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LESTATS User's Manual

Mark A. Christon and Thomas E. Voth

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Mark A. Christon and Thomas E. Voth
Computational Physics R & D Department
Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185-0819

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Abstract

LESTATS is a post-processing tool for deriving turbulence statistics from unstructured-grid large-eddy simulations. LESTATS has been developed to provide a simple, flexible means for deriving turbulence quantities such as the mean and fluctuating velocity, Reynolds stresses, turbulent kinetic energy, velocity–temperature and velocity–pressure correlations. In addition, higher-order statistics such as velocity skewness and flatness may be computed. LESTATS requires as input a "time-averaged" database that is generated by the large-eddy simulation code during the flow computation, and it provides the capability to select a time-averaging window for the generation of all the derived turbulence statistics.

[1]Keywords and Phrases: large-eddy simulation, turbulence, averaging, filtering sub-grid scale.

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Preface

The advent of terascale computational resources is making Large-Eddy Simulation (LES) a viable technology for multiple Sandia programs where turbulence plays a role. These programs encompass applications ranging from chemically reacting flows to z-pinches and aerodynamic design for long-haul trucks. LES is a promising alternative to traditional turbulence models because there are effectively no flow-calibrated parameters, little empiricism is required for a broad spectrum of flow regimes, and transitional and time-dependent flows can be treated.

LES directly computes the grid-resolvable features of the flow field and uses a sub-grid scale model to represent the flow physics associated with the unresolved scales of the flow field. Although LES has been demonstrated for simple geometries, the treatment of complex geometries with unstructured grids is just beginning to be explored. The interaction between dispersive errors, grid anisotropy, filters and filter scales, and sub-grid scale models has not been quantified in a rigorous way resulting in uncertainty for many LES predictions. These issues are compounded by Sandia applications that demand unstructured grids and accurate treatment of buoyancy, no-slip walls, and chemically reacting flows.

LESTATS computes time-averaged turbulence statistics suitable for comparison with experimental data and constitutes one component of an LES toolkit. The research behind the LES toolkit is seeking to advance LES models and methods by quantifying the effects of filters and filter scales for unstructured, non-orthogonal grids, under-resolved flow fields, and stochastic sub-grid scale models. This effort is relying on Sandia's large-scale computational capability, advanced numerical analysis techniques and controlled numerical experiments to develop an LES toolkit with models, algorithms, standard libraries for filters and derived flow statistics, and a suite of validation and verification problems.

Chapter 1

Introduction

LESTATS is a tool for deriving time-averaged turbulence statistics from unstructured-grid large-eddy simulations. It has been developed to provide a simple, flexible means for calculating quantities such as the mean and fluctuating velocity, Reynolds stresses, turbulent kinetic energy, velocity–temperature correlations and higher-order statistics such as velocity skewness and flatness.

LESTATS requires as input a "time-averaged" database that is generated by the large-eddy simulation code during the flow computation, and it provides the capability to select a time-averaging window for the generation of all the derived turbulence statistics.

1.1 Guide to the LESTATS User's Manual

The purpose for this document is to provide sufficient information for an experienced CFD analyst to use LESTATS in an effective way. The assumption is that the user is somewhat familiar with modern supercomputers, large-scale computing, common CFD practices, and large-eddy simulation. This document provides sufficient references to permit the interested reader to pursue the technical details of LESTATS.

In this document, an attempt is made to adhere to the convention that all keywords and defaults for input data appear in a **boldface** type, and sample computer input/output appears in a `typewriter` font. All other keywords, parameters and variables are defined in the context they are used.

In Chapters 2 and 3, a theoretical overview is presented as background for LESTATS while Chapter 4 presents information on the keyword input and how to execute LESTATS in a UNIX environment. Sample calculations are presented in Chapter 5 to illustrate some of the capabilities of LESTATS. Appendix A describes the contents of the input time-averaged data for LESTATS.

1.2 History of LESTATS Development

LESTATS was developed as a part of Sandia's LES toolkit for performing unstructured-grid large-eddy simulations. The development of LESTATS was done by Mark A. Christon and Thomas E. Voth using the existing software infrastructure for memory management and finite element calculations from GILA,[2] a parallel, unstructured-grid incompressible and low-Mach CFD code. The PXI/PDS/PIO libraries[6] were initially adopted to permit the treatment of large-scale, parallel databases that are typical of GILA's LES computations. Later, the EXODUS-II[5] libraries were integrated to permit compatibility with a broader suite of codes.

1.3 LESTATS Capabilities

LESTATS provides the capabilities to treat both 2-D and 3-D PXI or EXODUS-II databases that contain windowed time-averaged data generated during an LES calculation. Currently, LESTATS treats three levels of input data that range from mean quantities such as mean velocity, pressure, etc. to an intermediate level that includes correlations such as velocity and pressure, and the highest level that includes the higher-order correlations, $< u_i^3 >$ and $< u_i^4 >$. Details on the input data for LESTATS may be found in Appendix A.

The derived statistics generated by LESTATS are also provided to the user in three levels. The derived statistics are based on a user-specified window for time-averaging that is a subset of the input data from the large-eddy simulation. The lowest level of derived statistics yields mean quantities that are based on the user-specified time window. The mean quantities generated at this level include the velocity, $< u_i >$, pressure, $< p >$, vorticity $< \omega_i >$, enstrophy, $< 1/2\ \omega_i \omega_i >$, and helicity, $< \omega_i u_i >$. For thermal problems, the mean quantities also include the average temperature, $< T >$, and for species transport, the mean species concentration, $< Z_j >$.

At the intermediate level of derived statistics, second moments are computed in addition to the mean quantities. In this case, the turbulent stress tensor and scalar flux vectors are computed and output. That is, $< u_i u_j >$, $< u_i T >$, $< u_i Z_j >$, $< u_i p >$ are added to the output time average database. At the highest level of statistics, skewness and flatness of the velocity are computed in addition to the mean and derived flux quantities. Currently, the scalar dissipation is not calculated in LESTATS.

In addition to the computation of derived statistics, LESTATS provides the option to generate a two-scale decomposition of all of the turbulence statistics. The two-scale representation yields low-scale and "detail" output databases that are identified by "`_flt`" and "`_dif`" filename extensions respectively. The low-scale, or filtered, database contains the turbulence statis-

tics represented at one-half the grid resolution, while the detail database contains the difference between the turbulence statistics and the half-resolution statistics and provides a direct indication of where rapid changes in the turbulence statistics occur.

1.3.1 Database Interfaces

At this time, LESTATS reads and writes EXODUS-II and PXI files. For large-scale, parallel databases, the PXI file format may provide a more tractable solution. In contract, the EXODUS-II file format is strictly serial and requires a serial view of the computed LES data.

1.4 Running LESTATS

LESTATS has been developed to permit rapid configuration for many computer architectures. The common thread for all of these machines is a UNIX (or UNIX like) environment. LESTATS provides a single command line interface that accepts multiple command line arguments. LESTATS may be executed with the following command line options.

```
lestats -i inf -c cntl -o avg
```

LESTATS Command Line Arguments

Keyword	Meaning
-i *inf*	EXODUS-II/PXI file containing raw time-averaged data (*default*: **plot**)
-c *cntl*	LESTATS control file (*default*: **cntl**)
-o *avg*	EXODUS-II/PXI output file with derived LES statistics (*default*: **avg**)

On the command line, the individual command line arguments may include a path name in the file name as well. For example, the following command line makes use both absolute and relative paths for files.

```
lestats -i /tmp/flow1.exo -c../cntl1 -o/home/joe/plate.avg
```

Chapter 2

LES Derived Statistics

This chapter presents some of the tools that are available in LESTATS to analyze turbulent flow data. There are two primary objectives for analyzing data from a large-eddy simulation. The first is to develop an understanding of the flow field in question through the use of these tools. This may lead to design changes or implementation of turbulence controls. The second objective is to reveal pathologies caused by the numerical integration of the flow equations and concomitant closure models under realistic conditions. It is hoped that a clear understanding of these pathologies may lead to better simulation models.

In order to probe LES data, statistical analysis tools are needed that allows the distillation of the tremendous volume of data produced from simulation (or experiment) down to a few manageable quantities of interest that may be directly compared to experimental data. The nature of turbulent flows does not allow for a predictive solution in the strict sense of the word. One must therefore be content with the prediction of its statistics.

Some of the most important statistical quantities of interest (and the most physically revealing) correspond to the first moments of the flow variables, i.e., the mean values. Moments of flow variables such as the velocity are routinely measured in experiments and form the basis of the Reynolds Averaged Navier-Stokes (RANS) solution approach for turbulent flows. There are several techniques used to obtain these moments from raw data, e.g., LES data. Before proceeding with an overview of the derived statistics in LESTATS, several definitions are required.

2.1 Reynolds Averaged Statistics

Reynolds time averages, homogeneous spatial averages, ensemble averages and probability densities are four techniques commonly used to determine mean quantities (or moments) of a turbulent flow. Reynolds averaging is used

to derive the time invariant mean quantities of a stationary flow as a function of position. Ensemble averaging is suited for transient flows and describes the mean values as a function of both space and elapsed time. Spatial averaging describes the spatial invariance of mean values in a homogeneous flow that may or may not be stationary.

The fourth and most powerful technique for determining mean values is through the use of probability densities of stationary processes. If the probability density of the flow variables is known for the entire domain of interest, then all of the moments of the flow variables can be obtained from the probability density. In practice, this probability density is difficult to determine and contains more information than is desired, therefore it will not be considered further here. The remainder of this section will concentrate on the definition and use of the Rynolds, spatial and ensemble averaging.

A stationary flow is one in which mean values are independent of the initial time from which the means are determined. Stationary flows are also referred to as statistically steady. In other words, the mean values do not change with time. Consider the temporally and spatially varying quantity $\phi(x_i, t)$, its Reynolds time average is

$$< \phi(x_i) >= \lim_{T\to\infty} \frac{1}{T} \int_{t_0}^{t_0+T} \phi(x_i, t')dt' \tag{2.1}$$

where t_0 denotes an arbitrary starting time for the integration.

An example of a stationary flow is a jet flow issuing from the nozzle on a pipe at high Reynolds number with a fixed mass flow rate that is controlled by a valve. After some time, the flow settles down and a stationary flow is achieved. A probe designed to measure the velocity field placed at some location within the jet would measure a fluctuating velocity that if examined closely would seem to be oscillating randomly about a steady mean.

In contrast, for non-stationary flows, time-invariant mean can not be defined, i.e., the mean is time-dependent. For this type of flow, ensemble averaging may be used where flow data is accumulated over a number of trials, i.e., repeating the experiment until the mean values are independent of the number of experiments performed. At this point the mean values are said to have converged to a statistically reliable value. A formal definition of an ensemble average for a generic variable $\phi(x_i, t)$ is

$$< \phi(x_i, \tau) >_E= \lim_{N_E\to\infty} \frac{1}{N_E} \sum_{n=1}^{N_E} \phi(x_i, t = \tau) \tag{2.2}$$

where $\tau = t - t_0$ is the elapsed time from the start of the experiment t_0, and N_E is the number of experiments.

An example of a non-stationary flow may be seen in the turbulent flow around a moving body, e.g., a turning submarine. In this situation, the flow

can never become stationary. In contrast, the flow around a stationary bluff body would become stationary after an initial startup transient.

A homogeneous flow is one in which the statistical properties of the flow do not vary with spatial location. All the mean values are independent of location and can by described by a single value at an instant in time, instead of a value at each spatial location. The mean values of homogeneous flows are determined from a volume integral such as

$$\overline{\phi(t)} = \lim_{V \to \infty} \frac{1}{V} \int_V \phi(x_i, t) dV \tag{2.3}$$

where V is the volume of the domain and $dV = dx_1 dx_2 dx_3$. If in addition, the flow is isotropic then the properties of the flow do not vary with direction. In other words, the flow is invariant to a rotation in coordinate system. Homogeneous flow is an idealization because boundary conditions such as no-slip/no-penetration surfaces introduce inhomogeneities into the flow.

The best example of homogeneous flow is the flow behind a mesh in a wind tunnel, i.e., so-called "screen" turbulence. In the central region away from the tunnel walls, the flow approaches homogeneous and isotropic conditions. If we assume the flow to be incompressible, then the turbulence is entirely known from the velocity and pressure fields at an instant in time, which we refer to as a realization. If the flow is homogeneous the mean values can be obtained from a single realization of the flow instead of Reynolds time averaging over many realizations. The two techniques for measuring mean values are expected to be equivalent in a homogeneous flow.

The current version of LESTATS calculates Reynolds averaged statistics of stationary flows and provides spatial filtering for performing two-scale decompositions of the data. In the first implementation, spatial averaging of homogeneous data, ensemble averaging of transient flow data and calculation of probability densities have been neglected. The discussion above of the other techniques for determining mean quantities is meant to clarify the type of analysis that is being performed presently and set the stage for future developments in LESTATS. In addition, not all of the quantities of interest described below have been implemented at this point in time. Specifically, the higher order statistics such as velocity derivative skewness and flatness have been left for future development.

