DNS and LES of Transitional and Two-Phase Flows

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1 Introduction

Transition to turbulence, possibly followed by a relaminarization process, remains one of the most intriguing features found in many fluid flows. It is at the same time a highly relevant process for practical applications, since it will suddenly impact drag losses (along an aircraft wing), mixing properties (within a static mixer) or shear forces acting on cells (in a tubular bioreactor), to name just a few such cases. Additionally, it is still unclear how transition processes might be modified in the presence of an additional, disperse phase. Considering for instance blood [1], i.e., (with some simplification) a continuous liquid phase (plasma, mostly water) with a high loading of red blood cells ("particles"), is the tendency to undergo transition increased, decreased or unchanged, compared to a single-phase flow? Direct Numerical Simulation (DNS) is recognized as the best possible approach to investigate such questions. However, it is well-known that, due to the underlying computational requirements, DNS can only be carried out for relatively simple configurations and/or at relatively low Reynolds numbers. For other conditions, Large-Eddy Simulations (LES) constitute the logical alternative to DNS, but involve of course additional challenges concerning subgrid-scale modeling and near-wall resolution.

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D.G.E. Grigoriadis et al. (eds.), *Direct and Large-Eddy Simulation X*,
ERCOFTAC Series 24, https://doi.org/10.1007/978-3-319-63212-4_4

2 Flow Simulations

For this project, the 3rd-generation DNS code called DINO has been used. It has been developed within the last years based on our previous experience in DNS, obtained first by the developing the compressible code PARCOMB [2, 3], followed later by the low-Mach number code π^3 [4, 5].

It has been demonstrated during the last decades that DNS can be successfully employed to investigate numerically gaseous reactive flows. Nevertheless, many issues remain, since the underlying configuration is extremely challenging. As a consequence, high-performance computers are absolutely necessary to solve this problem. When considering a second phase, for instance for reacting sprays, the complexity becomes even higher [6].

Following previous work, DINO is able to take into account detailed reaction schemes, allowing an accurate description of kinetics. Then, the computational challenge becomes even worse compared to non-reacting flows or to crude approximations like single-step chemistry. For complex fuel molecules like n-heptane or ethylene, the computational overhead induced by chemistry dominates the overall computation time. Additionally, studies involving detailed chemistry require a comparable level of accuracy for all relevant molecular transport and thermodynamic properties, like diffusion coefficients, specific heat, thermal conductivity, and viscosity.

An Immersed Boundary Method (IBM) has been implemented in DINO. In this manner, DNS of configurations with a complex geometry become possible. Finally,

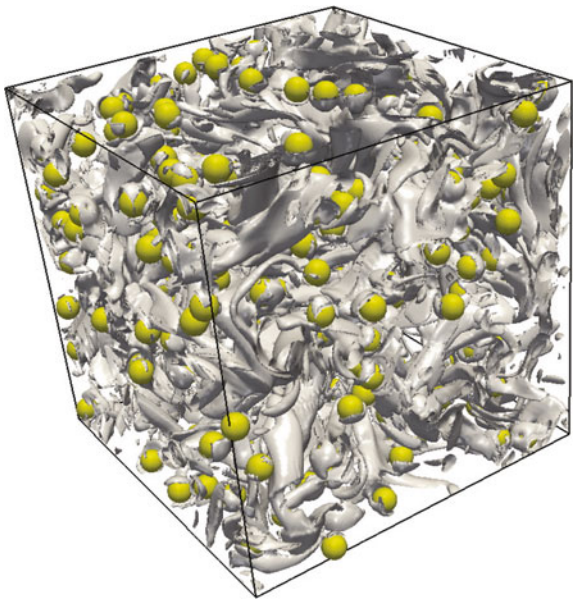

Fig. 1 Enstrophy field obtained by DINO in a particulate flow at a mass loading of 35% (fully resolved particles using IBM)

DINO has been employed for all simulations in this project. DINO solves the Navier–Stokes equations in the low-Mach number regime. It is possible to take into account the presence of a disperse phase (point particles, or particles resolved by direct-force IBM, allowing for 1-way up to 4-way coupling [7, 8]). Additionally, complex chemical schemes can be taken into account. An implicit time integration scheme is implemented to solve the usually very stiff chemistry source terms. For computing kinetic and transport properties, Cantera1.8 and Eglib3.4 have been coupled to DINO. More details on the code can be found in another chapter of this book [9]. DINO results for a heavily loaded particulate flow are shown in Fig. 1, while a turbulent flame is exemplarily shown in Fig. 2.

