Seeing the invisible through direct numerical simulation

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Introduction

In the scientific world, seeing is not necessarily believing. However, the ability to reproduce and visualise is vital to achieving full understanding of complex, unsteady and non-linear phenomena. Turbulence and other physical processes occurring in a turbulent medium, for example, are largely invisible to us and remain unsolved mysteries in engineering and physical sciences. Various experimental techniques such as high-speed cameras and laser-induced fluorescence are able to visualize turbulent phenomena to some extent, but they suffer from certain defects: (a) The spatial and temporal resolution is usually not sufficient to resolve small-scale phenomena; (b) Only basic quantities such as velocity and temperature are measurable while derived or high-order quantities (e.g. dissipation rate) are almost impossible to obtain; (c) Correlations between two or more variables are difficult to measure; and finally (d) seeding the flow field alters the phenomenon being investigated.

Computer visualization is a natural tool to complement experimental measurements, which can overcome the latter's inherent disadvantages (a)-(d), provided sufficient computer resources are made available. In the early days when computers were number-crunching below megaflops, only the Reynolds Averaged Navier-Stokes (RANS) calculations were possible. The results are not true visualization of turbulence, because the non-linear processes involved are not reproduced but represented by pre-determined turbulence models. Direct computer visualization of turbulent phenomena became a reality with the advent of gigaflops and now teraflops computers, which allowed Direct Numerical Simulation (DNS). As DNS solves the fundamental governing equations without the interference of empirical models, the simulation process is a reproduction of the physical "reality", and the non-linear turbulent processes are "seen" throughout the simulation. Analysis of any complex and unsteady phenomenon is greatly enhanced through access to the DNS data which contain full-field, time-dependent and accurate information of almost all quantities.

Current Research

Our work on computational fluids and combustion has benefited greatly from access to world class facilities provided by CSAR and HPCx. Generous support has been provided by CSAR staff, in particular, Dr. Neil Stringfellow who helped to port and optimize our codes on Green and Newton. Our research is conducted within two national consortia: the "UK Turbulence Consortium" (EPSRC Grant No. GR/R64964 with Prof. Neil Sandham as P.I.) and the "Consortium on Computational Combustion for Engineering Applications" (EPSRC Grant No. GR/R66197 with myself as P.I.). Each of these consortia consists of active researchers from up to eight universities in the UK, which provides an effective forum for dissemination of results to UK and international audience through regular meetings and international workshops. Current activities in our group fall into three main areas: (1) computational aerodynamics and aeroacoustics; (2) turbulent diffusion flames and partially premixed flames; and (3) mixing and dispersion of solid particles and liquid droplets in turbulent flow. Sample results from these numerical investigations are shown in the accompanying figures.

Direct computation of the invisible sound and its source generated by complex shear flows has always been desired, which presents a great challenge for numerical methods and requires massive computing power. Figure 1 shows results of a DNS of a compressible flow in and around