2.2 Mean and Fluctuating Quantities

All of the statistical measures of turbulent flows presented in this section are based upon the Reynolds average for stationary flows. With the definition of the Reynolds average given above, any variable can be decomposed into

its mean and fluctuating component,

$$\phi(x_i,t) =< \phi(x_i) > +\phi'(x_i,t) \tag{2.4}$$

and obeys the following Reynolds-averaging rules,

$$\begin{aligned} < \phi' > &= 0 && (2.5)\\ << \phi >> &= < \phi > && (2.6)\\ < \phi\psi > &= < \phi >< \psi > + < \phi'\psi' > && (2.7)\\ < \phi' < \psi >> &= < \psi' < \phi >>= 0. && (2.8) \end{aligned}$$

The time average is approximated by the discrete summation,

$$< \phi(x_i) >= \lim_{N\to\infty} \frac{\sum_{n=1}^{N} \phi_n(x_i,t_n)\Delta t_n}{\sum_{n=1}^{N} \Delta t_n} \tag{2.9}$$

where Δt_n is the time step increment for the nth time integration step and $t_n = \sum_{m=1}^{n} \Delta t_m$ is the accumulated time. Let ϕ represent a scalar quantity and let u_i, $(i = 1,2,3)$ represent the ith Cartesian component of the instantaneous velocity. The variance of a scalar is

$$\sigma^2 =< (\phi- < \phi >)^2 >=< \phi^2 > - < \phi >^2 \tag{2.10}$$

where the root mean square (r.m.s.) is σ. Similarly, the Reynolds stress tensor is

$$R_{ij} =< u_i'u_j' >=< u_iu_j > - < u_i >< u_j > \tag{2.11}$$

and the turbulent kinetic energy is one half of the trace of the Reynolds stress tensor

$$q' = \frac{1}{2} < u_k'u_k' >= \frac{1}{2}(< u_ku_k > - < u_k >< u_k >) \tag{2.12}$$

where repeated indices implies summation. The turbulent scalar flux vector is

$$< \phi'u_i' >=< \phi u_i > - < \phi >< u_i > . \tag{2.13}$$

The triple correlation between three independent scalars is defined as

$$\begin{aligned} < \phi'\psi'\lambda' > &= < \phi\psi\lambda > - < \phi >< \psi >< \lambda > && (2.14)\\ &\quad -(< \phi >< \psi'\lambda' > + < \psi >< \phi'\lambda' > + < \lambda >< \phi'\psi' >). \end{aligned}$$

Correlations of this type appear in second order moment closure models such as the Reynolds stress turbulence model. Higher order correlations can be defined in a similar manner.

2.2.1 Higher Order Statistics

Higher order moments of velocity, velocity differences and velocity derivatives have been used to analyze isotropic turbulence. The skewness of velocities is defined as

$$S_{0i} = \frac{\langle u_i^3 \rangle}{\langle u_i^2 \rangle^{3/2}} \tag{2.15}$$

and the flatness factor of velocities is

$$F_{0i} = \frac{\langle u_i^4 \rangle}{\langle u_i^2 \rangle^{2}}. \tag{2.16}$$

The skewness is a measure of the asymmetry of the fluctuations; $S_{0i} > 0$ are predominately positive and $S_{0i} < 0$ are predominately negative. The flatness is a relative measure of remotely occurring, symmetric spiking fluctuations.

The skewness of velocity derivatives is defined as

$$S_{1i} = \frac{\left\langle \left(\frac{\partial u_i}{\partial x_i} \right)^3 \right\rangle}{\left\langle \left(\frac{\partial u_i}{\partial x_i} \right)^2 \right\rangle^{3/2}} \tag{2.17}$$

and the flatness factor of velocity derivatives

$$F_{1i} = \frac{\left\langle \left(\frac{\partial u_i}{\partial x_i} \right)^4 \right\rangle}{\left\langle \left(\frac{\partial u_i}{\partial x_i} \right)^2 \right\rangle^{2}} \tag{2.18}$$

where there is no summation of indices.

Skewness and flatness of velocity differences have been also measured,[1]

$$S_{\Delta i}(r) = \frac{\langle (\Delta u_i)^3 \rangle}{\langle (\Delta u_i)^2 \rangle^{3/2}} \tag{2.19}$$

and the flatness factor is

$$F_{\Delta i}(r) = \frac{\langle (\Delta u_i)^4 \rangle}{\langle (\Delta u_i)^2 \rangle^{2}} \tag{2.20}$$

where $\Delta u_i = u_i(x_i + r_i, t) - u_i(x_i, t)$ and $r_i = x_i + r$.

For homogeneous and isotropic turbulence, the velocity fluctuations have a Gaussian probability distribution. Since this distribution is symmetric, all odd moments are zero. The nonzero moment higher than the variance is the flatness that obtains a value of 3.0. The derivative skewness is $\sim -0.3 - -0.5$ and the derivative flatness is $\sim 3 - 4$.[1] Velocity derivative skewness and flatness are dominated by the smaller scales in the flow so these statistics provide a good measure of how well the numerical scheme is resolving the smaller scales of the flow.

2.2.2 Anisotropic Stress Tensor

An intrinsic distinction exists between isotropic and anisotropic Reynolds stresses. The isotropic stress is $\frac{2}{3}q'\delta_{ij}$ and the deviatoric anisotropic part is

$$a_{ij} =< u_i'u_j' > -\frac{2}{3}q'\delta_{ij}. \tag{2.21}$$

The normalized anisotropy tensor is defined as $b_{ij} = \frac{a_{ij}}{2q'}$. It is readily seen that $a_{kk} = 0$ and any anisotropy is seen by non-zero values of the off-diagonal terms.

Chapter 3

Filters

This chapter begins with a brief description of the approach used to obtain a two-scale decomposition of the derived turbulent statistics. This decomposition provides direct indicators as to where rapid changes in the derived statistics occur and it is hoped that this capability will prove useful for a priori testing and development of physically consistent LES closure models. The following section provides an overview of the discrete filters used for the two-scale decomposition. In LESTATS, emphasis has been placed on filters that minimize commutative errors associated with filtering of the Navier-Stokes equations on unstructured grids. Although the LESTATS tool is not intended for explicit filtering of the LES equations, the filters included here may be implemented in such an unstructured grid code in the future. Thus LESTATS provides a framework for evaluation of these filters and a starting point for a priori testing of LES closure models. This chapter ends with a section outlining the operational details of the filters employed in LESTATS.

3.1 Two-Scale Decomposition

Following Liu et al.[4] two-scale decomposition refers to the separation of a field variable $u^a(\mathbf{x})$ into low-scale and detail components, $u^{2a}(\mathbf{x})$ and $\Delta u^{2a}(\mathbf{x})$ respectively. If $u^a(\mathbf{x})$ is the finest scale response available, then the two-scale decomposition of the response is given as,

$$u^a(\mathbf{x}) = u^{2a}(\mathbf{x}) + \Delta u^{2a}(\mathbf{x}) \tag{3.1}$$

Low-scale components are obtained from the fine (high) scale by discrete filtering of u^a,

$$u^{2a}(\mathbf{x}) = \sum_{i=1}^{Nnp} u^a(\mathbf{x}_i) w_i^{2a}(\mathbf{x}) \tag{3.2}$$

where Nnp is the number of grid points and $w_i^{2a}(\mathbf{x})$ is an appropriate low-pass filter as developed in the next section. Here, the finest scale available is

at the resolution of the grid. Thus, $u^a(\mathbf{x})$ in Eq. (3.2) are the time-averaged turbulent statistics as calculated by LESTATS.

3.2 Overview of Discrete Filters

This section summarizes the theory employed in developing discrete filters that satisfy the moment conditions necessary for commutation of filtering and differentiation. This commutation is necessary for the differential LES equations to have the same form as the Navier-Stokes equations.[7] Some of the details concerning commutation errors and LES filtering may be found in the work by Ghosal and Moin,[3] and the work by Vasilyev, et al.[7] For the sake of clarity, the following overview is limited to one spatial dimension although the formulation is easily extended to multi-dimensions. The LESTATS implementation includes both two and three-dimensional filters that may be used "in-line" with the computation of the derived statistics.

In one-dimension, the discrete filtering operation may be written as,

$$u^{2a}(x) = \sum_{i=1}^{Nnp} u^a(x_i) w_i^{2a}(x) \tag{3.3}$$

where $w_i^{2a}(x)$ is the filter (kernel) function centered at grid point i and evaluated at location x. The dilation parameter, $2a$, describes the width of (and hence scale represented by) the filter, Nnp is the number of filter functions, w_i^{2a}, which have x in their support, and u^{2a} is the filtered approximation to u^a at scale $2a$. As mentioned in § 3.1, u^a represent the LESTATS derived statistics variables evaluated at the grid points.

In general, it is necessary that the filtering operation described in Eq. (3.3) commute with the spatial differential operators of the Navier-Stokes equations for explicit filtering of these equations to be successful. Although it is not generally possible to reduce these commutative errors to zero, they can be controlled by enforcing "moment conditions" when generating the kernel functions. Leaving the details to the literature, we consider a class of filters that satisfy the following moment conditions,

$$m_0(x) = 1 \tag{3.4}$$

$$m_k(x) = 0, k = 1, ..., n, \tag{3.5}$$

$$m_k(x) \neq 0, k \geq n + 1. \tag{3.6}$$

imposed over the domain Ω. In Eq. (3.4)–(3.6), n is the order of the commutation error associated with filtering of the spatial first-derivative operator, and the moments are calculated as,

$$m_k(x) = \sum_{i=1}^{Nnp} (x - x_i)^k w_i^{2a}(x). \tag{3.7}$$

It remains to determine $w_i^{2a}(x)$ such that Eq. (3.4)– (3.5) are satisfied. Liu and co-workers have developed a methodology (the Reproducing Kernel Particle Method - RKPM) to generate kernel functions that satisfy the moment conditions to any order (n) for an arbitrary placement of nodes as typified by unstructured grids on finite domains, Ω, with complex geometry.

The RKPM kernel development begins with a parent kernel, ϕ, that generally does not satisfy the moment conditions. Though not strictly necessary, typical parent kernel functions are chosen to have compact support. Compact support of ϕ reduces the summation in Eq. (3.3) to a small number of neighboring points thereby reducing the computational cost involved in calculating u^{2a}. Commonly used choices for ϕ include the cubic B-spline and truncated Gaussian functions.

Following Liu et al., the reproducing kernel w is related to ϕ by,

$$w_i^{2a}(x) = \sum_{k=0}^{n} \beta_k(x)(x - x_i)^k \phi_i^{2a}(x), \tag{3.8}$$

where $\beta_k(x)$ are a set of correction functions that vary within the domain Ω to enforce the moment conditions. These correction functions are found by requiring that Eq. (3.3) reproduce polynomials to degree n,

$$\mathbf{p}(x) = \mathbf{P}\mathbf{W}(x) \tag{3.9}$$

where $\mathbf{p}^T = [1, x, x^2, ..., x^n]$, $\mathbf{P} = [\mathbf{p}(x_1), \mathbf{p}(x_2), ..., \mathbf{p}(x_{Nnp})]$ and $\mathbf{W}^T = [w_1^{2a}(x), w_2^{2a}(x), ..., w_{Nnp}^{2a}(x)]$. Depending on the **order** option set in the **filter** block of the LESTATS control file (cf. Chapter 4) linear ($\mathbf{p}^T = [1, x, y]$ two-dimensional; $= [1, x, y, z]$ three-dimensional) and bi-linear ($\mathbf{p}^T = [1, x, y, xy]$ two-dimensional domains) reproducing conditions are available. Substituting Eq. (3.8) into Eq. (3.9) yields,

$$\mathbf{B} = \mathbf{M}^{-1}\mathbf{P_0} \tag{3.10}$$

where $\mathbf{B}^T = [\beta_0, \beta_1, ..., \beta_n]$, $\mathbf{P_0}^T = [1, 0, ..., 0]$ and,

$$\mathbf{M} = \begin{bmatrix} M_0 & M_1 & ... & M_n \\ M_1 & M_2 & ... & M_{n+1} \\ \vdots & \vdots & ... & \vdots \\ M_n & M_{n+1} & ... & M_{n+n} \end{bmatrix} \tag{3.11}$$

is the moment matrix of the parent kernel and these moments are calculated as,

$$M_k(x) = \sum_{i=1}^{Nnp} (x - x_i)^k \phi_i^{2a}(x). \tag{3.12}$$

3.2.1 Filter Implementation in LESTATS

The filters (kernel functions) used in LESTATS are generated using the RKPM methodology outlined above. In order to reduce the computational cost associated with determining the connectivity between the kernel function and the nodes, the node-to-element connectivity is used yielding the "FAST-RKPM" filter. In this way, the kernel function associated with node i is generated as follows:

- The parent kernel function ϕ_i^{2a} is assumed to have compact support, being non-zero only at nodes j which share common elements with node i (cf. Figure 3.1). The node-to-element connectivity information is readily available in most unstructured-grid codes, eliminating the need for computationally expensive node-to-node searches. The magnitudes of parent kernel function at the nodes under its support are taken to be $\phi_i^{2a}(x_i) = 1$ and $\phi_i^{2a}(x_j) = 1/2$.