The wall-resolved LES simulations ($y^+ \simeq 1$) used for comparison have been systematically carried out with established software tools (OpenFOAM, Ansys-Fluent,

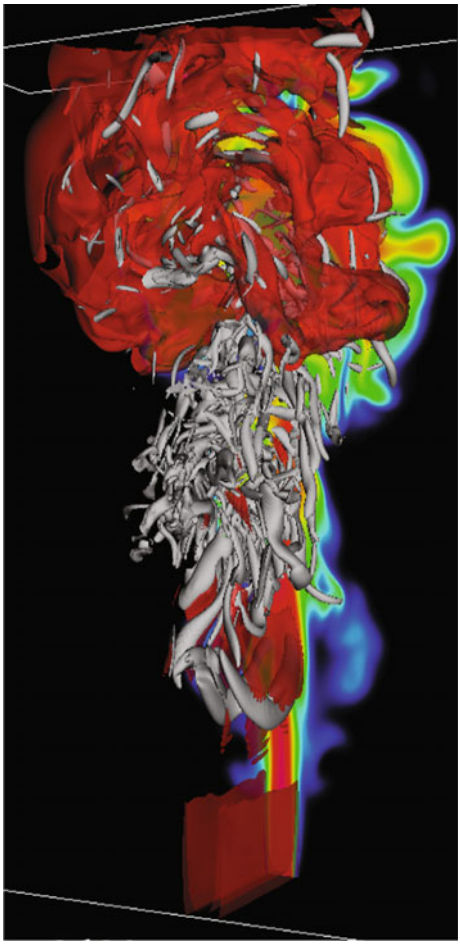

Fig. 2 Structure of a turbulent hydrogen jet flame computed with DINO using a full reaction scheme

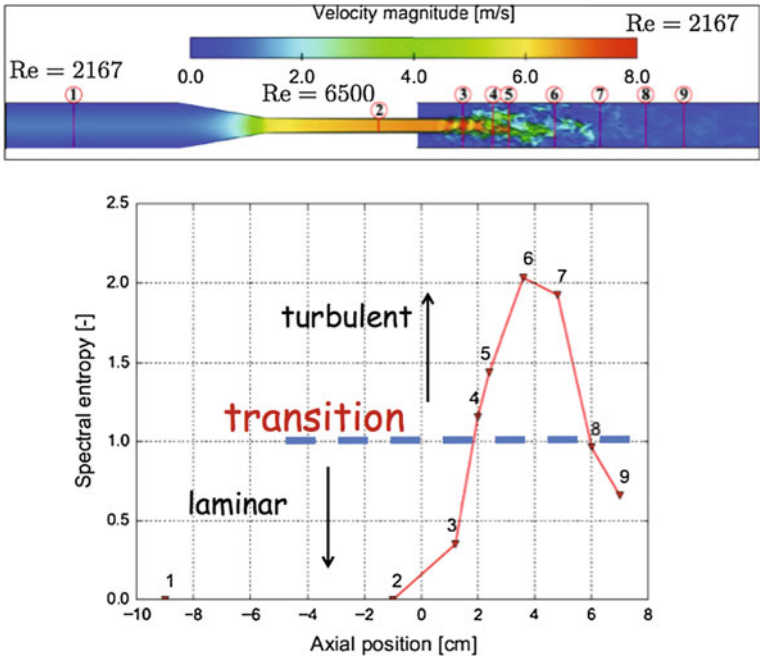

Fig. 3 Blood nozzle computed by LES used to check the validity of the criterion based on POD spectral entropy to delineate between different flow regimes (laminar, transition to turbulence followed by relaminarization)

STAR-CCM+), since they should be ultimately used for industrially-relevant applications. For the blood nozzle presented later in Fig. 3, Ansys-Fluent has been employed. All details of the computation can be found in [10].

3 Proper Orthogonal Decomposition

The software library used here for analysis and understanding of DNS and LES data is the in-house tool SIVAPOD developed and validated in previous projects to analyze both numerical and experimental data [11]. It allows for Proper Orthogonal Decomposition (POD), both as Snapshot POD (SPOD) and as Singular Value Decomposition (SVD). Those approaches, though very similar, involve subtle differences in the methodology used to handle the data. Therefore, one or the other might be more appropriate or efficient, depending on the available hardware and on the size of the problem (number of time instants, number of grid points, number of variables). In what follows, the SPOD has been employed.