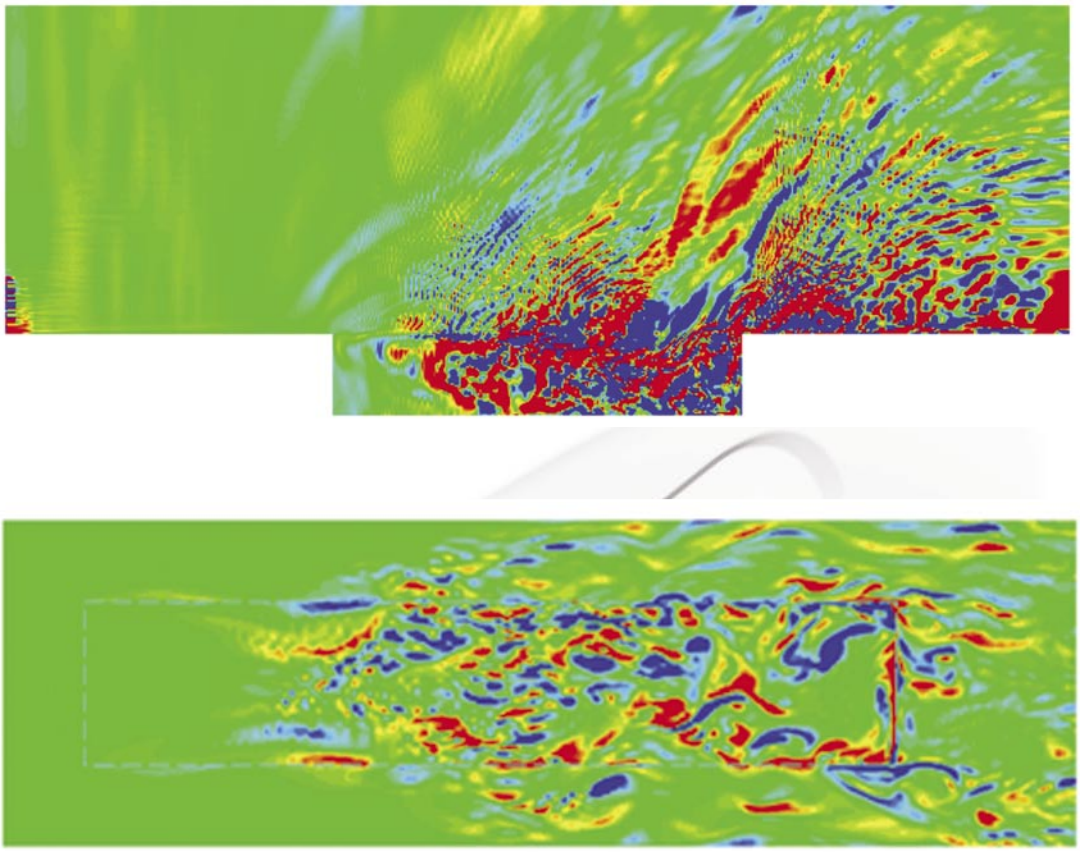


Figure 1: DNS of a compressible open cavity flow and its acoustic near-field at a Mach number 0.85 and a Reynolds number 5000, using 21 million grid points. The top plot shows a side view of the dilatation field and the lower plot a top view of the vorticity field (Lai and Luo, 2004).

an open cavity using a Reynolds number of 5000. The same configuration was used in a series of experimental measurements at DSTL. The geometry was fully three-dimensional, with side walls of the cavity included, which was very rare in numerical simulations. The side view of the dilatation field shows identifiable wave patterns in the near-field. The top view of the vorticity field demonstrates clear asymmetry of the flow in the spanwise direction, indicating strong three-dimensional effects, which were absent from a simulation at a lower Reynolds number of 1000. A Large Eddy Simulation (LES) under identical conditions was also performed. The predicted sound source of the cavity flow, as defined by Lilley, is shown in Figure 2 (overleaf). A comparison of DNS and LES predicted sound pressure level (SPL) with the DSTL measurements is also shown.

A series of direct numerical simulations have been performed to study the link among mixing, entrainment, vortex dynamics, combustion and the source configurations of transitional and turbulent buoyant diffusion flames. The full Navier-Stokes equations and chemical reactions governed by the Arrhenius law were solved by high-order numerical schemes. Figure 3 (overleaf) shows a diffusion flame from a rectangular source undergoing axis switching. The large number of grid points used, 256 x 256 x 768, is due to the fact that combustion

