Banff International Research Station

for Mathematical Innovation and Discovery

Connections Between Regularized and Large-Eddy Simulation Methods for Turbulence
May 14-18, 2012

MEALS

*Breakfast (Buffet): 7:00 – 9:30 am, Sally Borden Building, Monday – Friday
*Lunch (Buffet): 11:30 am – 1:30 pm, Sally Borden Building, Monday – Friday
*Dinner (Buffet): 5:30 – 7:30 pm, Sally Borden Building, Sunday – Thursday
Coffee Breaks: As per daily schedule, in the foyer of the TransCanada Pipeline Pavilion (TCPL)
***Please remember to scan your meal card at the host/hostess station in the dining room for each meal.**

MEETING ROOMS

All lectures will be held in the new lecture theater in the TransCanada Pipelines Pavilion (TCPL). LCD projector and blackboards are available for presentations.

SCHEDULE

Sunday

16:00 Check-in begins (Front Desk – Professional Development Centre - open 24 hours)
17:30-19:30 Buffet Dinner
20:00 Informal gathering in 2nd floor lounge, Corbett Hall (if desired)
Beverages and small assortment of snacks are available on a cash honor system.

Monday

7:00-8:45 Breakfast
8:45-9:00 Introduction and Welcome by BIRS Station Manager, TCPL
9:00 Lectures

09:00-09:45: Edriss Titi (Weizmann, Irvine): Analytical Sub-grid Scale Models of Turbulence and Inviscid Regularization of Hydrodynamic Equations
09:45-10:15 William Layton (U. of Pittsburgh): Modern ideas in turbulence confront legacy codes

Coffee Break, TCPL – available from 10:15-10:45

10:45-11:15: Bernard J. Geurts (U. of Twente/Eindhoven): Computational assessment of regularization models for turbulence

11:30-13:00 Lunch

13:00-14:00 Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall
14:00 Group Photo; meet in foyer of TCPL (photograph will be taken outdoors take a jacket).
Lectures

14:15-14:45: Roel Verstappen (U. of Groningen): On blending regularization and eddy dissipation
14:45-15:15: Luigi Berselli (U. of Pisa): LES and volcanic eruptions

Coffee Break, TCPL – available from 15:15

17:30-19:30 Dinner

Tuesday

7:00-9:00 Breakfast
9:00 Lectures

09:00-09:30: James Riley (U. of Washington): On the kinematics of flame surfaces in a turbulent flow
09:30-10:00: Lars Roehe (U. of Goettingen): Application and numerical analysis of weakly enforced boundary conditions for wall-bounded incompressible flow problems

Coffee Break, TCPL – available from 10:00-10:30

10:30-11:00: Volker John (WIAS/FU Berlin): On the analysis and numerical analysis of some turbulence models

11:00-11:30: Traian Iliescu (Virginia Tech): Approximate deconvolution large-eddy simulation of a barotropic ocean circulation

11:30-13:30 Lunch
14:00 Lectures

14:00-14:30: Jonathan Pietarila Graham (LANL): Spectral flux and error-landscape of 2D LES

14:30-15:00: Hans Kuerten (Eindhoven U. of Technology): The Leray model for turbulent channel flow

Coffee Break, TCPL – available from 15:00

17:30-19:30 Dinner

Wednesday

7:00-9:00 Breakfast
9:00 Lectures

09:00-09:30: Leo Rebholz (Clemson): Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering

09:30-10:00: Xavi Trias (Technical U. of Catalonia): Spectrally-consistent regularization modeling of turbulence and its connections with LES

Coffee Break, TCPL – available from 10:00

11:30-13:30 Lunch

Free Afternoon

17:30-19:30 Dinner

Thursday

7:00-9:00 Breakfast
9:00 Lectures

09:00-09:30: Helene Dallmann (U. of Goettingen): Turbulence models based on invariants of the strain rate tensor

09:30-10:00: Jonathan Gustafsson (McMaster): Integral invariants in homogeneous, isotropic, incompressible turbulence

Coffee Break, TCPL – available from 10:00-10:30

10:30-11:00: Assad Oberai (RPI): Variational multiscale formulation applied to large-eddy simulation

11:30-13:30 Lunch
Lectures

14:00-14:30: Erik Burman (U. of Sussex): Stabilized finite element methods for high Reynolds flow: hydrodynamic stability and computability