The aim of the snapshot POD is to find the function ϕ maximizing the value of $\langle|(\mathbf{u},\phi)|\rangle/\|\phi\|^2$, where $\langle\cdot\rangle$, $(\cdot,\cdot)$ and $\|\cdot\|$ are spatial average, inner product

and norm, respectively. The function ϕ spans a subspace of the original space of the snapshot $\mathbf{u}(t_k, \mathbf{x})$ such that the error of the orthogonal projection is minimized. Solving an optimization problem leads to an eigenvalue problem, where the functions ϕ are the eigenfunctions. In the snapshot POD ϕ can be described for one mode by

$$\phi(\mathbf{x}) = \sum_{k=1}^{N_s} a(t_k)\mathbf{u}(t_k, \mathbf{x}) \ , \tag{1}$$

where $a(t_k)$ is the entry k of the eigenvectors $\mathbf{A}$ of an eigenvalue problem,

$$\mathbf{CA} = \lambda \mathbf{A} \, , \tag{2}$$

$$\mathbf{A} = (a(t_1), a(t_2), ..., a(t_{N_s}))^T \, , \tag{3}$$

$$C_{ij} = \frac{\left(\mathbf{u}(t_i, \mathbf{x}), \mathbf{u}(t_j, \mathbf{x})\right)}{N_s} \ . \tag{4}$$

Solving this eigenvalue problem, Eq. (2), leads to a total of N_s eigenvalues, written λ_l, and eigenvectors, denoted $\mathbf{A}_l$ ($l \in 1, 2, 3, ..., N_s$).

The eigenvectors A_l are sorted by ordering the corresponding eigenvalues λ_l in descending order, and are then scaled as follows:

$$\sum_{k=1}^{N_s} a_i(t_k)a_j(t_k) = N_s \lambda_i \delta_{ij} \ , \tag{5}$$

where δ_{ij} is the Kronecker delta. In this way, the scaled entries, $a_l(t_k)$, represent the *temporal coefficients* for function ϕ_l, where subscripts l and k refer to the mode number and index of corresponding snapshot (or timestep), respectively. At the same time, λ_l quantifies the energy contained in mode ϕ_l, and this mode can be normalized to represent the corresponding *spatial eigenvector* (also called spatial or POD mode):

$$\phi_l(\mathbf{x}) = \frac{1}{N_s \lambda_l} \sum_{k=1}^{N_s} a_l(t_k)\mathbf{u}(t_k, \mathbf{x}) \ . \tag{6}$$

Using this approach the original signal (for us, the flow velocity) can be represented as follows, highlighting the connection between original data-set ($\mathbf{u}$), spatial mode ϕ_l and temporal coefficients a_l:

$$\mathbf{u}(t, \mathbf{x}) = \sum_{l=1}^{N_s} a_l(t)\phi_l(\mathbf{x}) \ . \tag{7}$$

In order to characterize now the intensity of the turbulence contained in the analyzed velocity field $\mathbf{u}$, the spectral entropy S_d classically used in information theory has been computed. This quantity should hopefully allow us to distinguish between

different flow regimes, from "highly disordered" (for us, turbulence), to "partially ordered" (for us, transition), or "well ordered" (for us, laminar flow). For the computation of the spectral entropy, the probability P_l of each mode is first computed, after ordering in decreasing order based on λ_l, as:

$$P_l = \frac{\lambda_l}{\sum_{j=1}^{N_s} \lambda_j} , \tag{8}$$

Then, the spectral entropy can be determined as:

$$S_d = -\sum_{l=1}^{N_s} P_l \ln P_l . \tag{9}$$

According to Eq. (3), the maximum possible value of S_d is reached when all eigenvalues are equal to each others, i.e., $P_l = 1/N_s$, and consequently $S_d = \ln(N_s)$. Physically, this means that the energy is equally distributed on all the N_s modes. The minimum value of S_d corresponds to the case where the original signal contains only one mode, the first one, meaning that the flow field is steady. Then, $S_d = 0$. Further discussions can be found in [12].

4 Results

To calibrate the approach, DNS simulations of homogeneous isotropic turbulence have been carried out with DINO. After checking the connection between POD spectral entropy and turbulence intensity by computing S_d for increasing values of the turbulent Reynolds number, as documented in Table 1, a very clear relationship can be established. There is indeed a monotonous relationship between S_d and the flow

Table 1 Computed spectral entropy S_d

Flow regime	Re_λ	Re_Λ	S_d
Quasi-laminar	1.01	1.780	0.057
	5.00	8.900	0.140
	15.2	26.80	0.470
	20.3	35.90	0.623
Transition	32.0	53.80	0.879
	40.7	71.80	1.089
	50.8	89.73	1.265
Turbulent	61.1	107.7	1.418
	81.5	143.7	1.660
	101.8	179.6	1.848

state, and specific thresholds can be associated to transition to turbulence ($S_d \approx 1$) and to fully turbulent flows ($S_d > 1.25$).