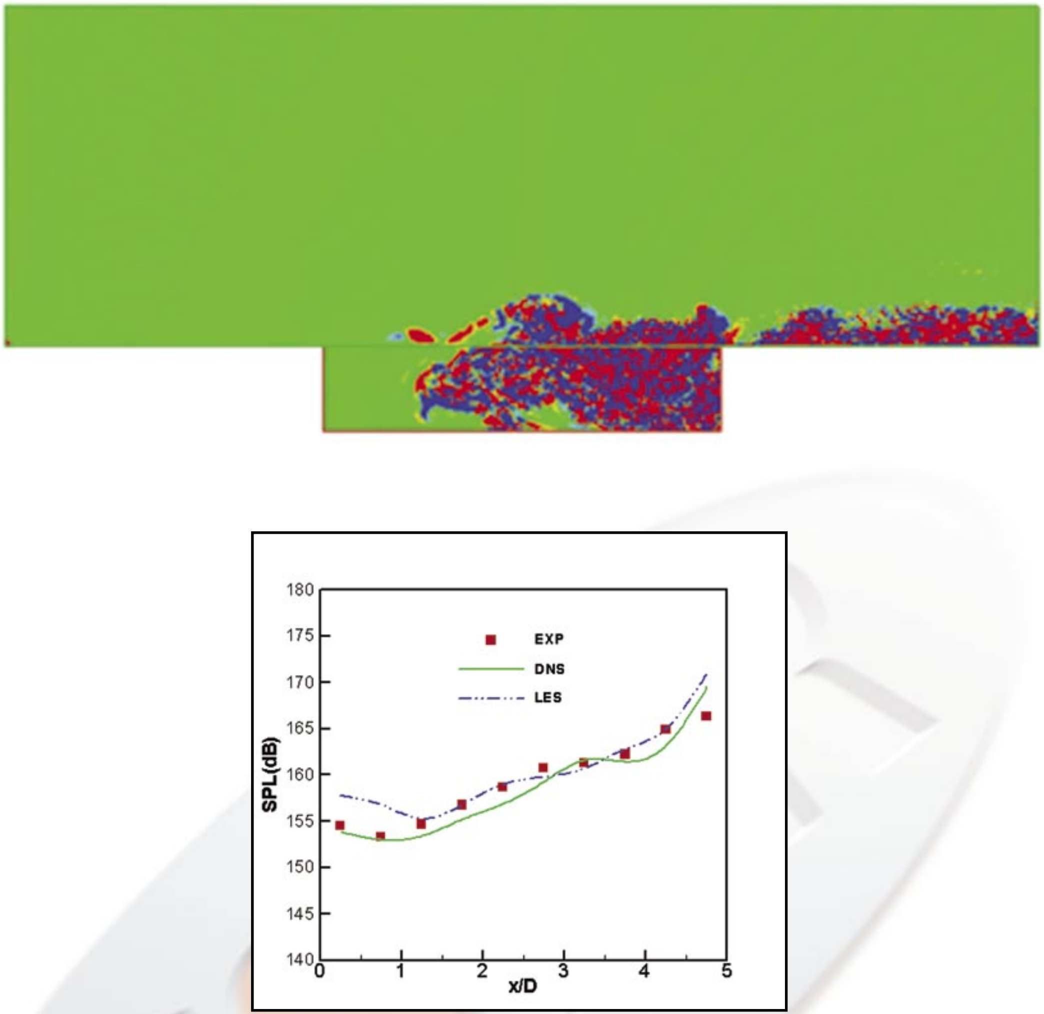


Figure 2: The acoustic source field obtained by LES of a compressible open cavity flow at a Mach number 0.85 and a Reynolds number 5000, using 5 million grid points and a comparison of the sound pressure level (SPL) from numerical predictions with the DSTL experimental data (Lai and Luo, 2004).

takes place at much smaller scales than the smallest scales of flow, the Kolmogorov scales.

Partially premixed flames are known to exist but direct proof by experiments or numerical simulations is not easy, due to the extremely small scales involved and the transient nature of the phenomena. Figure 4 shows a DNS of a lifted methane-air flame. Using the concept of cross-scalar dissipation rate, $\chi_{F,O} = D \nabla Y_F \bullet \nabla Y_O$, which is essentially the product of the gradient of the fuel concentration and the gradient of the oxidizer concentration, the lifted flame is seen to have partial premixing, if the reaction rate is conditioned on $\chi_{F,O}$. By following the evolution of the reaction zone numerically, the dynamics of partially premixed flames can be explained unambiguously.

Summary and Outlook

DNS has enabled unaltered views of fine details of turbulence and turbulence-related phenomena such as turbulent combustion, which are otherwise "invisible" to us. It is the only means by which complex unsteady phenomena in Thermofluids can be recreated with no or minimum empirical interference, providing a valuable tool for obtaining fundamental insight and for model validation. However, the computational cost is prohibitively high for most practical calculations. And despite the availability of today's teraflops hypercomputers,

