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December 2002

LES INVESTIGATION OF COHERENT
STRUCTURES IN BOUNDARY LAYERS AND
WAKES

VOLUME IV: SUMMARY OF WORK ACCOMPLISHED
AND FINAL CONCLUSIONS

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Dr. Patrick PURTELL
Office Naval Research
Ballston Center Tower One,
800 North Quincy Street
Arlington VA 22217-5660
U.S.A.

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Dear Dr Purtell,

Please, find, here enclosed, copy of the Summary and Conclusion of Performance/
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"LES investigation of coherent structures in boundary layers and wakes"

which completes the detailed technical report sent on the 10th January 2003.

We remain, of course, at your disposal for any further information you might
require.

Sincerely yours,

Carlo BENOCCI,
Professor

Gerard DEGREGZ,
Adjunct Professor

C/o

Administrative Office

Office of Naval Research Regional Office Boston
495 Summer Street Room 627
Boston MA 02210-2109
U.S.A

Defense Technical Information Center

8725 John J Kingman Road Ste 0994
Fort Belvoir VA 22060-6218

Office of Naval Research

ATTN: ONR 363

Ballston Center Tower One,
800 North Quincy Street
Arlington VA 22217-5660
U.S.A.

Patent Office

Office of Naval Research
ATTN: ONR 00CC
Ballston Center Tower One,
800 North Quincy Street
Arlington VA 22217-5660
U.S.A.

von Karman Institute for Fluid Dynamics
Chaussée de Waterloo, 72
B - 1640 Rhode Saint Genèse - Belgium

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**VOLUME IV: SUMMARY OF WORK ACCOMPLISHED
AND FINAL CONCLUSIONS**

C. Benocci & G. Degrez

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Abstract

Present text summarizes the work performed during the present investigation to assess the feasibility to simulate and study coherent structures in turbulent shear layers making use of Large Eddy Simulations (LES), and whose results are detailed in the three companion volumes R. Giammanco and C. Benocci (2003a), R. Giammanco and C. Benocci (2003b) and G. Degrez and D. Snyder (2003), which complete the present report. General conclusions are offered together suggesting on possible future work on this topics. The comments are organized in two chapters: one devoted to the application of a structured LES code and the development of original algorithms for the detection and analysis of coherent structures present within flow fields created by the former code; the second one details the development and the application of the unstructured LES code also considered for the present application

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1. Simulation and analysis of coherent structures in shear layers by a structured LES code. Summary of work accomplished and final conclusion

C. Benocci & R. Giammanco

Purpose of present research had been to investigate the feasibility to apply the Large Eddy Simulation to the study of coherent structures in shear layers. The aim was to develop numerical tools able to detect, recognize and define all the coherent structures present with the instantaneous flow fields create by LES as well to extract quantitative information and relevant statistics of the resulting population whose results are detailed in the two companion volumes R. Giammanco and C. Benocci (2003a) and R. Giammanco and C. Benocci (2003b).

Instantaneous realization of turbulent flow fields is made by the mean an existing LES code, developed by the Von Karman Institute, which solves the transport equations for resolved turbulence in cartesian frame. A set of original algorithms have been developed for the study of coherent structures.

The which main steps of the proposed procedures are:

- all the nodes of the LES grid are tested to check whether satisfy an identification criterion (the procedure is compatible with all identification criteria proposed by the literature, but most of the actual work was performed with Q criterion).
- strongly connected regions which satisfy the above criterion are defined vortex cores and becomes the pivot of further search
- all the other grid points which satisfy the identification criterion are test to check whether they can be connected to a vortex core and added to this structure. The most complex and critical point of the whole procedure is to check all the possible conflicts and establish whether the examined grid point actually belong to a structures; at the end of the process the grid points so rejected are considered numerical noise.
- the population of so defined structures are analyzed of extract: the global quantities, such as turbulent kinetic energy, vorticity and enstrophy, of the whole field versus the ones for the surrounding un-coherent background; statistics of the physical proprieties of the individual structures, such as size, orientation and distribution across the flow field; statistics of the dynamic proprieties of the individual structures such as vorticity and enstrophy. A software allow to visualize and examine all the structures one by one