- Next, the parent kernel function moment matrices are generated at each node within the domain via Eq. (3.12).

- The set of correction functions for each node j are determined using Eq. (3.10) and the filter functions $w_i^{2a}(x_j)$ are calculated from Eq. (3.8).

- The filtered statistics variables, u^{2a} are calculated using Eq. (3.3), and the results are output to the low-scale database as the low-scale part of the two-scale decomposition.

- The "detail" data is calculated as the difference between the spatially un-filtered data and the filtered data, $\Delta u^{2a} = u^a - u^{2a}$. The results are output in the detail database.

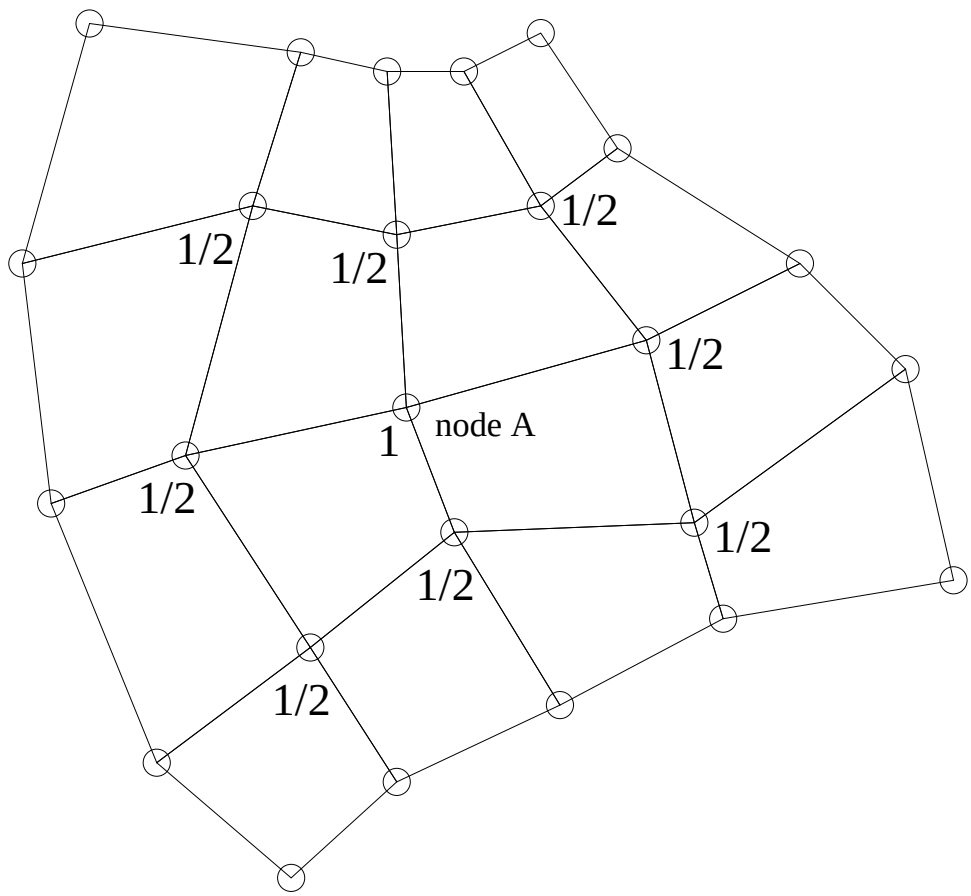


Figure 3.1: FAST-RKPM parent kernel function values for the function centered about node A. The kernel function is shown on a two-dimensional unstructured grid.

Chapter 4

LESTATS Control File

The necessary input data for LESTATS is split into multiple files. The first file, the "control file", contains all of the control information for selection of the statistics to be generated from the LES data. The second file is a PXI file and contains raw time-average data from the LES calculation that is to be post-processed. Appendix A presents a description of the input time-average data. From this data, a variety of turbulence statistics may be generated ranging from simple time-averages of primitive variables, i.e., velocity, pressure and temperature, to Reynolds stresses, turbulent kinetic energy, velocity skewness and flatness.

In the ensuing description, **bold** text denotes keywords, while *italic* text identifies keyword parameters or optional data in the control file. Primary sections of the control file are delimited by a **keyword** – **end** sequence that may contain a series of **keyword** – *parameter* sequences. The presence of a keyword and a parameter implies that the parameter is expected as input. Where possible, default values have been identified in order to minimize the number of keywords that are necessary in the input file. Comments in the control file must be preceded by a "$" symbol or a "#" symbol, or may be enclosed in a pair of braces "{ }". All input in the control file is case insensitive. Figure 4.1 shows the typical format of an LESTATS control file.

```
# starts a comment line

$ starts a comment line

{ Comments may be enclosed in braces as well }

# Define the file format
pltype exodus

average
# The average-end block describes the type of derived statistics
...
end

# The filter-end block activates the two-scale filtering procedure
filter
...
end

# The exit command terminates input from the control file
exit
```

Figure 4.1: A Sample LESTATS Control File

4.1 Primary Keywords

4.1.1 pltype

pltype *file_type*

LESTATS permits the selection of file formats for reading/writing the time-averaged data. Valid values for *file_type* are:

exodus: Selects the Exodus-II file format,

pxi: Selects the PXI file format.

4.2 Time Averaging Parameters (average – end)

The averaging parameters define the type of statistics to be derived, and the starting and ending indices for the time-average window. The level of

statistics to be derived must be consistent with the input time-average data in the PXI file. The lowest common level of statistics between the control file and input PXI file will be used. All of the time-averaging parameters are specified in the **average** − **end** block in the control file.

average Start the **average** − **end** block.

end Terminate the time-average block.

An example of how the **average** − **end** block would appear in the input file is shown below.

```
average
   stats   10
   starti   5
   endi   100
   ...
end
```

4.2.1 stats

stats *level_id*

Set the level of statistics to derive.

stats=10: The mean statistical quantities generated at this level include the velocity, $< u_i >$, pressure, $< p >$, vorticity $< \omega_i >$, enstrophy, $< 1/2\ \omega_i \omega_i >$, and helicity, $< \omega_i u_i >$. For thermal problems, the mean quantities also include the average temperature, $< T >$, and for species transport, the mean species concentration, $< Z_j >$. Table 4.1 shows the output mean variables and the associated database variables.

stats=20: At this level of statistics, second moments are computed during the computation and output at the time-average dump interval. In addition to the mean quantities, for **stats=10**, the turbulent stress tensor and scalar flux vectors are computed and output. That is, $< u_i u_j >$, $< u_i T >$, $< u_i Z_j >$, $< u_i p >$ are added to the time average database. Table 4.2 shows the additional output variables associated with **stats=20**. At this time, the scalar dissipation is not included in the time average database.

stats=30: In addition to the mean and derived flux quantities, the higher-order averages are generated that include $< u_i^3 >$ and $< u_i^4 >$. Table 4.3 shows the additional output variables associated with **stats=30**.

Variable Name	Quantity	PXI Database Label
X-velocity	$< u_1 >$	`<u1>`
Y-velocity	$< u_2 >$	`<u2>`
Z-velocity	$< u_3 >$	`<u3>`
Pressure	$< p >$	`<pnode>`
X-vorticity	$< \omega_1 >$	`<w1>`
Y-vorticity	$< \omega_2 >$	`<w2>`
Z-vorticity	$< \omega_3 >$	`<w3>`
Enstrophy	$< 1/2\ \omega_i \omega_i >$	`<enstrophy>`
Helicity	$< u_i \omega_i >$	`<helicity>`
Stream Function	$< \psi >$	`<stream>`
Temperature	$< T >$	`<temp>`
Density	$< \rho >$	`<rho>`
Species-1	$< Z_1 >$	`<Z1>`
Species-2	$< Z_2 >$	`<Z2>`

Table 4.1: LESTATS **stats**=10 output variables and database labels.

4.2.2 starti

starti *index*

Set the time index of the input time average data where the derived turbulence statistics will begin.

4.2.3 endi

endi *index*

Set the PXI index of the simulation time to end the turbulence statistics.

4.2.4 exit

exit

This keyword terminates parsing of the control file. Any keywords following the **exit** keyword will be ignored.

Variable Name	Quantity	PXI Database Label
Velocity Correlations	$< u_1 u_1 >$	`<u1u1>`
	$< u_1 u_2 >$	`<u1u2>`
	$< u_1 u_3 >$	`<u1u3>`
	$< u_2 u_2 >$	`<u2u2>`
	$< u_2 u_3 >$	`<u2u3>`
	$< u_3 u_3 >$	`<u3u3>`
Reynolds Stresses	$< u_1' u_1' >$	`<u1'u1'>`
	$< u_1' u_2' >$	`<u1'u2'>`
	$< u_1' u_3' >$	`<u1'u3'>`
	$< u_2' u_2' >$	`<u2'u2'>`
	$< u_2' u_3' >$	`<u2'u3'>`
	$< u_3' u_3' >$	`<u3'u3'>`
Turbulent Kinetic Energy	q'	`TKE`
Velocity – Pressure Correlations	$< u_1 p >$	`<u1p>`
	$< u_2 p >$	`<u2p>`
	$< u_3 p >$	`<u3p>`
	$< u_1' p' >$	`<u1'p'>`
	$< u_2' p' >$	`<u2'p'>`
	$< u_3' p' >$	`<u3'p'>`
Velocity – Temperature Correlations	$< u_1 T >$	`<u1T>`
	$< u_2 T >$	`<u2T>`
	$< u_3 T >$	`<u3T>`
	$< u_1' T' >$	`<u1'T'>`
	$< u_2' T' >$	`<u2'T'>`
	$< u_3' T' >$	`<u3'T'>`
Velocity – Species Correlations	$< u_1 Z_1 >$	`<u1Z1>`
	$< u_2 Z_1 >$	`<u2Z1>`
	$< u_3 Z_1 >$	`<u3Z1>`
	$< u_1' Z_1' >$	`<u1'Z1'>`
	$< u_2' Z_1' >$	`<u2'Z1'>`
	$< u_3' Z_1' >$	`<u3'Z1'>`
	$< u_1 Z_2 >$	`<u1Z2>`
	$< u_2 Z_2 >$	`<u2Z2>`
	$< u_3 Z_2 >$	`<u3Z2>`
	$< u_1' Z_2' >$	`<u1'Z2'>`
	$< u_2' Z_2' >$	`<u2'Z2'>`
	$< u_3' Z_2' >$	`<u3'Z2'>`

Table 4.2: LESTATS **stats=**20 output variables and database labels.

Variable Name	Quantity	PXI Database Label
Third Moments	$< u_1^3 >$	`<u1^3>`
	$< u_2^3 >$	`<u2^3>`
	$< u_3^3 >$	`<u3^3>`
Velocity Skewness	$< u_1^3 > / < u_1^2 >^{3/2}$	`<S01>`
	$< u_2^3 > / < u_2^2 >^{3/2}$	`<S02>`
	$< u_3^3 > / < u_3^2 >^{3/2}$	`<S03>`
Fourth Moments	$< u_1^4 >$	`<u1^4>`
	$< u_2^4 >$	`<u2^4>`
	$< u_3^4 >$	`<u3^4>`
Velocity Flatness	$< u_1^4 > / < u_1^2 >^2$	`<F01>`
	$< u_2^4 > / < u_2^2 >^2$	`<F02>`
	$< u_3^4 > / < u_3^2 >^2$	`<F03>`

Table 4.3: LESTATS **stats**=30 output variables and database labels.

4.3 Filter Options (filter – end)

The specification of a filter and two-scale decomposition occurs in the *filter - end* block in the control file. In the specification of a filter *type* and the associated degree of consistency, *deg*, must be prescribed.

filter Start the **filter – end** block.

type *type* Specify the filter type to be used.

order *deg* Specify the degree of filter consistency to be used.

end Terminate the material block.

An example of how the **filter – end** block would appear in the input file is shown below.

```
filter
   type    10
   order   10
   ...
end
```

Filter Parameters

The following keyword – parameter commands are provided to set filter properties.

4.3.1 type

type *id*

Set the filter *id* to be used. (*default:* **type=10**).

type=10**:** FAST-RKPM filter is used. This is currently the only filter type available.

4.3.2 order

order *deg*

Set the filter order, *deg*, that is to be used. (*default:* **order=10**).

order=10**:** Linear consistency of the filter is enforced. For two-dimensional domains, the filter enforces exact reproduction of $[1, x, y]$. Three-dimensional filters of this order enforce exact reproduction of $[1, x, y, z]$.

order=20**:** Bi-linear consistency of the filter is enforced. For two-dimensional domains, the filter exactly reproduces the polynomial bases $[1, x, y, xy]$. This option is not available for three-dimensional domains.

Chapter 5

Example Calculations

Several example calculations are included in this chapter to demonstrate the use of the control file and some of the capabilities of LESTATS.

