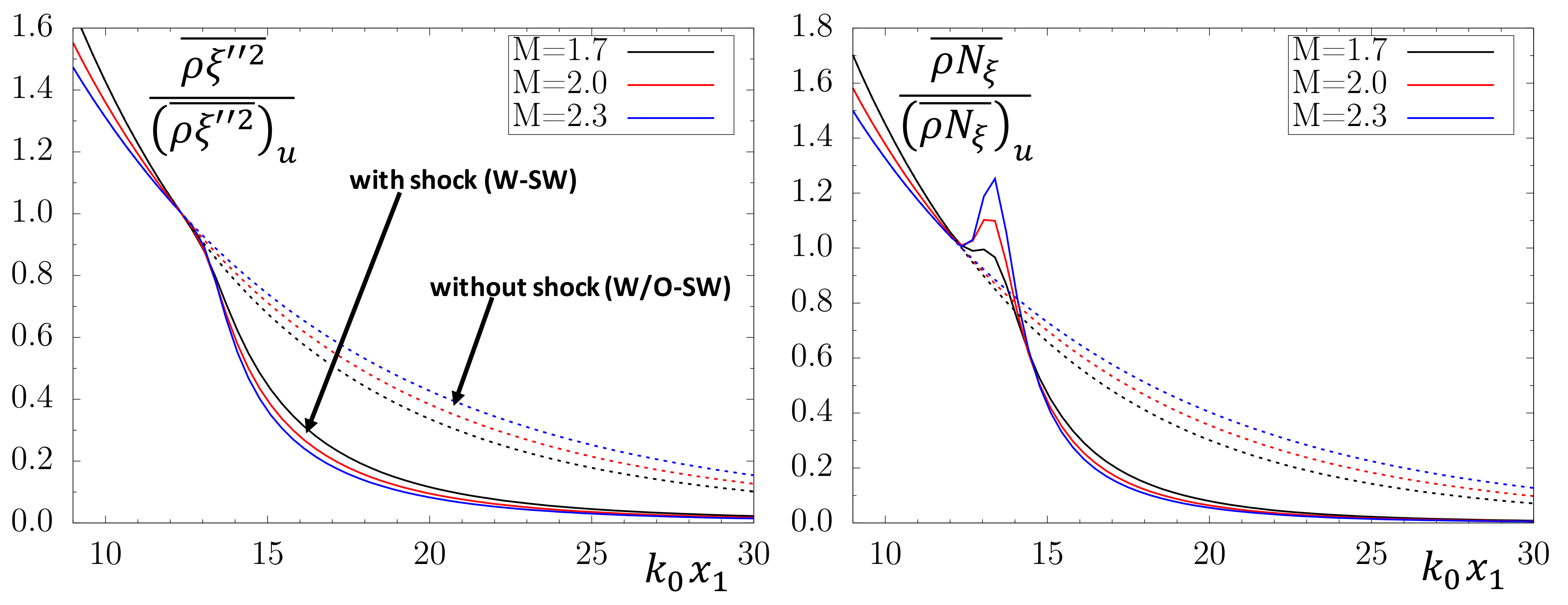
Same position (case 1-W/-SW)



Scalar dissipation rate (SDR) $N_\xi = D \dfrac{\partial \xi}{\partial x_i} \dfrac{\partial \xi}{\partial x_i}$

Characteristics of **shocked scalar turbulence**

Normalized scalar variance and SDR evolutions



R. Boukharfane, Z. Bouali, A. Mura, Scalar and velocity dynamics evolutions in planar shock-turbulence interaction, ***Shock Waves***, vol. 28(6), pp. 1117–1141 (2018)

2- Shock-turbulence interactions

Characteristics of **shocked scalar turbulence**

Scalar dissipation rate evolution (SDR)

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{N}_{\xi}\right) + \frac{\partial}{\partial x_j}\left(F_j^{\widetilde{N}_{\xi}}\right) = \cdots - 2\overline{\rho N_{\xi}^{ij}\frac{\partial u_i}{\partial x_j}} - 2\overline{\rho D^2 \frac{\partial^2 \xi}{\partial x_i \partial x_j}\frac{\partial^2 \xi}{\partial x_i \partial x_j}}$$