This procedure has been extensively tested for the case of turbulent plane channel at equilibrium, at different Reynolds number. The main findings of are consistent with the present literature:

- organized structures are, indeed, present within flow fields and are clustered in the buffer layer and the inner part of the inertial layer
- the most common shape for the structures is an entity elongated along the stream-wise direction, which could be modeled as ellipsoid; surprising the most common size of the structures was found to be far smaller than the longitudinal macro-scale
- the so-identified structure correspond to the most active of the turbulent field : a typical value would be they correspond to 10% of volume of computational field, but 20% of its turbulent kinetic energy and 30% of its enstrophy. Therefore their importance on the dynamic behavior of the flow is demonstrated.

Different simulation parameters were tested to assess their possible influence on present results: it was found that the most important, indeed critical, parameter is resolution of the LES grid, while influence of choice of accuracy of LES discretization, SGS model and identification for structures are found to be of relatively minor effect.

The importance of grid refinement became evident when dealing with the next programmed test case, namely turbulent flows such the one around a cylinder of square cross section at moderately high Reynolds number.

In this case, present simulations were only partially successful.

In what concerns the behavior of dynamic field , visualizations with Q criterion have proved the Large Eddy Simulation approach capable of reproducing the principal mechanisms of flow separation over an obstacle and of formation of a wake dominated by large scale, inherently coherent, structures; onset and development of 'Kelvin-Helmholtz' class instability and formation and interaction of rib-roll structure are well put in evidence. Tracking of span-wise vortices trough pressure field has proved the coherent and persistent character of these structures.

The algorithms developed to identify, define, classify all the organized structures in flow-field and extract all relevant statistics of this population were found unable to resolve and identify the all present structures, as it had been the case of the plane channel: again this defect can be attributed, in large part, to insufficient grid resolution which has posed unresolvable conflicts to the definition algorithm. Useful global statistics have been obtained relaxing the constraints posed to the procedure, confining the analysis to strongly defined vortex cores and rejecting as numerical noise a large number of the nodes which satisfy the Q criterion. The consequence is, however, to worsen the signal-to-noise ratio with respect the one obtained in simulations of plane channel (Volume I).

However, it can be concluded, that present simulations, in spite of their shortcomings, have been able to show that an very important part of the entire turbulent field lies within very active structures, which, by themselves, cover a very small part of the entire flow field.

It can be advanced that the characteristics of these structures are the ones which define and control the wake behavior, and their identification could be key to understand and possibly identify and recognize specific wakes.

It could be suggested that a general and affordable procedure might pass through the adoption of the afore-mentioned approach (computing only the strongly connected vortex cores), while the full process initially developed and proposed in Volume I might prove itself non-affordable or impossible to apply to complex flow field without introducing ad hoc, case by case, adaptations.

Most of the defects remarked for present simulation can be attributed to insufficient available computer power, which has limited the size of computational field and the resolution of the grid, primarily along the critical span-wise direction; increasing the size of the computational domain by 50% ($L_y=6H$ against $L_y=4H$) and doubling the corresponding resolution (96 nodes against 32) are quite likely to yield a full satisfactory simulation of flow field, not only in terms of the eulerian statistics, but most probably in terms of detection and identification of the coherent structures. For the second task, assuming that the computational resources would allow the increase of span-wise number of nodes from 32 to 96, an increase in resolution in the wake should also be undertaken.

Continuing increase of computer capabilities on open market allows to assume that the requirements could soon be available for possible future investigations, as more and more inexpensive clustering technology is made available from both software and hardware vendors, operating within area of the GNU/Linux Operating System. At the present moment, available computational resources would allow to compute the configuration proposed above in a massively parallel environment, where the latent parallel capabilities of the code would be exploited.