5.1 Vortex Shedding

This example consists of a moderate Reynolds number, $Re = 100$, laminar flow past a circular cylinder that was computed using GILA.[2] The grid used for this computation is shown in Figure 5.1. At this Reynolds number, a time-dependent von Karman vortex street develops in the wake of the cylinder after about 100 non-dimensional time units. Figure 5.2 shows the kinetic energy for the flow problem as a function of time. In this example, the flow establishes a steady-periodic behavior associated with the vortex shedding process. For this computation, the averaging was started at 100 time units and carried out with a window size corresponding to 500 time steps in GILA.

For this computation, the basic statistics level was selected along with the FAST-RKPM filter and linear consistency. The control file for LESTATS is shown in Figure 5.3. The screen output from LESTATS is shown in Figure 5.4. Figures 5.5 – 5.6 show the instantaneous velocity, pressure and stream function at $t = 500$ time units. In contrast, the time-averaged velocity, pressure and stream function are shown in Figures 5.7 – 5.8. The differences between the symmetric time-averaged wake and the instantaneous wake are striking in this calculation.

In this example, a two-scale decomposition of the time-averaged data was also computed. The representation of the x-velocity at the $2a$ scale is shown in Figure 5.9(a) and the difference between the averaged x-velocity at full resolution and the filtered data at the $2a$ resolution is shown Figure 5.9(b). Here the plot of the difference between scales indicates where the largest gradients in the time-averaged x-velocity field will occur.

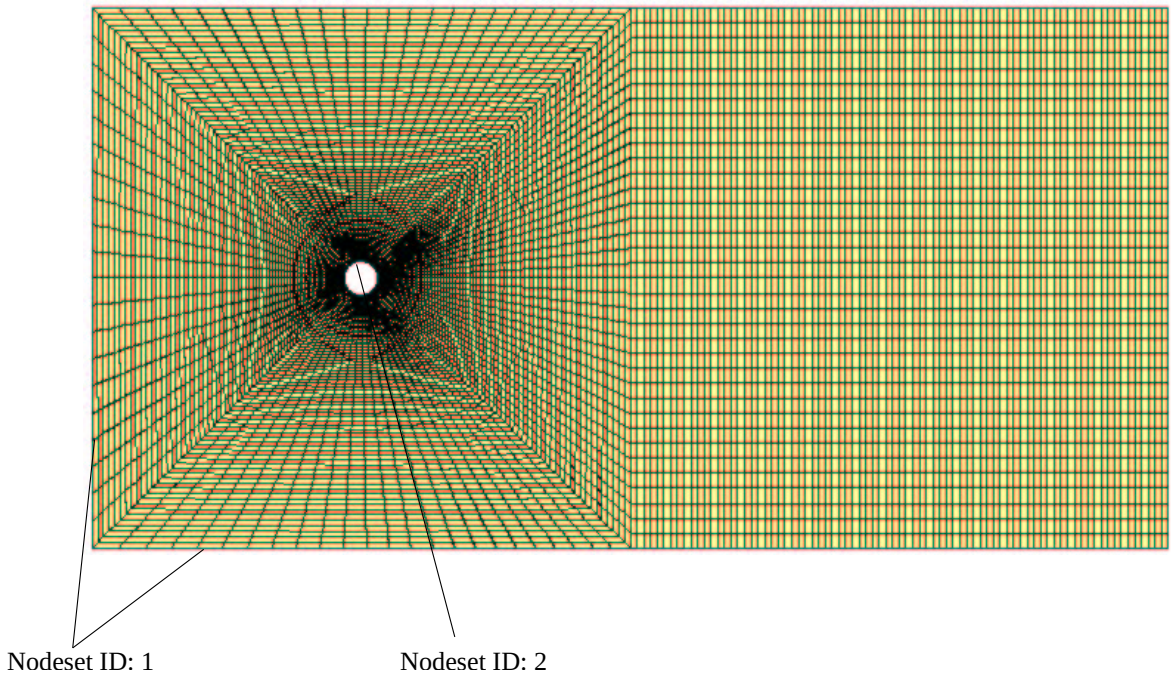


Figure 5.1: Mesh used for $Re = 100$ flow past a cylinder.

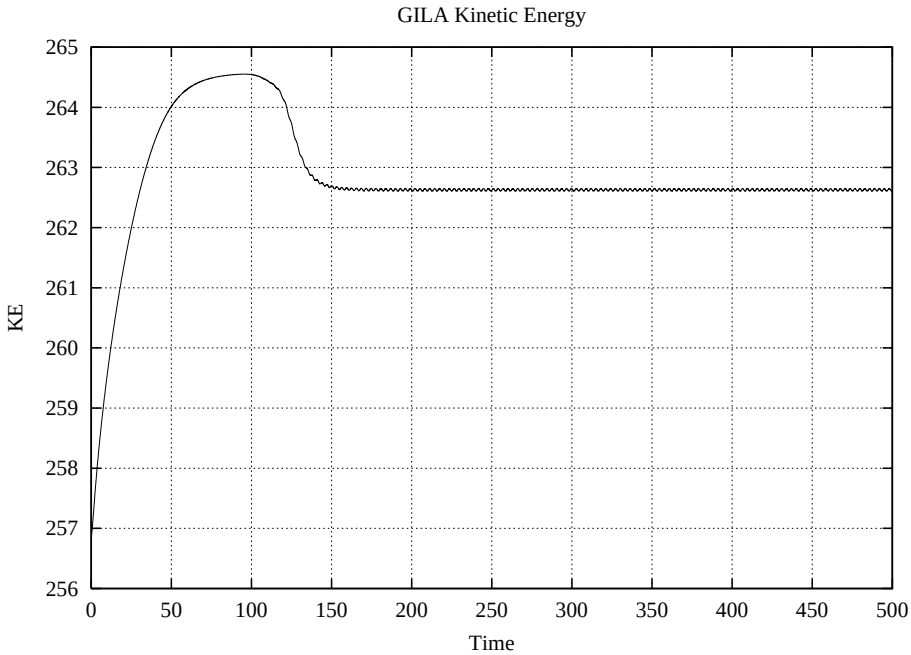


Figure 5.2: Kinetic energy ($1/2\ \mathbf{u}^T M_L \mathbf{u}$) vs. time for $Re = 100$ flow past a cylinder.

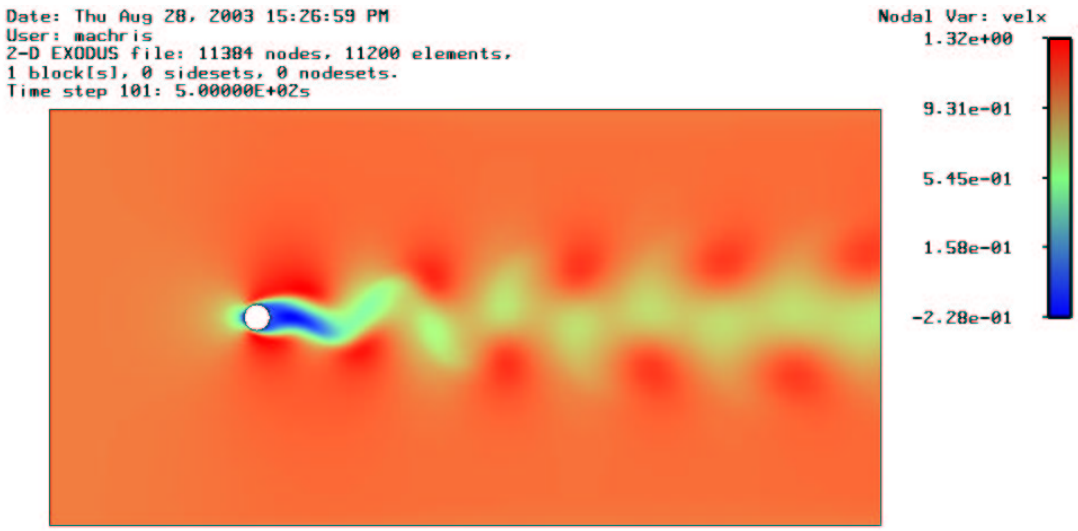
```
{ Sample control file for vortex shedding }

{ Select exodus format input/output }
pltype exodus

{ Specify the averaging parameters }
average
  stats 10
  starti 1
  endi 20
end

{ Activate filtering and two-scale decomposition }
filter
  type 10
  order 10
end

exit
```

Figure 5.3: LESTATS control file for the two-dimensional vortex shedding example.

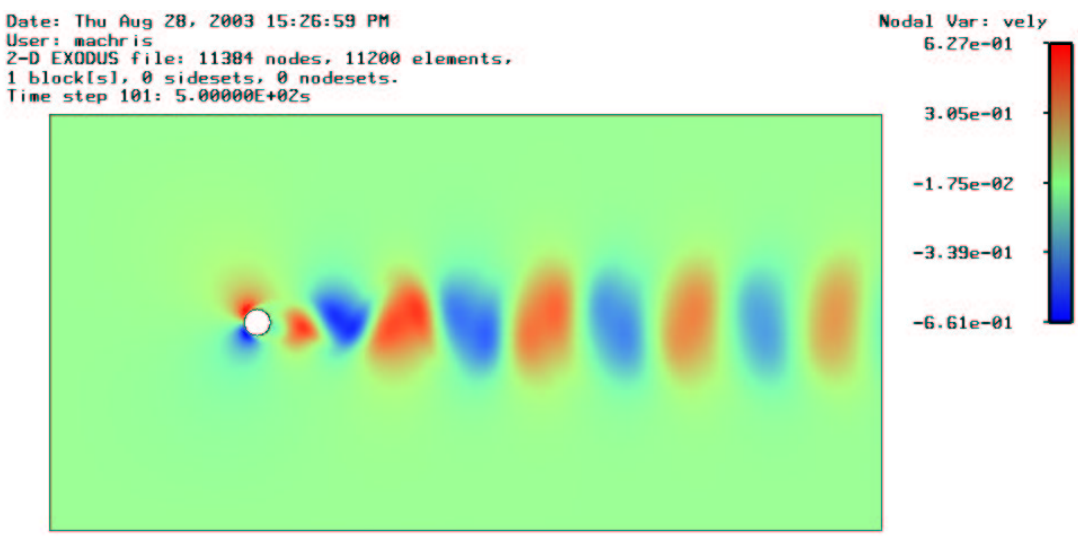
```
=====================================================================

        LL      EEEEEEE  SSSSSS TTTTTT   AAAAA  TTTTTT   SSSSSS
        LL      EE      SS        TT    AA   AA   TT    SS
        LL      EE      SS        TT    AA   AA   TT    SS
        LL      EEEEE    SSSSS    TT    AAAAAAA   TT     SSSSS
        LL      EE          SS   TT    AA   AA   TT         SS
        LL      EE           SS  TT    AA   AA   TT         SS
        LLLLLLL EEEEEEE SSSSSS    TT    AA   AA   TT    SSSSSS


        LESTATS Version : 1.1
        Generated on    : Fri Jan 22 19:39:10 MST 1999

=====================================================================



   LESTATS Path  : /home/machris/fem/cfd/gila/lestats/src/lestats
   Date & Time   : Thu Aug 28 14:21:42 2003

   Input   File  : plot_avg.exo
   Output  File  : avg.exo
   Control File  : cntl
   Filtered File : avg_flt.exo
   Two-Scale File: avg_dif.exo


    C o n t r o l   I n f o r m a t i o n


        MESH PARAMETERS
        ===============

        Number of dimensions .........................          2

        Number of nodes ..............................      11384

        Number of elements ...........................      11200

        Connectivity dimension .......................          4

        Number of element blocks .....................          1

        Number of node sets ..........................          0

        Number of side sets ..........................          0

        Number of materials ..........................          1

        Number of Global Variables ...................          2

        Number of Nodal Variables ....................          6


        INPUT NODAL VARIABLES
        =====================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     3 - Name:         <w3>
             Index:     4 - Name:         <enstrophy>
             Index:     5 - Name:         <stream>
             Index:     6 - Name:         <pnode>


        TIME AVERAGING PARAMETERS
        =========================

             Statistics Level .........................         10

             Database Statistics Level ................         10

             Averaging Start Index ....................          1

             Averaging End Index ......................         20


        TIME AVERAGING WINDOW
        =====================

        Time Average Samples in Database ...

             INDEX     TIME       PERIOD
             =====  ==========  ==========

                 1  2.5000E+01  2.5000E+01
                 2  5.0000E+01  2.5000E+01
                 3  7.5000E+01  2.5000E+01
                 4  1.0000E+02  2.5000E+01
                 5  1.2500E+02  2.5000E+01
                 6  1.5000E+02  2.5000E+01
                 7  1.7500E+02  2.5000E+01
                 8  2.0000E+02  2.5000E+01
                 9  2.2500E+02  2.5000E+01
                10  2.5000E+02  2.5000E+01
                11  2.7500E+02  2.5000E+01
                12  3.0000E+02  2.5000E+01
                13  3.2500E+02  2.5000E+01
                14  3.5000E+02  2.5000E+01
                15  3.7500E+02  2.5000E+01
                16  4.0000E+02  2.5000E+01
                17  4.2500E+02  2.5000E+01
                18  4.5000E+02  2.5000E+01
                19  4.7500E+02  2.5000E+01
                20  5.0000E+02  2.5000E+01


        Selected Time Average Samples

             Start Time Index .........................          1

             Start Time ...............................  2.5000E+01

             End   Time Index .........................         20

             End   Time ...............................  5.0000E+02
```

```
             INDEX     TIME       PERIOD
             =====  ==========  ==========

                 1  2.5000E+01  2.5000E+01
                 2  5.0000E+01  2.5000E+01
                 3  7.5000E+01  2.5000E+01
                 4  1.0000E+02  2.5000E+01
                 5  1.2500E+02  2.5000E+01
                 6  1.5000E+02  2.5000E+01
                 7  1.7500E+02  2.5000E+01
                 8  2.0000E+02  2.5000E+01
                 9  2.2500E+02  2.5000E+01
                10  2.5000E+02  2.5000E+01
                11  2.7500E+02  2.5000E+01
                12  3.0000E+02  2.5000E+01
                13  3.2500E+02  2.5000E+01
                14  3.5000E+02  2.5000E+01
                15  3.7500E+02  2.5000E+01
                16  4.0000E+02  2.5000E+01
                17  4.2500E+02  2.5000E+01
                18  4.5000E+02  2.5000E+01
                19  4.7500E+02  2.5000E+01
                20  5.0000E+02  2.5000E+01


        M e m o r y   U s a g e

        Memory Usage [MWords] ........................ 2.5517E+02

        Memory Usage [MBytes] ........................ 2.0414E+03


    T i m e   A v e r a g e d   V a r i a b l e s

        OUTPUT NODAL VARIABLES
        ======================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     6 - Name:         <pnode>
             Index:     3 - Name:         <w3>
             Index:     4 - Name:         <enstrophy>
             Index:     5 - Name:         <stream>


    F i l t e r e d   V a r i a b l e s

        OUTPUT NODAL VARIABLES
        ======================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     6 - Name:         <pnode>
             Index:     3 - Name:         <w3>
             Index:     4 - Name:         <enstrophy>
             Index:     5 - Name:         <stream>


    D i f f e r e n c e d   V a r i a b l e s

        OUTPUT NODAL VARIABLES
        ======================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     6 - Name:         <pnode>
             Index:     3 - Name:         <w3>
             Index:     4 - Name:         <enstrophy>
             Index:     5 - Name:         <stream>


        FILTERING PARAMETERS
        ====================

             Filter Type ..............................         10

             Number of Correction Betas................          3


        N o d a l   E q u a t i o n   S t a t i s t i c s

             Nodal 1/2 bandwidth ......................       6781

             Node w. Max. Connections .................          2

             Maximum nodal row entries ................          9

             Maximum edges connected to a node ........          4

             Maximum elements connected to a node .....          4

             Number of entries in coefficient matrix ..     102456

             Number of zero entries ...................       1104


    T i m i n g   I n f o r m a t i o n


        Total CPU  time used [sec.] ................... 1.6000E-01

        Total User time used [sec.] ................... 8.0000E-02
```