(TSI) (Dissipation)

Determination of the **eigen-frame** of the **strain-rate tensor (symmetric part of the VGT)**

$\det\left(S_{ij} - \lambda\,\delta_{ij}\right) = 0$ eigen-vectors associated to compression and straining

Expression of the **turbulence-scalar interaction** (TSI) term in the eigenframe of the strain-rate tensor

$$\boxed{(\mathrm{TSI}) = -2\overline{\rho N_{\xi}^{ij} S_{ij}} = -2\overline{\rho N_{\xi}\lambda_k \cos^2\theta_k}}$$

$$\theta_k = \left(\boldsymbol{n}_{\xi}, \boldsymbol{e}_k\right)$$

$$\boldsymbol{n}_{\xi} = \boldsymbol{\nabla}\xi / \|\boldsymbol{\nabla}\xi\|$$

Characteristics of **shocked scalar turbulence**

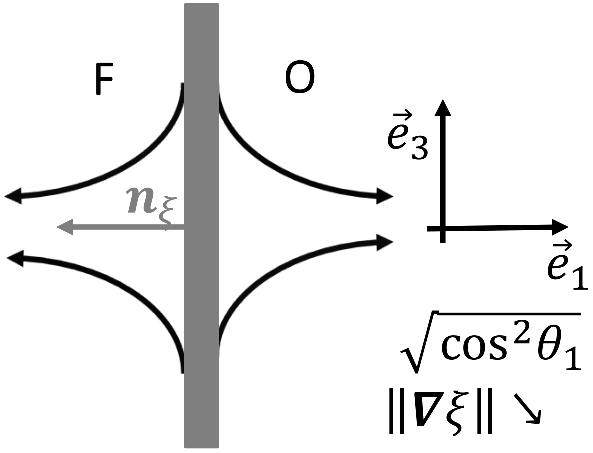
Orientations statistics of the scalar gradient in the strain-rate eigenframe

Let us consider **two principal directions** (only for the sake of simplicity)

- one principal direction of **straining**,
  eigenvalue and eigenvector $\lambda_1 > 0 \,;\, \boldsymbol{e}_1$
- one principal direction of **compression**,
  eigenvalue and eigenvector $\lambda_3 < 0 \,;\, \boldsymbol{e}_3$

$$\theta_k = (\boldsymbol{n}_\xi , \boldsymbol{e}_k)$$

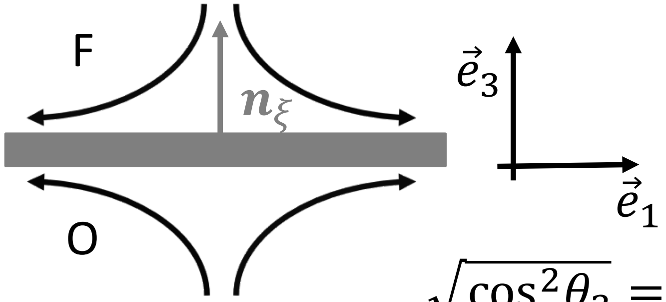
Scalar gradient $\boldsymbol{\nabla}\xi$ // $\boldsymbol{e}_1$ (straining)



$$\sqrt{\cos^2\theta_1} = 1$$

$\|\boldsymbol{\nabla}\xi\| \searrow$ SDR $\searrow$

Scalar gradient $\boldsymbol{\nabla}\xi$ // $\boldsymbol{e}_3$ (compression)