If, however, assuming that exists the possibility of setting up a simulation in a parallel context, spending necessary resources in terms of manpower to polish the parallel version of the code, the speed-up that it could be possible to obtain cannot mask the deficiency of the scalar version of the code: explicit treatment of viscous term, absence of an up-to date dynamic SGS model, bottle neck generated by the upwinding procedure, grid conformity between different domains, are all factors that should be faced and solved before planning to use a parallel context to speed-up computations.

It can, however, be concluded that, even in case of complex flows, it is indeed feasible to identify and quantify the contribution of organized turbulence versus non-coherent background through the Large Eddy Simulation approach; whether the results found are deeply linked to the filtering operator and to the grid dimensions, only a careful campaign of test simulations could provide a definitive answer. Concerning the eulerian statistics, it is found that even high order ones, such the turbulent kinetic energy budget (defined in Volume I, §2) cannot be used to separate coherent behavior from non-coherent one.

It could be possible, according to some suggestions given in literature, by spectral analysis of the two fields, which was found impossible

2. Development of a parallel unstructured grid LES code. Summary of work accomplished and final conclusion

G. Degrez & D. Snyder

The essential contribution of this work was the development of a parallel LES solver for the simulation of turbulent flows over arbitrary two-dimensional geometries, using a piecewise linear finite element representation on unstructured triangular meshes combined with a Fourier decomposition in the transverse (periodic) direction whose results are detailed in the companion volume G. Degrez and D. Snyder (2003). The development of the solver involved the following steps:

Two-dimensional unsteady laminar flow solver SFE2D The first step of the research was the development of a 2D incompressible unsteady laminar flow solver, that would serve as a building block for the development of the subsequent 3D flow solver. The spatial discretization is formulated using a SUPG/PSPG FE approach. This formulation has been heavily developed in the last decade and has the advantage of allowing equal-order elements as well as having convective stability without the over-diffusive characteristics of typical upwinding schemes. Linear triangle elements are utilized, resulting in second-order accuracy. As a result of this spatial discretization, very complex geometries can be easily accommodated via unstructured triangle meshes.

The temporal discretization uses a consistent mass matrix and is second-order accurate. An implicit Crank-Nicholson scheme is used for the pressure and diffusion terms, while an explicit second-order Adams-Bashforth scheme is used for the convective terms. Though the explicit treatment of the convective terms introduces a stability limit on the time step size, it affords several advantages when the algorithm is extended to 3D.

Solution of the algebraic system arising at each time step is performed using the SPARSKIT toolkit. This kit is a "black box" GMRES iterative solver package written in Fortran 77 that includes compact matrix storage formats and many preconditioning algorithms. The best performance in terms of robustness and speed in this application was realized using the ILUT preconditioner.

SFE2D was validated against published benchmark lid-driven cavity numerical results at Reynolds numbers between 100 and 5000; as well as published experimental and numerical results for backward-facing step flow at Reynolds numbers between 150 and 1000, and circular cylinder flow at Reynolds numbers between 20 and 140.

Three-dimensional unsteady laminar flow solver SFE3D Starting from the 2D flow solver, the 3D unsteady laminar solver was then developed. With the two basic assumptions of a 2D (cylindrical) geometry and periodicity in the transverse direction, the natural choice for the discretization was to combine the stabilised FE discretization

of the 2D solver in the plane perpendicular to the periodic direction, and a Fourier decomposition in that direction. In order to reduce computational costs, all nonlinear terms are treated using a pseudo-spectral approach where the terms are evaluated in physical space and then transformed into Fourier space. The in-plane and temporal discretizations are identical to the SFE2D solver and are described above. The use of explicit temporal treatment for the nonlinear terms decouples the matrix equations in Fourier space, reducing computational cost and allowing for a novel parallelization scheme where the work is partitioned in Fourier space. The parallelization is implemented using OpenMP, an emerging standard for shared-memory parallelism that allows parallelization with little programming overhead.

SFE3D was validated against published numerical and experimental results for flow past a circular cylinder at Reynolds numbers 195 and 300, where mode-A and mode-B 3D instabilities are present in the wake, respectively.