Figure 5.4: LESTATS screen output for two-dimensional vortex shedding example.

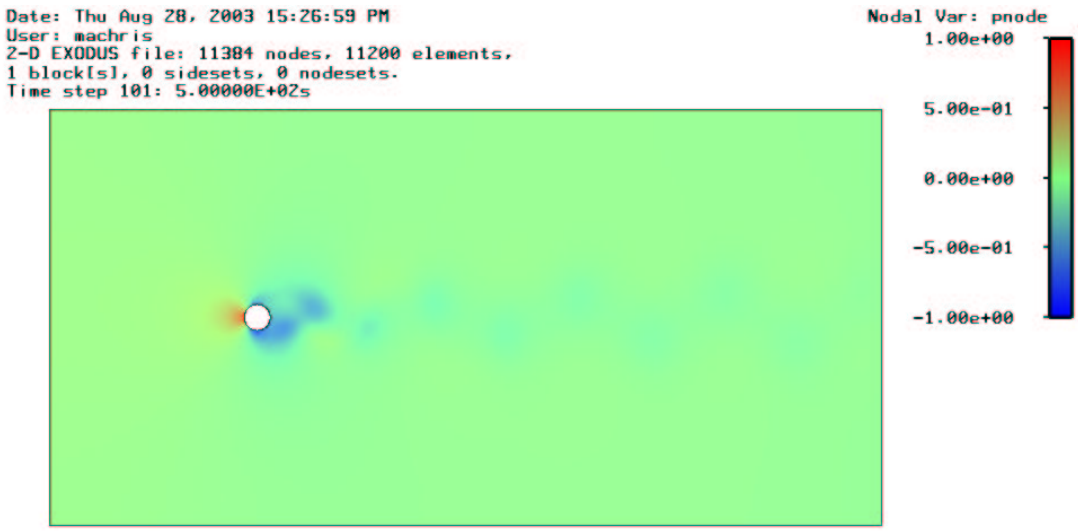


(a)

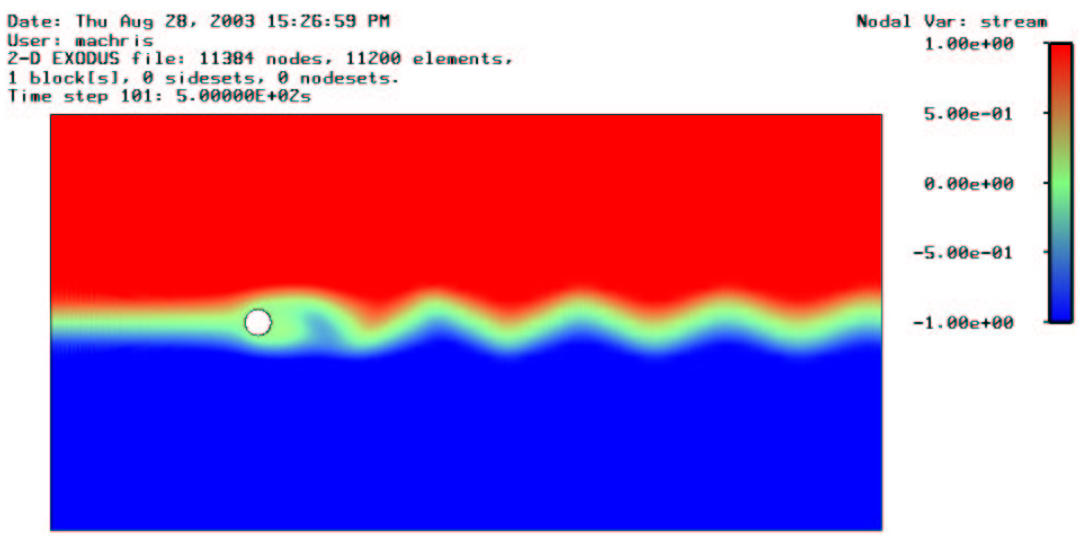


(b)

Figure 5.5: Snaphots of the instantaneous (a) x-velocity and (b) y-velocity for the $Re = 100$ flow.

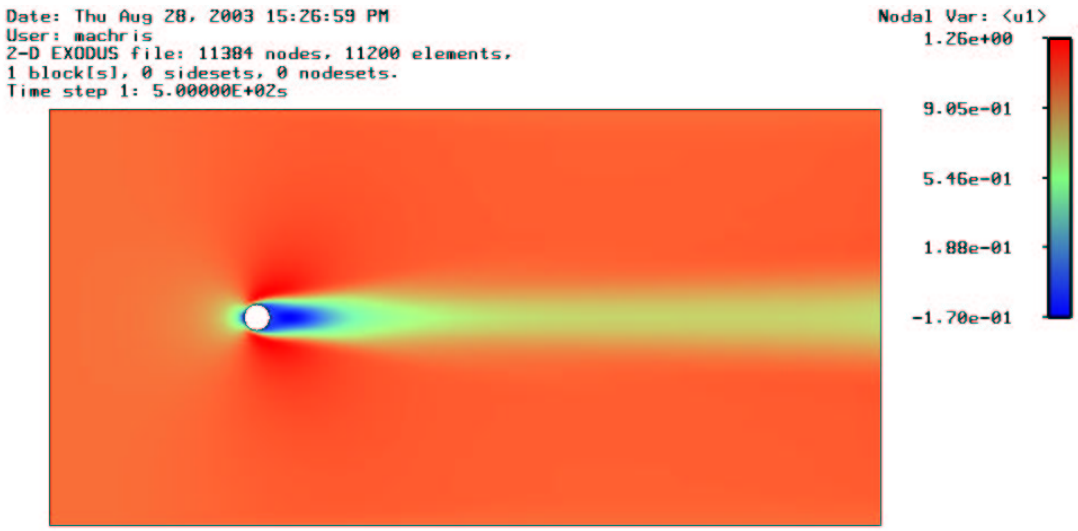


(a)

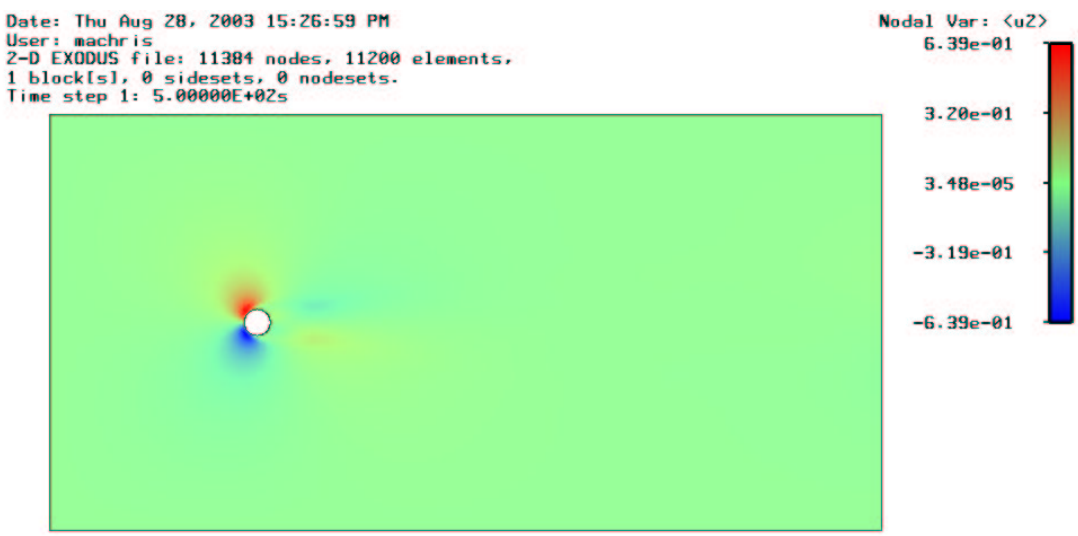


(b)

Figure 5.6: Snaphots of the instantaneous (a) pressure and (b) stream function for the $Re = 100$ flow.

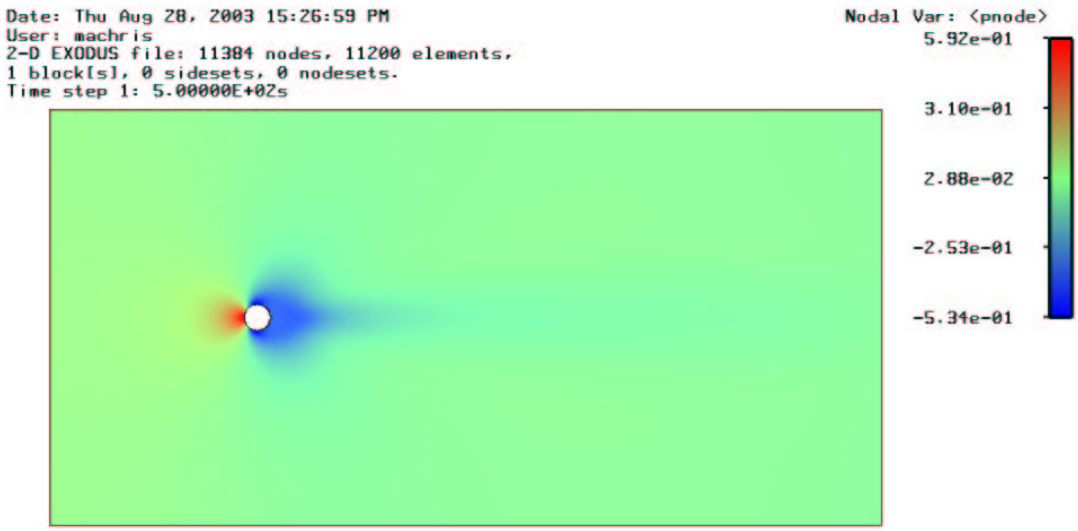


(a)

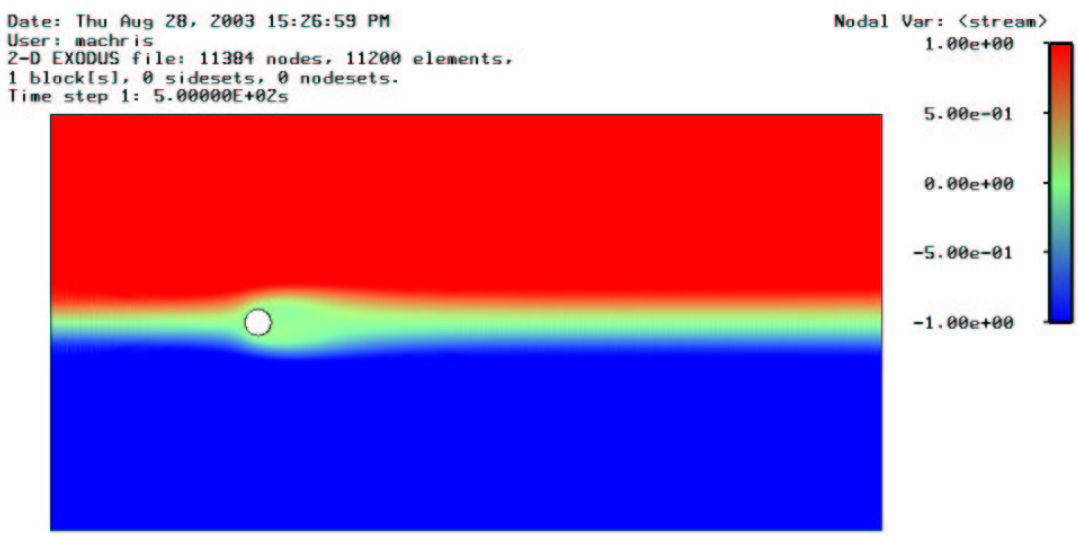


(b)

Figure 5.7: Snaphots of the time-averaged (a) x-velocity and (b) y-velocity for the $Re = 100$ flow.