14:30-15:00: Johan Hoffman (KTH): Adaptive finite element LES with implicit turbulence modeling

Coffee Break, TCPL – available from 15:00

17:30-19:30 Dinner

Friday

7:00-9:00 Breakfast
9:00 Lectures (if desired)

09:00-09:30: Gantumur Tsogtgerel (McGill): On well posedness of the Navier-Stokes-αß equations with the wall-eddy boundary conditions: Preliminary results

09:30-10:00: Tae-Yeon Kim, Eliot Fried, Leo Rebholz (McGill): Numerical study of the influence of the separation of length scales in the Navier-Stokes-αß model

Coffee Break, TCPL – available from 10:00

11:30-13:30 Lunch

Checkout by 12 noon.

** 5-day workshop participants are welcome to use BIRS facilities (BIRS Coffee Lounge, TCPL and Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon. **

Connections Between Regularized and Large-Eddy Simulation Methods for Turbulence
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ABSTRACTS

(in alphabetic order by speaker surname)

Author Luigi Berselli (U. of Pisa)
Title: LES and volcanic eruptions

Abstract:
We present some result of a work in progress with the National Institute for Geophysics and Volcanology to perform reliable numerical simulations of some of the phenomena involved in volcanic eruptions. In particular, we will consider reduced models (as the Dusty gas one) for motion of mixtures of a compressible fluid and solid particles.

Author: Erik Burman (U. of Sussex)
Title: Stabilized finite element methods for high Reynolds flow: hydrodynamic stability and computability

Abstract:
The computation of high Reynolds flows remains an important challenge in scientific computation. It is generally believed that so called Large Eddy Simulation, i.e. a simulation where only the larger scales of the flow are computed, is feasible and that useful information can be extracted from such a computation. The underlying idea is that the flow is dominated by large scale structures and that resolving those structures is sufficient for the computation of relevant quantities. Although there appears to be computational evidence giving support to this hypothesis, no analytical results, in the form of error estimates that are uniform in the Reynolds number, validating the theory exist in the literature. One reason for this is the appearance of huge exponential error constants reflecting the hydrodynamic instability. In this talk we will consider stabilized finite element methods as a tool for large eddy simulation. We will show that these methods allow for optimal error estimates that are independent of the viscosity for smooth solutions of the Navier-Stokes' equations. Unfortunately the constants of these estimates blow up in case the solution loses regularity, i.e. the solution develops layers or becomes turbulent. To get better insight in this instability, triggered by the nonlinearity, we will study the viscous Burgers' equation. First we show that the same huge constants appear for error estimates in the L2-norm. Then we consider L2-norm error estimates of filtered quantities, and show that in this case we can derive error estimates that have moderate constants, depending only on the initial data. This shows that for filtered quantities, error bounds may be obtained that are uniform in the Reynolds number and independent of the solution regularity. It also leads naturally to a relation between the filter width and the convergence order of the method. The talk will end with a brief overview of possible extensions and ongoing work.

Author: Helene Dallmann (U. of Goettingen)
Title: Turbulence models based on invariants of the strain rate tensor

Abstract:
In [Ver11] a LES-model is presented that is constructed such that the influence of non-resolved scales is dissipated. Here two invariants of the strain rate tensor arise: the trace and the determinant. As pointed out e.g. in [CPC90] they can be used to detect the local behaviour of the flow. We present a derivation of the model and provide some error analysis, which is similar to [RL10]. Furthermore the performance of the model is demonstrated for two common test cases, the homogeneous decaying turbulence and the channel
flow. In the latter experiments we also explore the quality of structure detection provided by the model. This is especially relevant for implementations using isotropic meshes and weak boundary conditions; see e.g. [BH07]. What is more we compare this LES-model with Vreman's eddy-viscosity model ([Vre04]) which makes use of an invariant-based classification of flow structures as well.