To check the generality of the developed approach, the resulting thresholds have then been employed to predict the flow state in a completely different case, a complex blood nozzle proposed as a benchmark by the Food and Drug Administration. As shown in Fig. 3, a perfect agreement is obtained compared with a user-based analysis of the flow, showing that S_d can be used to characterize in an automatic manner the state of an unsteady, three-dimensional flow.

5 Conclusions

Based on these first tests, it appears that the spectral entropy computed from the POD decomposition can be used to quantify the flow state (laminar, transitional or turbulent) in an automatic, user-independent manner. Starting from a three-dimensional, unsteady velocity field, a single scalar quantity S_d is obtained in this manner. A value of S_d around unity denotes a transitional value, while $S_d > 1.25$ characterizes full-developed turbulence, the parameter S_d increasing in a monotonic way with the turbulence intensity. Further tests will be needed in order to check that these thresholds are generally applicable.

Acknowledgements All the results discussed in this paper have been obtained in close collaboration with A. Abdelsamie, P. Arányi, P. Berg, G. Fru, G. Martello and G. Janiga from my own research group. The financial support of the DFG (Deutsche Forschungsgemeinschaft) within the Forschergruppe (Research unit) number 1447 as well as the computer resources provided by the Gauss Center for Supercomputing/Leibniz Supercomputing Center Munich under grant pro84qo are highly acknowledged.

References

1. Berg, P., Abdelsamie, A., Yu, H., Janiga, G. Thévenin, D.: Multi-phase blood flow modeling in intracranial aneurysms considering possible transition to turbulence. 8th International Symposium on Turbulence and Shear Flow Phenomena, BIOE/1–6, Poitiers (F) (2013)
2. Thévenin, D., Behrendt, F., Maas, U., Przywara, B., Warnatz, J.: Development of a parallel direct simulation code to investigate reactive flows. Comput. Fluids **25**(5), 485–496 (1996)
3. Hilbert, R., Thévenin, D.: Influence of differential diffusion on maximum flame temperature in turbulent non-premixed hydrogen/air flames. Combust. Flame **138**, 175–187 (2004)
4. Thévenin, D., Gicquel, O., de Charentenay, J., Hilbert, R., Veynante, D.: Two- versus three-dimensional direct simulations of turbulent methane flame kernels using realistic chemistry. Proc. Combust. Inst. **29**, 2031–2039 (2003)
5. Thévenin, D.: Three-dimensional direct simulations and structure of expanding turbulent methane flames. Proc. Combust. Inst. **30**, 629–637 (2005)
6. Reveillon, J., Pera, C., Bouali, Z.: Examples of the potential of DNS for the understanding of reactive multiphase flows. Int. J. Spray Combust. Dyn. **3**(1), 63–92 (2011)

7. Abdelsamie, A., Thévenin, D.: Turbulence modulation by fully resolved particles using immersed boundary methods. In: EUROMECH/ERCOFTAC Colloquium Immersed Boundary Methods, pp. 145–147. Leiden (NL) (2013)
8. Abdelsamie, A., Thévenin, D.: Modulation of isotropic turbulence by resolved and non-resolved spherical particles. In: Fröhlich, J., Kuerten, H., Geurts, B.J., Armenio, V. (eds.) Direct and Large-Eddy Simulation IX, pp. 621–629. Springer, Berlin (2015)
9. Abdelsamie, A., Thévenin, D.: Direct numerical simulation of turbulent lean premixed syngas flames at elevated pressure. In: Direct and Large-Eddy Simulation X. Springer, Berlin. (This same book)
10. Janiga, G.: Large-eddy simulation of the FDA benchmark nozzle for a Reynolds number of 6500. Comput. Biol. Med. **47**, 113–119 (2014)
11. Arányi, P., Janiga, G., Zähringer, K., Thévenin, D.: Analysis of different POD methods for PIV-measurements in complex unsteady flows. Int. J. Heat Fluid Flow **43**, 204–211 (2013)
12. Abdelsamie, A., Janiga, G., Thévenin, D.: Spectral entropy as a flow-state indicator. Int. J. Heat Fluid Flow, (2016). Submitted for publication