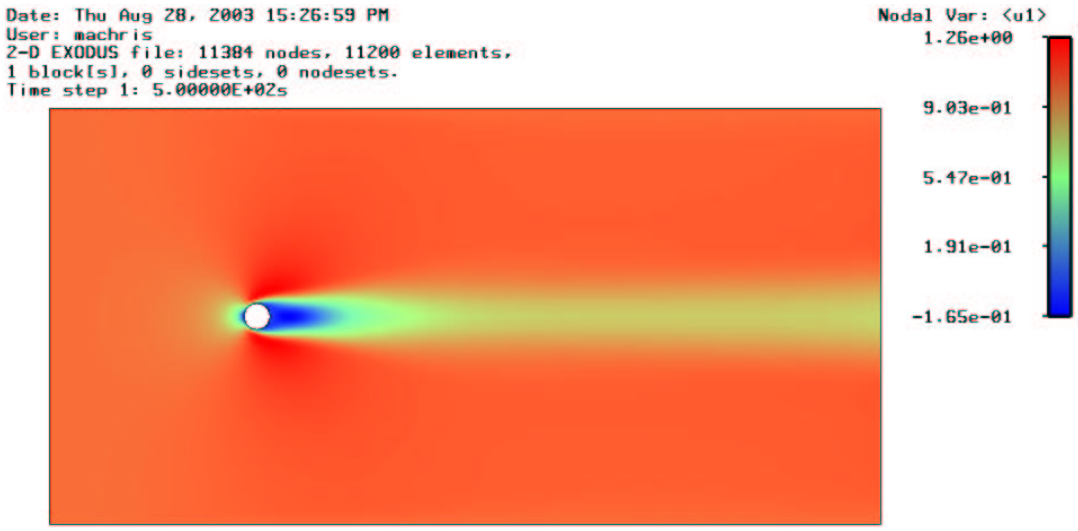


(a)

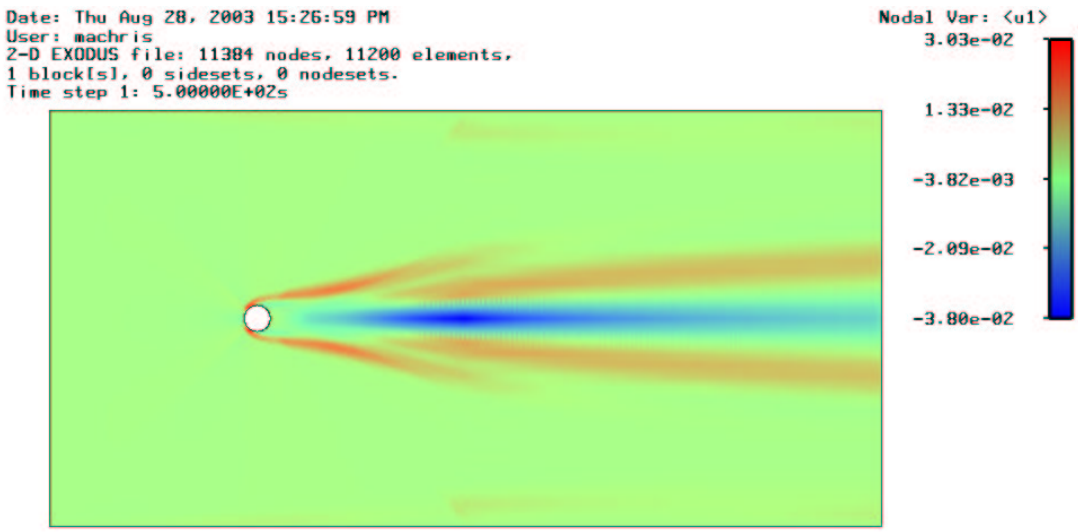


(b)

Figure 5.8: Snaphots of the time-averaged (a) pressure and (b) stream function for the $Re = 100$ flow.



(a)



(b)

Figure 5.9: Snapshots of the x-velocity showing the (a) filtered time-averaged field and (b) difference between the time-averaged and filtered x-velocity fields for the $Re = 100$ flow.

5.2 Lid-Driven Cavity

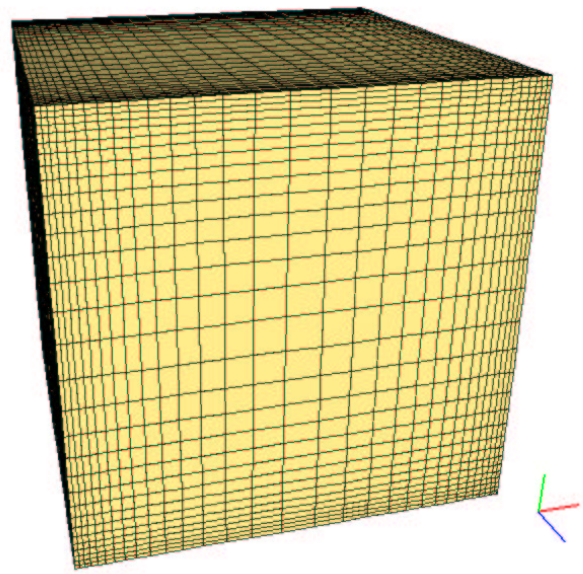
In this example, a large-eddy simulation of a $Re = 10,000$ flow in a lid-driven cavity was performed using GILA.[2] For the simulation, the dimensionless lid velocity was assumed to be $u_1 = 1$. Cavity dimensions were 1 unit in the x, y and z directions. Additional details on this problem may be found in Zang, Street and Koseff.[8] A grid with $32 \times 32 \times 32$ elements was used and the simulation was run for approximately 400 dimensionless time units with 32 time planes containing average statistics being written. The LESTATS control file used to process the GILA output is shown in Figure 5.10.

The computational grid for this calculation is shown in Figure 5.11(a) and the time-history of kinetic energy is shown in Figure 5.11(b). As indicated in the LESTATS control file, time planes 200 through 400 were used to derive the statistics at level 30. The screen output from LESTATS is shown in Figure 5.12.

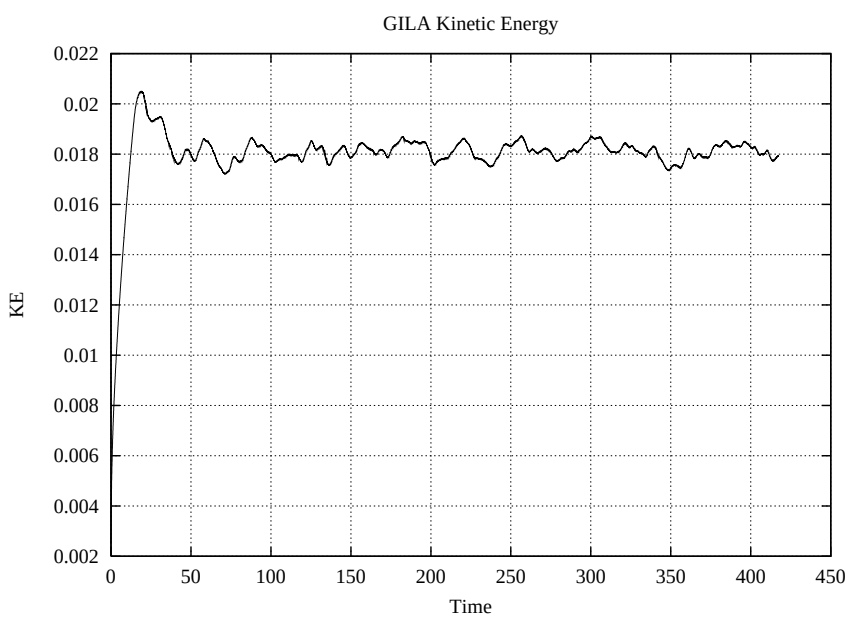
Snapshots of the instantaneous vorticity are shown in Figure 5.13, and the corresponding images showing the time-averaged vorticity are presented in Figure 5.14. The time-averaged z-vorticity and turbulent kinetic energy are shown in Figure 5.15. The $< u_1' u_1' >$ and $< u_2' u_2' >$ components of the Reynolds stress tensor are presented in Figure 5.16.

```
# LESTATS Control File

pltype exodus

average
  stats 30 # use highest level of statistics
  starti 16 # start averaging at time-plane 16 (t=200 s)
  endi 32 # end averaging at time-plane 32 (t=400 s)
end

# Activate the two-scale filtering procedure
filter
  type 10 # use the FAST-RKPM filter
  order 10 # use linear-consistency
end

# Terminates input from the control file
exit
```

Figure 5.10: Control File for Lid-Driven Cavity Example Problem.



(a)



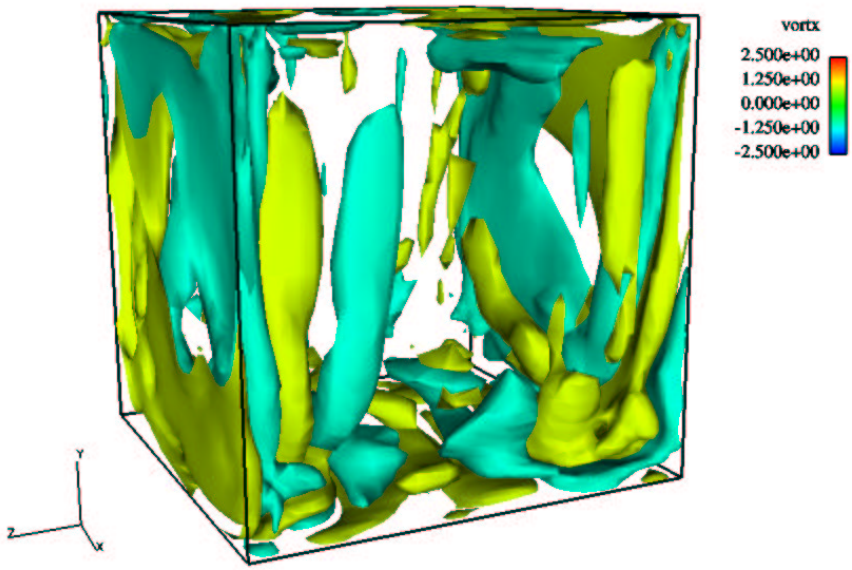
(b)

Figure 5.11: $Re = 10,000$ lid-driven cavity (a) the computational grid and (b) kinetic energy vs. time.