References
[BH07] Y. Bazilevs and T.J.R. Hughes, Weak imposition of Dirichlet boundary conditions in mechanics , Computers and Fluids 36 (2007), 12
[CPC90] M.S. Chong, A.E. Perry, and B.J. Cantwell, A general classification of three dimensional flow fields , Physics of Fluids 2 (1990), 765
[RL10] L. Rohe and G. Lube, Analysis of a variational multiscale method for large-eddy simulation and its application to homogeneous isotropic turbulence, Computer Methods in Applied Mechanics and Engineering 199 (2010), 2331
[Ver11] Roel Verstappen, When does eddy viscosity damp subfilter scales sfficiently? , Journal of Scientific Computing 49 (2011), 94
[Vre04] A.W. Vreman, An eddy-viscosity subgrid-scale model for turbulent shear flow: Algebraic theory and applications , Physics of Fluids 16 (2004), 3670-3681

Author: Bernard J. Geurts (U. of Twente/Eindhoven)
Title: Computational assessment of regularization models for turbulence

Abstract:
An overview of the filtering approach to LES is given and a connection is made with recent regularization principles for the nonlinear convective terms in the Navier-Stokes equations. The implications of Leray-type regularizations for commutator errors in inhomogenously filtered LES are discussed. Generalized Leray regularizations are applied to LES of homogeneous, isotropic, decaying turbulence and the accuracy of predictions is compared with filtered DNS. The trade-off between efficiency and accuracy as determined by the selected filter-width is analyzed. We include the Leray, the modified Leray and the modified Bardina model in the comparison. We indicate what increase in the Reynolds number is possible at given accuracy requirements, using regularization LES.

Author: Jonathan Pietarila Graham (LANL)
Title: Spectral flux and error-landscape of 2D LES

Abstract:
We measure the error-landscape of the subgrid spectral transfers of 5 different LES for forced-dissipative simulations of the barotropic vorticity equation (2D Navier-Stokes equation). Of the studied LES, the dissipative methods perform the best. In contrast, the Lagrangian-averaged alpha regularization does not work as a LES for this system due to no reduction in the build-up of small-scale structures and a reduction in the capability to dissipate them: it continues to create small-scale vortex filaments via stretching by the large scales, but by removing small-scale vorticity from the advecting field, oppositely-signed vortex filaments are not spun into close proximity where they can be acted upon by diffusion. The form of the anticipated vorticity method employed functions as an LES, even with regards to back-scatter, but its dissipative effects are not scale selective enough.

Author: Jonathan Gustafsson (McMaster)
Title: Integral invariants in homogeneous, isotropic, incompressible turbulence

Abstract:
This talk will start with an introduction to turbulence theory for freely homogeneous, isotropic, incompressible decaying turbulence. The two-point velocity correlations, the dynamic von Karman-Howarth equations and integral invariants will be introduced. Which leads to the definition of the three dimensional energy function. Then the three dimensional energy spectrum function for small wave numbers or large scales will be examined, which can be approximated by a polynomial. By the use of fractional derivatives together with the integrals of moments of the two-point correlation function, it is possible to obtain the form of this polynomial. This polynomial can only be even. The dynamic of the three dimensional energy function can be related to the decay of turbulent kinetic energy by a length scale using the theory proposed by George. This can be related to more recent results about integral invariants by Vassilicos.

Author: Johan Hoffman (KTH)
Title: Adaptive finite element LES with implicit turbulence modeling

Abstract:
In this talk we present our work on the development of adaptive finite element methods for simulation of turbulent flow, a framework which we refer to General Galerkin methods (G2), with the key features of implicit turbulence modeling through numerical stabilization of the residual, with a posteriori error control of functional output using adjoint techniques. The finite element approximations are weak solutions to the Navier-Stokes equations that dissipate kinetic energy proportional to the residual of the equations, and that are well-posed with respect to mean value output. In the framework of LES, the G2 methodology can be interpreted as Implicit LES. We also discuss appropriate boundary conditions in the G2 framework. Examples are presented from incompressible and compressible flow, and fluid-structure interaction.