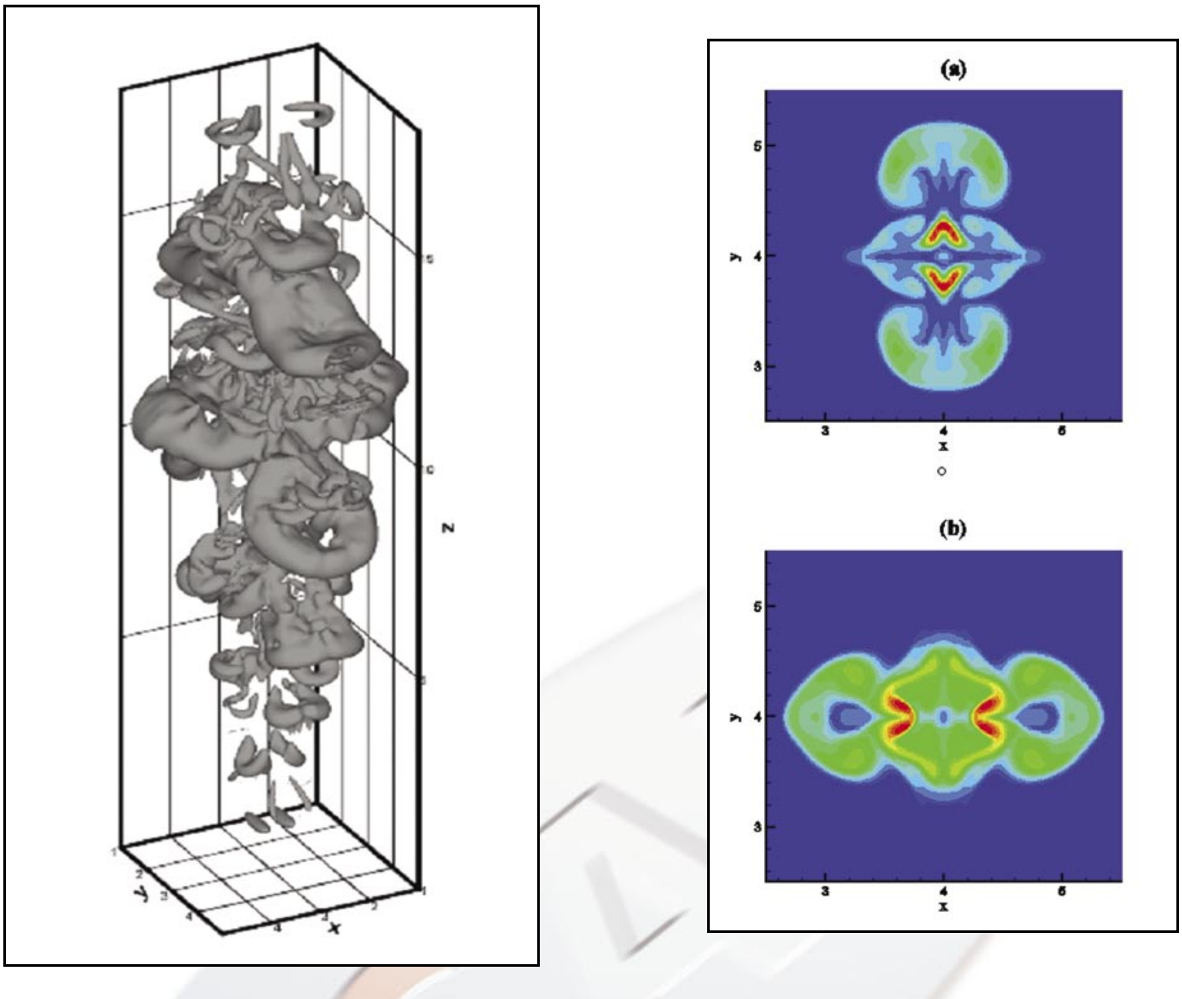
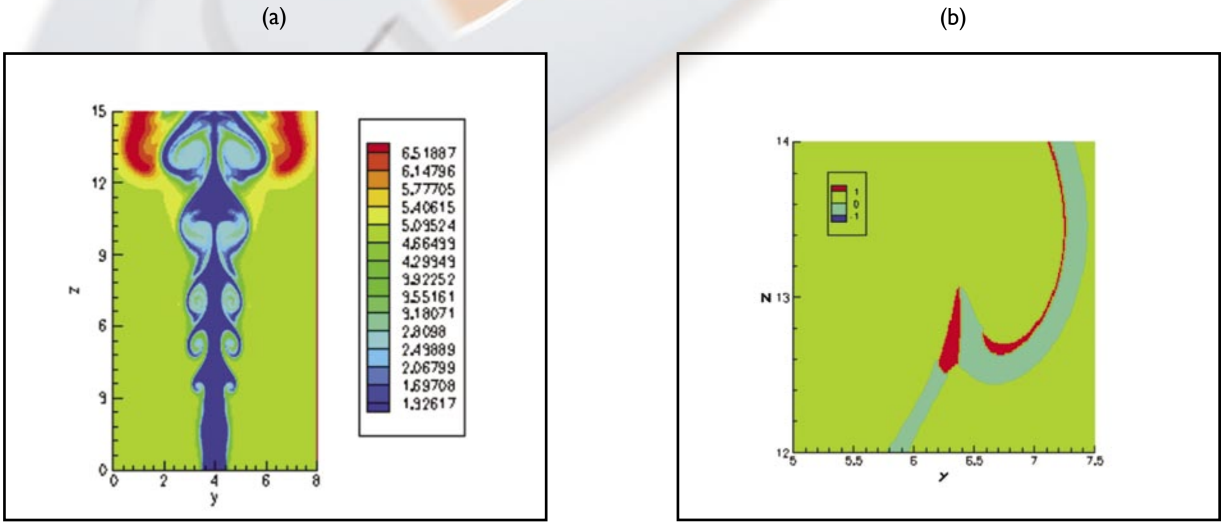


Figure 3: DNS of a buoyant diffusion flame from a rectangular source showing axis switching. Left --- pressure iso-surfaces showing the vortex structures; Right --- combustion product distributions in two vertical planes before and after the axis switching (Luo, 2004).