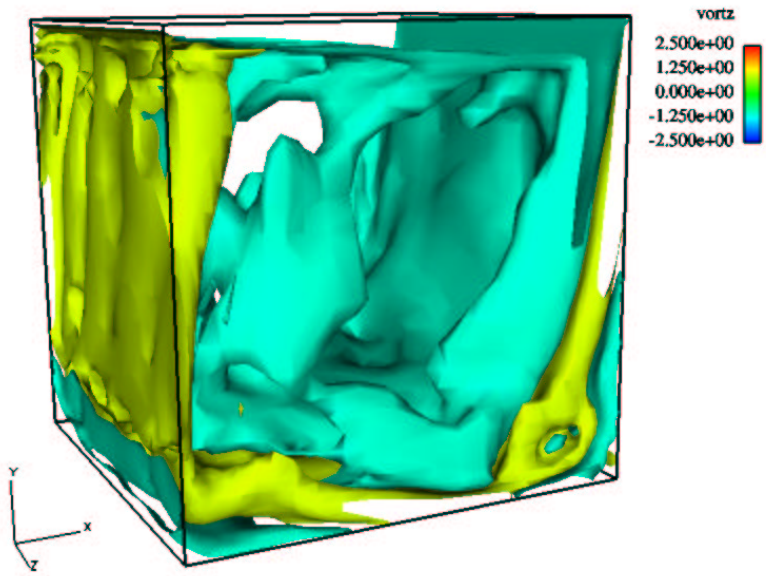
```
=====================================================================

        LL      EEEEEEE  SSSSSS TTTTTT   AAAAA  TTTTTT   SSSSSS
        LL      EE      SS        TT    AA   AA   TT    SS
        LL      EE      SS        TT    AA   AA   TT    SS
        LL      EEEEE    SSSSS    TT    AAAAAAA   TT     SSSSS
        LL      EE           SS   TT    AA   AA   TT         SS
        LL      EE           SS   TT    AA   AA   TT         SS
        LLLLLLL EEEEEEE SSSSSS    TT    AA   AA   TT    SSSSSS


        LESTATS Version : 1.1
        Generated on    : Fri Jan 22 19:39:10 MST 1999

=====================================================================



   LESTATS Path  : /home/machris/fem/cfd/gila/lestats/src/lestats
   Date & Time   : Fri Aug 29 10:25:08 2003

   Input   File  : plot.exo.avg
   Output  File  : avg.exo
   Control File  : cntl
   Filtered File : avg_flt.exo
   Two-Scale File: avg_dif.exo


    C o n t r o l   I n f o r m a t i o n


        MESH PARAMETERS
        ===============

        Number of dimensions .........................          3

        Number of nodes ..............................      32768

        Number of elements ...........................      29791

        Connectivity dimension .......................          8

        Number of element blocks .....................          1

        Number of node sets ..........................          0

        Number of side sets ..........................          0

        Number of materials ..........................          1

        Number of Global Variables ...................          2

        Number of Nodal Variables ....................         24


        INPUT NODAL VARIABLES
        =====================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     3 - Name:         <u3>
             Index:     4 - Name:         <w1>
             Index:     5 - Name:         <w2>
             Index:     6 - Name:         <w3>
             Index:     7 - Name:         <helicity>
             Index:     8 - Name:         <enstrophy>
             Index:     9 - Name:         <pnode>
             Index:    10 - Name:         <u1u1>
             Index:    11 - Name:         <u1u2>
             Index:    12 - Name:         <u1u3>
             Index:    13 - Name:         <u2u3>
             Index:    14 - Name:         <u2u2>
             Index:    15 - Name:         <u3u3>
             Index:    16 - Name:         <u1p>
             Index:    17 - Name:         <u2p>
             Index:    18 - Name:         <u3p>
             Index:    19 - Name:         <u1^3>
             Index:    20 - Name:         <u2^3>
             Index:    21 - Name:         <u3^3>
             Index:    22 - Name:         <u1^4>
             Index:    23 - Name:         <u2^4>
             Index:    24 - Name:         <u3^4>


        TIME AVERAGING PARAMETERS
        =========================

             Statistics Level .........................          30

             Database Statistics Level ................          30

             Averaging Start Index ....................          16

             Averaging End Index ......................          32


        TIME AVERAGING WINDOW
        =====================

        Time Average Samples in Database ...

             INDEX     TIME       PERIOD
             =====  ==========  ==========

                 1  1.2500E+01  1.2500E+01
                 2  2.5000E+01  1.2500E+01
                 3  3.7500E+01  1.2500E+01
                 4  5.0000E+01  1.2500E+01
                 5  6.2500E+01  1.2500E+01
                 6  7.5000E+01  1.2500E+01
                 7  8.7500E+01  1.2500E+01
                 8  1.0000E+02  1.2500E+01
                 9  1.1250E+02  1.2500E+01
                10  1.2500E+02  1.2500E+01
                11  1.3750E+02  1.2500E+01
                12  1.5000E+02  1.2500E+01
                13  1.6250E+02  1.2500E+01
                14  1.7500E+02  1.2500E+01
                15  1.8750E+02  1.2500E+01
```

```
                16  2.0000E+02  1.2500E+01
                17  2.1250E+02  1.2500E+01
                18  2.2500E+02  1.2500E+01
                19  2.3750E+02  1.2500E+01
                20  2.5000E+02  1.2500E+01
                21  2.6250E+02  1.2500E+01
                22  2.7500E+02  1.2500E+01
                23  2.8750E+02  1.2500E+01
                24  3.0000E+02  1.2500E+01
                25  3.1250E+02  1.2500E+01
                26  3.2500E+02  1.2500E+01
                27  3.3750E+02  1.2500E+01
                28  3.5000E+02  1.2500E+01
                29  3.6250E+02  1.2500E+01
                30  3.7500E+02  1.2500E+01
                31  3.8750E+02  1.2500E+01
                32  4.0000E+02  1.2500E+01
                33  4.1250E+02  1.2500E+01
                34  4.2500E+02  1.2500E+01


        Selected Time Average Samples

             Start Time Index .........................          16

             Start Time ...............................  2.0000E+02

             End   Time Index .........................          32

             End   Time ...............................  4.0000E+02

             INDEX     TIME       PERIOD
             =====  ==========  ==========

                16  2.0000E+02  1.2500E+01
                17  2.1250E+02  1.2500E+01
                18  2.2500E+02  1.2500E+01
                19  2.3750E+02  1.2500E+01
                20  2.5000E+02  1.2500E+01
                21  2.6250E+02  1.2500E+01
                22  2.7500E+02  1.2500E+01
                23  2.8750E+02  1.2500E+01
                24  3.0000E+02  1.2500E+01
                25  3.1250E+02  1.2500E+01
                26  3.2500E+02  1.2500E+01
                27  3.3750E+02  1.2500E+01
                28  3.5000E+02  1.2500E+01
                29  3.6250E+02  1.2500E+01
                30  3.7500E+02  1.2500E+01
                31  3.8750E+02  1.2500E+01
                32  4.0000E+02  1.2500E+01


        M e m o r y   U s a g e

        Memory Usage [MWords] ......................... 1.2840E+00

        Memory Usage [MBytes] ......................... 1.0272E+01

    T i m e   A v e r a g e d   V a r i a b l e s

        OUTPUT NODAL VARIABLES
        ======================

             Index:     1 - Name:         <u1>
             Index:     2 - Name:         <u2>
             Index:     3 - Name:         <u3>
             Index:     9 - Name:         <pnode>
             Index:     4 - Name:         <w1>
             Index:     5 - Name:         <w2>
             Index:     6 - Name:         <w3>
             Index:     8 - Name:         <enstrophy>
             Index:     7 - Name:         <helicity>
             Index:    10 - Name:         <u1u1>
             Index:    11 - Name:         <u1u2>
             Index:    14 - Name:         <u2u2>
             Index:    12 - Name:         <u1u3>
             Index:    13 - Name:         <u2u3>
             Index:    15 - Name:         <u3u3>
             Index:    16 - Name:         <u1p>
             Index:    17 - Name:         <u2p>
             Index:    18 - Name:         <u3p>
             Index:    19 - Name:         <u1^3>
             Index:    20 - Name:         <u2^3>
             Index:    21 - Name:         <u3^3>
             Index:    22 - Name:         <u1^4>
             Index:    23 - Name:         <u2^4>
             Index:    24 - Name:         <u3^4>
             Index:    25 - Name:         TKE
             Index:    26 - Name:         <u1'u1'>
             Index:    27 - Name:         <u1'u2'>
             Index:    28 - Name:         <u2'u2'>
             Index:    29 - Name:         <u1'u3'>
             Index:    30 - Name:         <u2'u3'>
             Index:    31 - Name:         <u3'u3'>
             Index:    32 - Name:         <u1'p'>
             Index:    33 - Name:         <u2'p'>
             Index:    34 - Name:         <u3'p'>
             Index:    35 - Name:         S01
             Index:    36 - Name:         S02
             Index:    37 - Name:         S03
             Index:    38 - Name:         F01
             Index:    39 - Name:         F02
             Index:    40 - Name:         F03

    . . .

    T i m i n g   I n f o r m a t i o n


        Total CPU  time used [sec.] ................. 8.6000E-01

        Total User time used [sec.] ................. 8.5000E-01
```

Figure 5.12: LESTATS screen output for lid-driven cavity example.

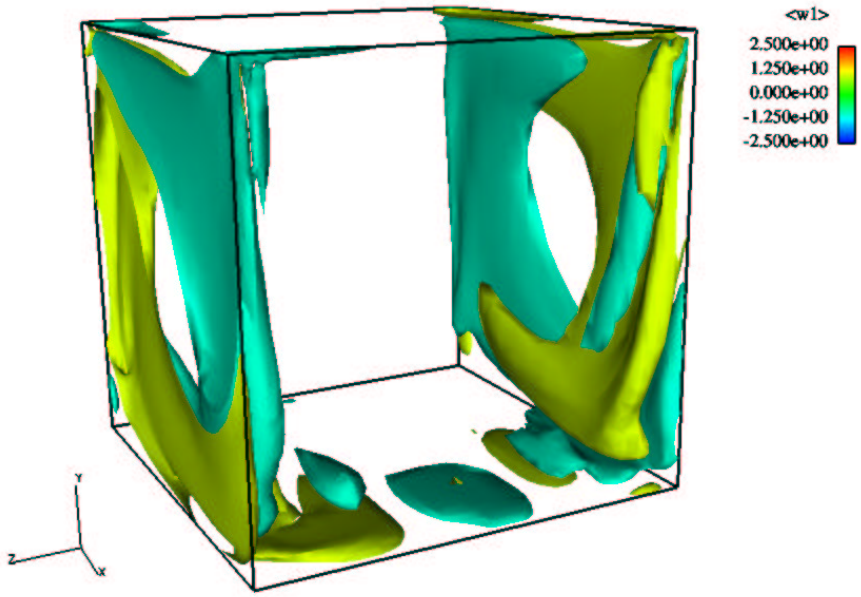


(a)

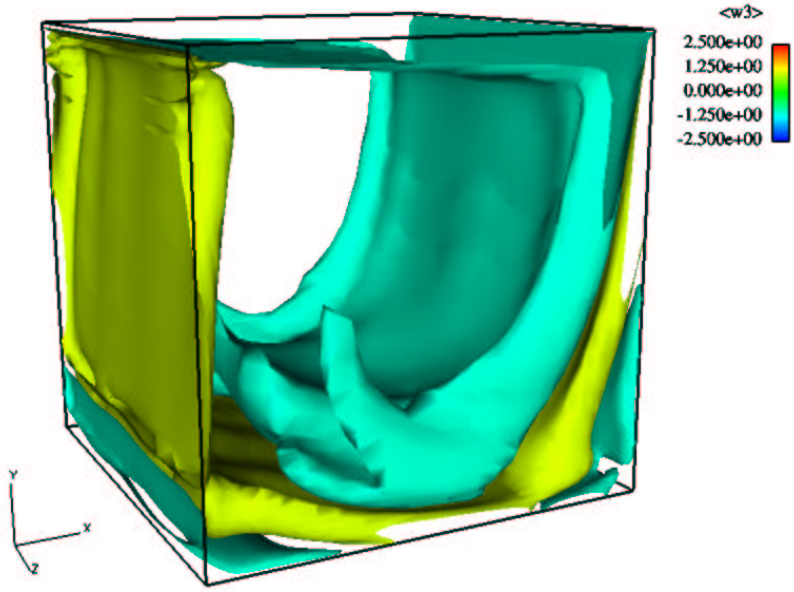


(b)

Figure 5.13: Snapshots of the instantaneous (a) x-vorticity and (b) z-vorticity (isosurface levels at ± 1) at $t = 400$ time units.