Author: Traian Iliescu (Virginia Tech)
Title: Approximate deconvolution large-eddy simulation of a barotropic ocean circulation

Abstract:
This talk introduces a new large eddy simulation closure modeling strategy for two-dimensional turbulent geophysical flows. This closure modeling approach utilizes approximate deconvolution, which is based solely on mathematical approximations and does not employ phenomenological arguments, such as the concept of energy cascade. The new approximate deconvolution model is tested in the numerical simulation of the wind-driven circulation in a shallow ocean basin, a standard prototype of more realistic ocean dynamics. The model employs the barotropic vorticity equation driven by a symmetric double-gyre wind forcing, which yields a four-gyre circulation in the time mean. The approximate deconvolution model yields the correct four-gyre circulation structure predicted by a direct numerical simulation, on a much coarser mesh and at a fraction of the computational cost. This first step in the numerical assessment of the new model shows that approximate deconvolution could represent a viable alternative to standard eddy viscosity parameterizations in the large eddy simulation of more realistic turbulent geophysical flows.

Author: Volker John (WIAS/FU Berlin)
Title: On the analysis and numerical analysis of some turbulence models

Abstract:
Turbulence models extend the (discretized) incompressible Navier--Stokes equations with additional terms or additional equations. The goal of this approach consists in incorporating important properties of the flow field, which cannot be capturedby standard discretizations of the Navier--Stokes equations on coarser grids, into the simulations. For the extended systems of equations,

questions of existence and uniqueness of solutions arise. In addition, the convergence of numerical schemes has to be studied.

This talk considers a number of selected turbulence models, like the Smagorinsky model, some Large Eddy Simulation (LES) models, and variational multiscale (VMS) methods.
A survey on results concerning the analysis and the finite element error analysis will be given.

Author: Tae-Yeon Kim, Eliot Fried, Leo Rebholz (McGill)
Title: Numerical study of the influence of the separation of length scales in the Navier-Stokes-ab model

Abstract:
We present a numerical study of the Navier-Stokes-ab model, which is a multiscale variation of the Navier-Stokes-a model that attempts to recapture scales lost through over-regularization by separately modeling dissipation-range scales. We develop a similarity theory shows that the Navier-Stokes-ab model is better equipped than the Navier-Stokes-a model to capture smaller-scale behavior. In particular, we examine the effect of the length scales a and b on the energy spectrum in three-dimensional homogeneous and isotropic turbulent flows in a periodic cubic domain. The limiting cases of the Navier-Stokes-a and Navier-Stokes equations are included as special cases. A significant increase in the accuracy of the energy spectrum at large wave numbers arises for b < a. Finally, numerical studies of two- and three-dimensional channel flows over a forward-backward step show that the NS-ab model, at low resolutions, closely approximates flow features obtained from the highly-resolved simulations based on the Navier-Stokes equations.

Author: Hans Kuerten (Eindhoven U. of Technology)
Title: The Leray model for turbulent channel flow

Abstract:
The Leray model was first proposed by Geurts and Holm [1] as a subgrid model in large-eddy simulation of turbulent flow. It is based on a regularized form of the Navier-Stokes equation, in which one velocity in the convective term of the equation is replaced by a filtered velocity, which implies that the solution is convected with a smoothed velocity field. The subgrid model follows from filtering the regularized Navier-Stokes equation. The properties of the Leray model were illustrated by Geurts and Holm for the turbulent compressible mixing layer. The model has not often been applied to large-eddy simulation of turbulent channel flow. In the presentation I will show the properties of solutions of this model for channel flow and analyze the behavior of the model. In particular the role of the inverse filter operation will be studied, as well as
the relation between the solution of the large-eddy simulation model and the solution of the Navier-Stokes equation.

1. B.J. Geurts and D. Holm, Regularization modeling for large-eddy simulation, Phys. Fluids 15, L13–L16 (2003).

Author: William Layton (U. of Pittsburgh)
Title: Modern ideas in turbulence confront legacy codes

Abstract:
The accurate, efficient and reliable simulation of turbulent flows in complex geometries and modulated by other effects is a recurring challenge. Often these simulations must be done with legacy codes written a generation of programmers ago. The question then becomesHow are modern models and methods to be used in such a setting This talk will present one path to doing so that is very efficient [low cost] in both computer time and programmer effort. The new algorithms involved lead to new models of turbulence.

Author: Leo Rebholz (Clemson)
Title: Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering

Abstract:
We study adaptive nonlinear filtering in the Leray regularization model for incompressible, viscous Newtonian flow. The filtering radius is locally adjusted so that resolved flow regions and coherent flow structures are not `filtered-out', which is a common problem with these types of models. A numerical method is proposed that is unconditionally stable with respect to time step, and decouples the problem so that the filtering becomes linear at each time step and is decoupled from the system. Several numerical examples are given that demonstrate the effectiveness of the method.