LES turbulent flow solver SFELES The LES solver SFELES is derived from the unsteady laminar flow solver by including a subgrid scale (SGS) model for the unresolved turbulent fluctuations. The classic Smagorinski SGS Reynolds stress model with van Driest damping near the solid walls is used. Because it is a direct extension of SFE3D, SFELES utilizes a second-order SUPG/PSPG formulation in the 2D plane and a spectral formulation in the transverse direction. The temporal accuracy is second-order, with the eddy viscosity terms being treated using an explicit Adams-Bashforth scheme. An unstructured mesh in the 2D plane allows for LES calculations to be run on complex 2D geometries such as arbitrary bluff bodies, arrays, or complex multi-element airfoils. This capability to feasibly perform LES on unstructured meshes is currently very rare due to the high computational costs associated with both LES and unstructured meshes. The SFELES solver was validated by comparison with published experimental and numerical studies of flow past a circular cylinder at $Re = 3900$.

Finally, the added value of unstructured mesh LES capabilities has been illustrated via a brief investigation of turbulent flow past a circular cylinder with an attached wake splitter plate at $Re = 3900$. This geometry configuration (assuming a finite-thickness splitter plate) cannot be well modeled with a single-block structured mesh, but rather needs an unstructured or block-structured mesh. This represents an original contribution of the present work as, to the author's knowledge, no other computational results exist for this flow configuration. This work contributes information in terms of the physical mechanisms of vortex formation in the presence of splitter plates as well as shedding frequency and drag characteristics for multiple splitter plate lengths. Numerical results are found in very good agreement with experimental measurements and observations of 3D turbulent flow past cylinders with splitter plates.

Although the potentialities of the code have been clearly demonstrated, work remains to be done to improve its efficiency up to the point where it can be used on a daily basis for the

investigation of turbulent flows over complex 2D geometries, First, the iterative linear solver is presently too slow for practical use. Block or algebraic multigrid preconditioners have the potential of cutting the linear systems solution time by an order of magnitude. Linear systems solution time could even further be reduced, at the expense of an increased storage requirement, by factorizing the system matrices and storing the LU factors. Secondly, due to the recent development of affordable and highly powerful distributed memory systems such as PC clusters, a parallel version for distributed memory architectures needs to be developed. Both the Fourier domain parallelization strategy used in the present work and the finite element mesh partitioning strategy should be investigated.

Once the code computational efficiency will have been optimized, much additional research will become possible:

Development of feature detection algorithms The coherent structures detection algorithms developed in the first part of the present work should be extended to the unstructured mesh discretization used in the SFELES code.

Implementation of wall functions and additional boundary conditions In its current form, SFELES contains no wall functions and limited boundary conditions. The addition of wall functions will allow higher Reynolds number simulations to be performed without requiring exorbitant numbers of nodes in the near-wall region. Boundary conditions such as convective outflow and far-field inflow/outflow will also enlarge the class of problems that can be solved with this solver.

Implementation of additional SGS Reynolds stress models This work has focused on the development of the FE/spectral algorithm rather than on achieving the most accurate LES solutions. The Smagorinski model implemented in SFELES is a very basic SGS model, and has a number of shortcomings. SGS model development is an area of intense research, and SFELES can provide an excellent test bed for application of these models to complex geometries.

Extension to axisymmetric configurations The FE/spectral discretization used in SFELES can easily be adapted to cylindrical coordinates, where a FE discretization is used in the meridional plane and a spectral method used in the azimuthal direction. This would expand the class of problems that can be solved to include turbulent flow in pipes and nozzles, including swirling flows such as vortex breakdown, and also external flows over bodies of revolution such as reentry capsules.

Application to airfoil problems High-lift aerodynamics has received much attention in the past decade, both in experimental studies and numerical predictions. The difficulties in obtaining acceptable numerical solutions are twofold. First, the multi-element geometry is difficult to mesh properly, particularly when using structured grids. Secondly, the complex separation and reattachment of the flow on multiple bodies is problematic

for RANS turbulence models. Once sufficient progress has been made in terms of computational speed, boundary conditions, and SGS models, SFELES will be well-suited for high-lift airfoil performance prediction.

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