$$\sqrt{\cos^2\theta_3} = 1$$

$\|\boldsymbol{\nabla}\xi\| \nearrow$ SDR $\nearrow$

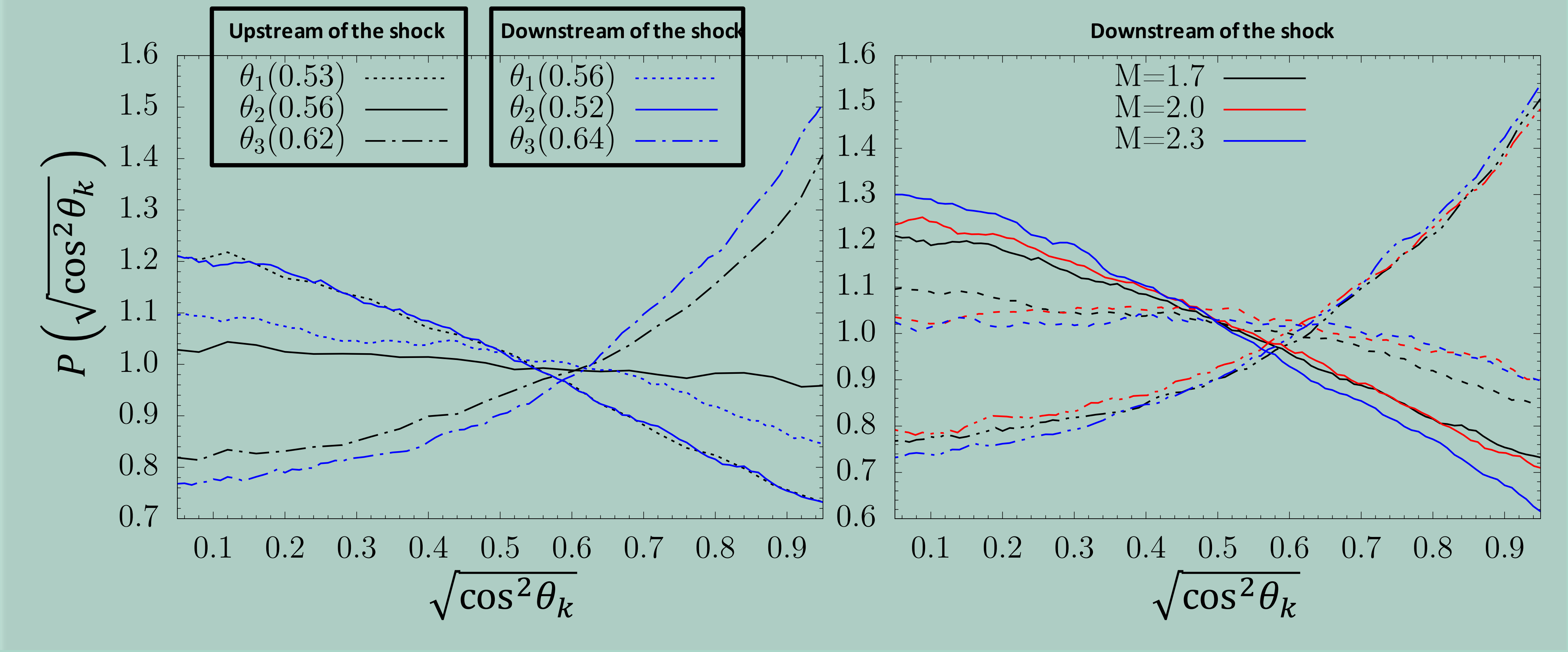
2- Shock-turbulence interactions

Characteristics of **shocked scalar turbulence**

Turbulence-scalar interaction (TSI) may increase or decrease the scalar mixing rate

Analysis in the eigen-frame of the **strain-rate tensor** (symmetric part $\boldsymbol{S}$ of the VGT)

$$\mathrm{TSI} = -2\rho N_\xi \sum_{k=1}^{k=3} \lambda_k \cos^2\theta_k \qquad \theta_k = (\boldsymbol{n}_\xi, \boldsymbol{e}_k)$$