Author: James Riley (U. of Washington)
Title: On the kinematics of flame surfaces in a turbulent flow

Abstract:
An important aspect of the dispersive influence of turbulent flows is their ability to rapidly increase the area of fluid surfaces. An example of such a surface is the stoichiometric surface in a non-premixed, chemical reaction, which approximates the flame surface. The stoichimetric surface can itself be approximated by a surface of constant value of a passive scalar, the mixture fraction. In this presentation results will be presented for the growth and decay of iso-surfaces in turbulent flow. Direct measurements of iso-surfaces from numerical simulation will be presented, along with their indirect measurement using Rice's theorem (1944). This theorem leads to two separate modeling approaches to predict the evolution of the iso-surfaces. Comparisons of the predictions of these models with simulation results will be presented.

Author: Lars Roehe (U. of Goettingen)
Titlte: Application and numerical analysis of weakly enforced boundary conditions for wall-bounded incompressible flow problems

Abstract:
For the three-dimensional incompressible Navier{Stokes equations, we consider a formulation with weakly enforced Dirichlet boundary conditions [1] as well as fluid structure coupling problems [3]. For this problem we prove stability and an a priori estimate for di_erent turbulence models and obtain a parameter choice of the model paramters from the analysis. As an application we present results in a turbelent channel flow and discuss the influence of the weak treatment of the boundary conditions and a possible anisotropy of the underlying grid. This talk is an extension of the results in [2, 4].

References
[1] Bazilevs, Y., Michler, C., Calo, V.M., Hughes, T.J.R , Isogeometric variational multiscale modeling of wall-bounded turbulent flows with weakly-enforced boundary conditions on unstretched meshes. Comput. Meths. Appl. Mech. Engrg. 199 (2010), 780-790.
[2] Braack, M., Lube, G., Rohe, L. , Divergence preserving interpolation on anisotropic quadrilateral meshes. accepted for CMAM (2012).
[3] Girault, V., Riviere, B. , DG approximation of coupled Navier{Stokes and Darcy equations by Beaver/Joseph/Saffman interface condition. SIAM J. Num. Anal. 47 (2009), 2052-2089.
[4] Rohe, L., Lube, G. , Layer-adapted meshes vs. weak Dirichlet conditions in low-turbulent flow simulation. accepted for ENUMATH 2011 Proceedings (2012).

Author: Edriss Titi (Weizmann, Irvine)
Title: Analytical Sub-grid Scale Models of Turbulence and Inviscid Regularization of Hydrodynamic Equations

Abstract:
In recent years many analytical sub-grid scalemodels of turbulence were introduced based on the Navier--Stokes-alpha model (also known as a viscous Camassa--Holm equations or the Lagrangian Averaged Navier--Stokes-alpha (LANS-alpha)). Some of these are the Leray-alpha, the modified Leray-alpha, the simplified Bardina-alpha and the Clark-alpha models. In this talk we will show the global well-posedness of these models and provide estimates for the dimension of their global attractors, and relate these estimates to the relevant physical parameters. Furthermore, we will show that up to certain wave number in the inertial range the energy power spectra of these models obey the Kolmogorov -5/3 power law, however, for the rest the inertial range the energy spectra are much steeper.

In addition, we will show that by using these alpha models as closure models to the Reynolds averaged equations of the Navier--Stokes one gets very good agreement with empirical and numerical data of turbulent flows for a wide range of huge Reynolds numbers in infinite pipes and channels.

It will also be observed that, unlike the three-dimensional Euler equations and other inviscid alpha models, the inviscid simplified Bardina model has global regular solutions for all initial data. Inspired by this observation we will introduce new inviscid regularizing schemes for the three-dimensional Euler, Navier--Stokes and MHD equations, which does not require, in the viscous case, any additional boundary conditions. This same kind of inviscid regularization is also used to regularize the Surface Quasi-Geostrophic model.

Finally, and based on the alpha regularization we will present, if time allows, some error estimates for the rate of convergence of the alpha models to the Navier-Stokes equations, and will also present new approximation of vortex sheets dynamics.