(a)

(b)

Figure 4: DNS of a lifted flame at a Reynolds number 9500. (a) A representative temperature field showing the reaction zone detached from the source and (b) a close-up view of the conditional reaction rate field showing partially premixed flame (Luo, 2003).

DNS is limited to a small range of physical parameters. The desire of extending such limits is curbed by the fact that the pace of demand from the physical point of view is always exceeding even the very rapid advancement in computer technology. For DNS of turbulence only, the computational cost (memory x CPU requirements) scales with the turbulent Reynolds number to the power of 3. In other words, an order of magnitude increase in the Reynolds number would increase the computational cost by a factor of 1000, which in turn would require the computer industry roughly 10 years to achieve on a constant-cost basis. Nevertheless, the current computing techniques coupled with development of higher-order numerical schemes have enabled DNS to pass the threshold of being able to simulate physical conditions comparable to the lower range of conditions in experiments. Moreover, it is the sole method that can compute 2nd and higher order quantities accurately. In comparison, the RANS approach can only calculate the mean quantities (zero order) and the LES may compute the first derivatives (1st order), with acceptable accuracy. In a word, the desire of the scientific and engineering communities to seek truth and to break the limits will continue to drive the development of DNS and related modelling approaches such as LES.

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References

[1] X. Zhou, K. H. Luo and J. J. R. Williams (2002). "Vortex dynamics in spatio-temporal development of reacting plumes," Combustion and Flame, 129: 11-29.

[2] Y. M. Chung and K. H. Luo (2002). "Unsteady heat transfer analysis of an impinging jets," Transactions of ASME: J. Heat Transfer, 124 (6): 1039-1048.

[3] Y. M. Chung, K. H. Luo and N. D. Sandham (2002). "Direct numerical simulation of an impinging jet," Intl. J. Heat and Fluid Flow, 23 (5): 592-600.

[4] Z. W. Hu, X. Y. Luo and K. H. Luo (2002). "Numerical simulation of particle dispersion in a spatially-developing mixing layer," Theoret. Comput. Fluid Dynamics, 15(6): 403-420.

[5] X. Jiang and K. H. Luo (2003). "Dynamics and structure of transitional buoyant jet diffusion flames with side-wall effects," Combustion and Flame, 133 (1-2): 29-45.

[6] K. H. Luo (2003). "New opportunities and challenges in fire dynamics modelling," Proc. 4th Intl. Seminar on Fire and Explosion Hazards, 15 pages, Londonderry, N. Ireland, 8-12 September (Invited keynote speech).

[7] K. H. Luo (2003). "A study of partial premixing in flames by direct numerical simulation," European Combustion Meeting 2003, Orleans, France, October 25-28.

[8] X. Jiang, E. Avital and K. H. Luo (2004). "Direct computation and aeroacoustic modelling of a subsonic axisymmetric jet," J. Sound and Vibration , 270 (3): 525-538.

[9] X. Jiang, E. Avital and K. H. Luo (2004). "Sound generation by vortex pairing in subsonic axisymmetric jets," AIAA J., 42 (2): 241-248.

[10] K. H. Luo (2004). "Enhancement of mixing and combustion in buoyant non-circular jets," in ERCOFTAC Series: Direct and Large-Eddy Simulation V, 9, 375-384, R. Friedrich, B. J. Geurts and O. Metais (Eds.), Kluwer Academic Publishers, Dordrecht. ISBN 1-4020-2032-5.

[11] K. H. Luo (2004). "Instabilities, entrainment and mixing in buoyant reacting jets," European J. Mechanics B: Fluids , 23 (3): 443-460.

[12] K. H. Luo (2004). "Axis switching in buoyant diffusion flames," Proc. Combust. Inst., 30: 1-7 (in press).

[13] H. Lai and K. H. Luo (2004). "Direct numerical simulation of three-dimensional compressible flows in an open cavity," in Recent Advances in Fluid Mechanics, F. Zhuang and J. Li (eds.), Tsinghua University Press & Springer, Beijing, pp. 790-793.

[14] K. H. Luo (2004). "Fluid dynamics effects on lifted flames," in Recent Advances in Fluid Mechanics, edited by F. Zhuang and J. Li (eds.), Tsinghua University Press & Springer, Beijing, pp. 381-385.

[15] H. Lai and K. H. Luo (2004). "Large eddy simulation of a compressible flow over a fully three-dimensional open cavity," Flow, Turbulence and Combustion (to be submitted).