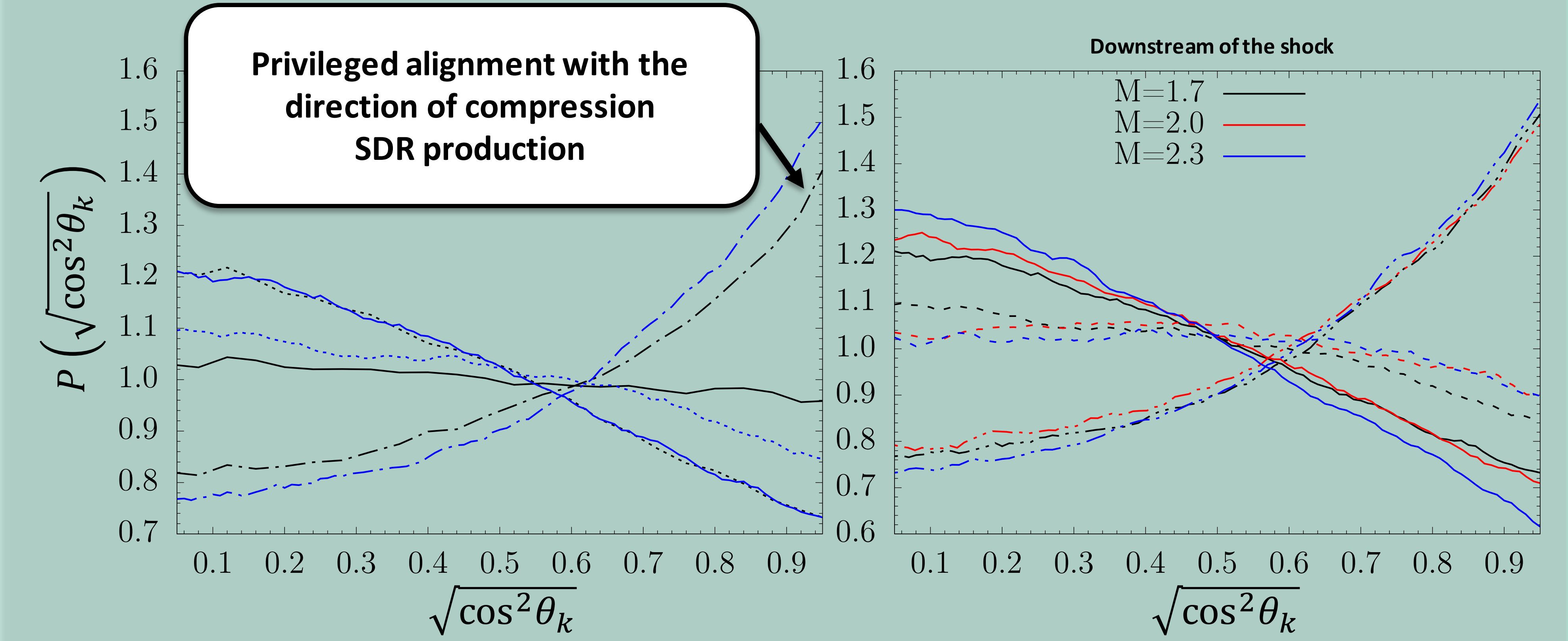
2- Shock-turbulence interactions

Characteristics of **shocked scalar turbulence**

Turbulence-scalar interaction (TSI) may increase or decrease the scalar mixing rate

Analysis in the eigen-frame of the **strain-rate tensor** (symmetric part $\boldsymbol{S}$ of the VGT)

$$\mathrm{TSI} = -2\rho N_{\xi} \sum_{k=1}^{k=3} \lambda_k \cos^2\theta_k \qquad \theta_k = (\boldsymbol{n}_{\xi}, \boldsymbol{e}_k)$$



Privileged alignment with the direction of compression
SDR production

3- Conclusions and prospects

Available computational databases and post-processing tools

- Fully premixed flame kernels development in homogeneous turbulence
- Vaporizing two-phase flows in homogeneous turbulence
- Interaction of homogenous (velocity and scalar) turbulence with a planar shock

Inspection of the DNS data and physical analyses (still ongoing work …)

- Unconditional and conditional characterization of the turbulence (TKE, Reynolds stresses, characteristic scales, spectra, structure functions, etc.)
- Topology of the turbulent flow-field: portrays of the JPDF of Q and R, Lagrangian evolution
- Scalar gradient orientations statistics and dynamics

The ultimate objective is to end up with modelling proposals

Acknowledgements

The input of Song Zhao, Radouan Boukharfane, Aimad Er-raiy, Zakaria Bouali and Guillaume Lehnasch is gratefully acknowledged

Acknowledgements

The input of Song Zhao, Radouan Boukharfane, Aimad Er-raiy, Zakaria Bouali and Guillaume Lehnasch is gratefully acknowledged

Thank you for your kind attention