Author: Xavi Trias (Technical U. of Catalonia)
Title: Spectrally-consistent regularization modeling of turbulence and its connections with LES

Abstract:
Regularizations of the Navier-Stokes (NS) equations that preserve the symmetry and conservation properties constitute a promising approach for turbulence modeling [1, 2]. The C4 approximation proposed in [1] is an example of thereof: the convective term in the NS equations is replaced by a fourth order accurate approximation involving the residual of a self-adjoint linear filter. Note that the C4 approximation is also a skew-symmetric operator like the original convective operator. Hence, it preserves all the invariant transformations of the original NS equations, except the Galilean transformation. This usual feature of regularizations [3] can be repaired by means of a proper modification of the time-derivative term. With this idea in mind, and following the same principles as in [1], new regularizations have been recently proposed in [4]. They can be viewed as a generalization of the regularizations proposed in [1] where the Galilean invariance is partially recovered by means of a modification of the diffusive term. In this way, the dissipation is reinforced by means of a hyper-viscosity term. This basically acts at the tail of the energy spectrum and therefore helps to mitigate the additional hump observed for the original C4 regularization [1]. Even more importantly, the

regularizations can be related to the “small-small” variational multiscale method [5]. This type of connections between regularization and Large-Eddy Simulation will be analyzed during the workshop. In the same vein, new eddy-viscosity-type models will be also presented and discussed.

References

[1] Roel Verstappen. On restraining the production of small scales of motion in a turbulent channel flow. Computers & Fluids , 37:887–897, 2008.
[2] F. X. Trias, R.W. C. P. Verstappen,A. Gorobets,M. Soria, and A. Oliva. Parameter-free symmetry preserving regularizationmodeling of a turbulent differentially heated cavity. Computers& Fluids, 39:1815–1831, 2010.
[3] J. L. Guermond, J. T. Oden, and S. Prudhomme. An interpretation of the Navier-Stokes-alpha model as a frame-indifferent Leray regularization. Physica D , 177:23–30, 2003.
[4] F. X. Trias, A. Gorobets, R. W. C. P. Verstappen, and A. Oliva. Symmetry-preserving regularization of wall-bounded turbulent flows. In 13th European Turbulence Conference, Warsaw, Poland, September 2011.
[5] T. J. R. Hughes, L. Mazzei, A. A. Oberai, and A. A. Wray. The multiscale formulation of large-eddy simulation: Decay of homogeneous isotropic turbulence. Physics of Fluids , 13(2):505–512, 2001

Author: Gantumur Tsogtgerel (McGill)
Title: On well posedness of the Navier-Stokes-αß equations with the wall-eddy boundary conditions: Preliminary results

Abstract:
Generalizing the Navier-Stokes-α model, Fried and Gurtin recently introduced the Navier-Stokes-αß equations, as a turbulence model with a solid continuum mechanical foundation. An attractive feature of this model is that boundary conditions arise naturally. In this talk, we consider the so-called wall-eddy boundary conditions, a replacement of the no-slip boundary conditions. We will discuss some preliminary results on the well posedness of the problem.

Author: Roel Verstappen (U. of Groningen)
Title: On blending regularization and eddy dissipation

Abstract:
A large-eddy simulation (LES) with an eddy-viscosity model differs from a Navier-Stokes simulation only in the use of a modified viscosity. Therefore regularization techniques that have been applied to the convective nonlinearity in the Navier-Stokes equation may also be applied to LES. The desired solution should contain only scales of size smaller than the user-chosen truncation scale. Since both the regularization of the convective term and the eddy dissipation reduce the number of degrees of freedom, we expect that the combination allows to use less eddy viscosity than the classical non-regularized LES-approach. The scale truncation properties of the classical approach were analyzed in Ref. [1]. The combined approach including eddy-viscosity can be analyzed along the same lines. A lower bound for the eddy viscosity is determined from the requirement that the production of any eddies of size smaller than the filter-width by the regularized nonlinear mechanism is counteracted by the eddy dissipation. Poincare's inequality shows that this can be achieved by damping the velocity gradient.

References

[1] Roel Verstappen, When does eddy viscosity damp sub-filter scales sufficiently? Journal of Scientific Computing 49 :94 (2011).
[2] Roel Verstappen, On restraining the production of small scales of motion in a turbulent channel Computers & Fluids 37 :887