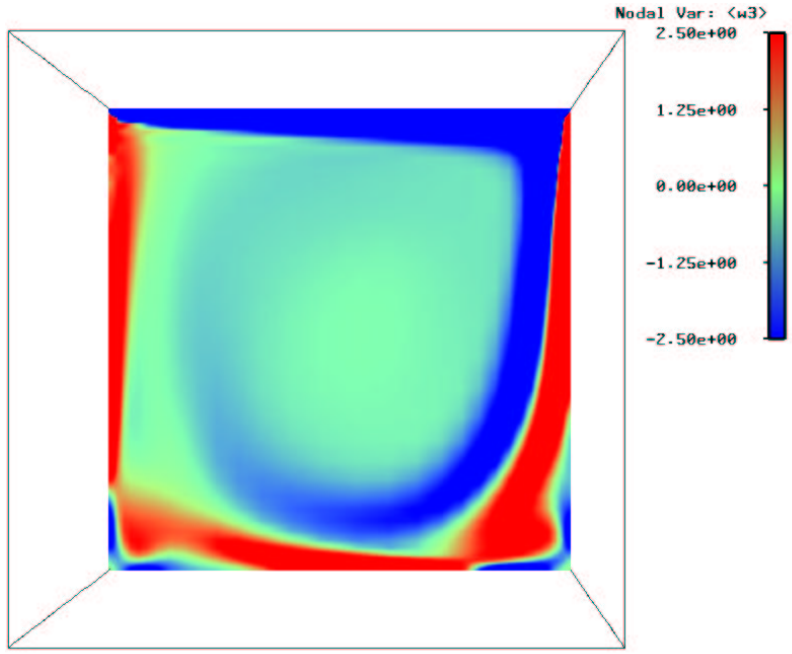


(a)

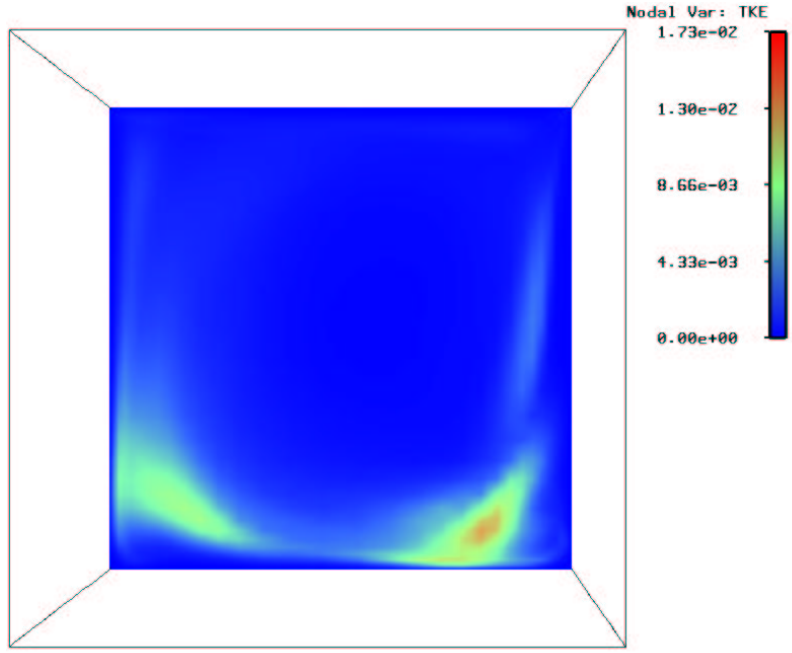


(b)

Figure 5.14: Snapshots of the time-averaged (a) x-vorticity and (b) z-vorticity (isosurface levels at ± 1).

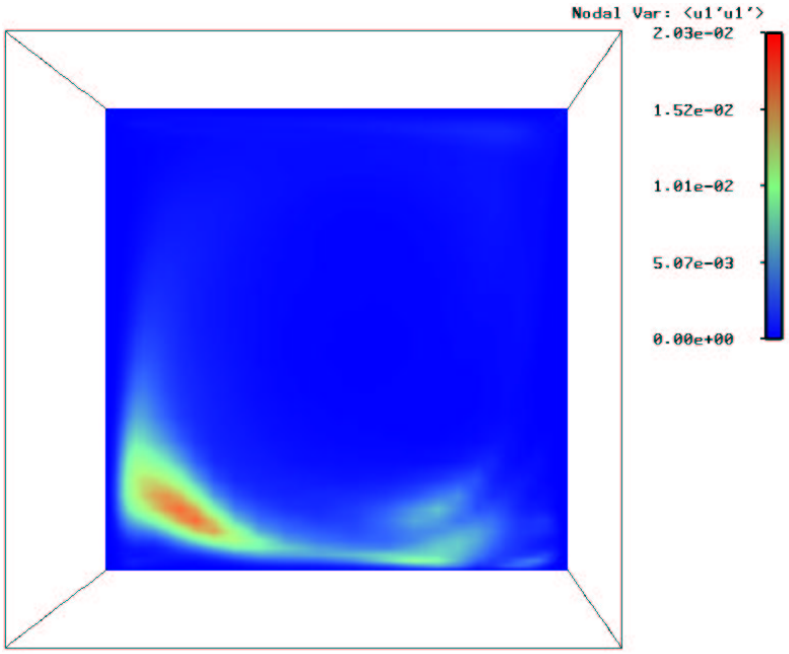


(a)

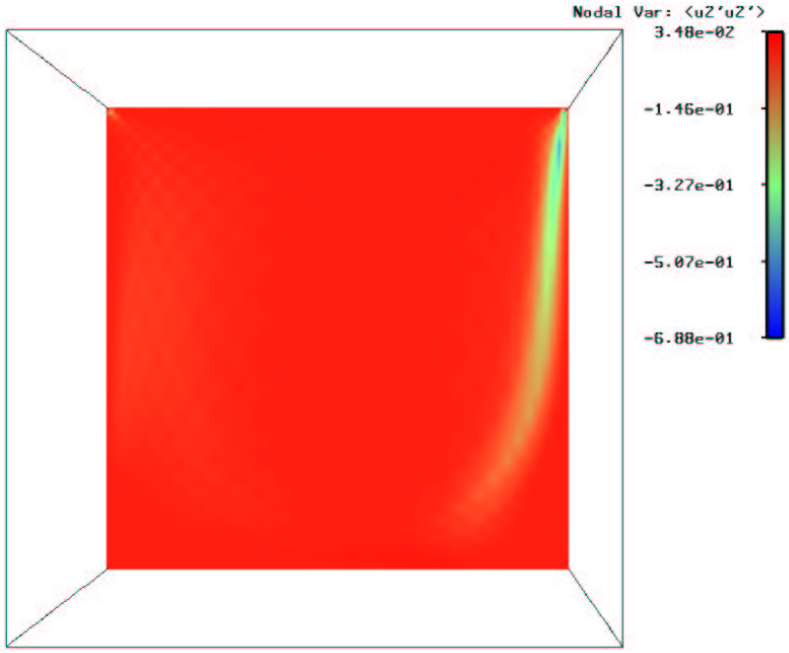


(b)

Figure 5.15: Cutplanes showing the time-averaged (a) z-vorticity and (b) turbulent kinetic energy.



(a)



(b)

Figure 5.16: Cutplanes showing the time-averaged Reynolds stress components (a) $< u_1' u_1' >$ and (b) $< u_2' u_2' >$.

Appendix A

LESTATS Input Data

LESTATS requires an input data file that contains raw time-averaged data that has been collected during the course of a simulation. In order to facilitate the computation of a windowed time-average for the derived statistics, LESTATS assumes that the input time-averaged data has been collected over a series of time windows as shown in Figure A.1. In this example, the time averaging procedure starts at t_1 and is restarted after the data for a time window is written to disk. This approach permits the exclusion of start-up transients in the computation of the derived turbulence statistics.

For each time-window, the application code is expected to collect the raw statistics for the active time window. Considering a generic variable, $\phi(x_i, t)$, the time-average for a given window is simply

$$< \phi(x_i) >= \frac{1}{t_{n+Navg} - t_n} \sum_{j=n}^{n+Navg} \phi(x_i, t_j)\Delta t_j. \tag{A.1}$$

The input data for LESTATS is presented in the following sections in terms of global data associated with the time windows and the three levels of output statistics generated by LESTATS (see Chapter 4).

A.1 Global Data

For each time window, the application code is expected to write the time associated with the end of the time window, the elapsed time associated the window, and the number of samples collected in the window. The elapsed time, $t_{n+Navg} - t_n$, and the number of time samples, $Navg$ is written in the first two words of the global data in the EXODUS-II/PXI database.

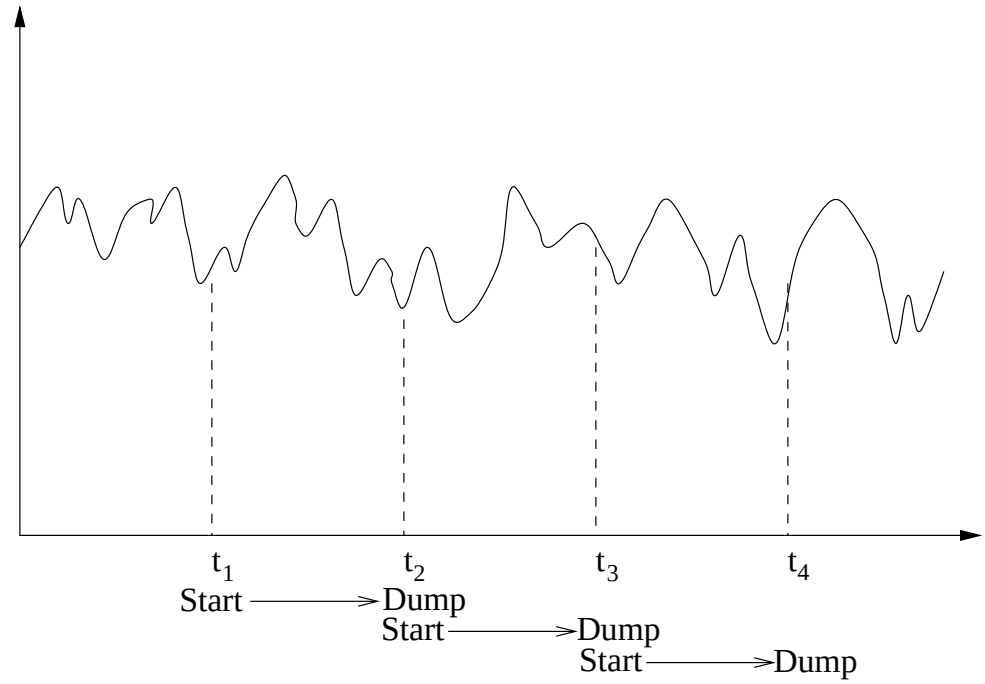


Figure A.1: Time windows for the collection the raw time-average data for LESTATS.

A.2 Mean Statistics

The computation of the derived mean statistics is described in Chapter 2 and uses only the variables that have been registered in the database. Table A.2 shows the variables and their associated database labels for the mean statistics.

A.3 Second Moment Statistics

The computation of the second-moment statistics relies on the variables listed in Table A.3. This data must be present in the input time-average database in order for the statistics associated with **stats** = 20 to be computed.

A.4 Higher-Order Statistics

The computation of the second-moment statistics relies on the variables listed in Table A.4. This data must be present in the input time-average database in order for the statistics associated with **stats** = 20 to be computed.

Variable Name	Quantity	Database Label
X-velocity	$< u_1 >$	`<u1>`
Y-velocity	$< u_2 >$	`<u2>`
Z-velocity	$< u_3 >$	`<u3>`
Pressure	$< p >$	`<pnode>`
X-vorticity	$< \omega_1 >$	`<w1>`
Y-vorticity	$< \omega_2 >$	`<w2>`
Z-vorticity	$< \omega_3 >$	`<w3>`
Enstrophy	$< 1/2\ \omega_i \omega_i >$	`<enstrophy>`
Helicity	$< u_i \omega_i >$	`<helicity>`
Stream Function	$< \psi >$	`<stream>`
Temperature	$< T >$	`<temp>`
Density	$< \rho >$	`<rho>`
Species-1	$< Z_1 >$	`<Z1>`
Species-2	$< Z_2 >$	`<Z2>`

Table A.1: LESTATS **stats**=10 input variables and database labels.

Variable Name	Quantity	Database Label
Velocity Correlations	$< u_1 u_1 >$	`<u1u1>`
	$< u_1 u_2 >$	`<u1u2>`
	$< u_1 u_3 >$	`<u1u3>`
	$< u_2 u_2 >$	`<u2u2>`
	$< u_2 u_3 >$	`<u2u3>`
	$< u_3 u_3 >$	`<u3u3>`
Velocity – Pressure Correlations	$< u_1 p >$	`<u1p>`
	$< u_2 p >$	`<u2p>`
	$< u_3 p >$	`<u3p>`
Velocity – Temperature Correlations	$< u_1 T >$	`<u1T>`
	$< u_2 T >$	`<u2T>`
	$< u_3 T >$	`<u3T>`
Velocity – Species Correlations	$< u_1 Z_1 >$	`<u1Z1>`
	$< u_2 Z_1 >$	`<u2Z1>`
	$< u_3 Z_1 >$	`<u3Z1>`
	$< u_1 Z_2 >$	`<u1Z2>`
	$< u_2 Z_2 >$	`<u2Z2>`
	$< u_3 Z_2 >$	`<u3Z2>`

Table A.2: LESTATS **stats**=20 input variables and database labels.

Variable Name	Quantity	Database Label
Third Moments	$< u_1^3 >$	`<u1^3>`
	$< u_2^3 >$	`<u2^3>`
	$< u_3^3 >$	`<u3^3>`
Fourth Moments	$< u_1^4 >$	`<u1^4>`
	$< u_2^4 >$	`<u2^4>`
	$< u_3^4 >$	`<u3^4>`

Table A.3: LESTATS **stats**=30 input variables and database labels.

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Mechanical Engineering Dept.
Colorado State University
Ft. Collins, CO 80523

Philip M. Gresho, Ph.D.
Lawrence Livermore National Laboratory
P.O. Box 808, L-262
Livermore, California 94551

Prof. Thomas J. R. Hughes
Institute for Computational Engineering and Sciences
The University of Texas
201 East 24th Street, ACES 6.412
1 University Station, C0200 Austin, Texas 78712-0027

Prof. Wing Kam Liu
Mechanical Engineering Dept.
Northwestern University
2145 Sheridan Road
Evanston, Illinois 60208-3111

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