Large Numerical Database Generated by Direct Numerical Simulation

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Why Direct Numerical Simulations ?

- More insight in the physics of complex flows
- Complementary data not available from experiments
  - experiments in the lab : full investigation of the physical parameters but limited available data
  - numerical simulation : limitation of changes in the physical and numerical parameters but full 3D unsteady velocity and pressure fields available
- A priori test of turbulence models : new models ?

Outline

- Motivations and definitions
  - Numerical requirements for physically relevant simulation
  - Current capabilities in direct numerical simulation
  - Direct numerical simulations at LIN-EPF (Lausanne)
  - Post-processing of the DNS data : database analysis
- Databases : lid-driven cavity and square duct
  - Visualisation
  - Mean flow statistics and Reynolds stress equations
  - Conditional sampling
  - A priori test of turbulence models

Definition : the DNS approach consists of solving the full non-linear, time-dependent Navier-Stokes equations without any empirical closure assumptions

$$\begin{cases} \dfrac{\partial u}{\partial t} + u.\nabla u = \dfrac{1}{\mathrm{Re}}\Delta u - \nabla p + f & \text{for}(x,t)\,\text{in}\,\Omega\times(0,T) \\ \nabla . u = 0 \end{cases}$$

Boundary Condition : $u = U$ for (x,t) in $\partial\Omega\times(0,T)$

Initial Condition : $u(x, t=0) = U^0$ for x in Ω

where f includes all/any body force terms

Definition : a database is a collection of files (called dump) containing space-time results i.e. of instantaneous discrete velocity and pressure fields produced by direct numerical simulation of the Navier-Stokes equations

- The database is organised by attaching to each file a time iteration counter
- One access to the database corresponds to load one of the dump
- **One** database corresponds to **one** numerical experiment i.e. **one** simulation for **one** set of fixed parameters (like the Reynolds number, rotation, etc…)
- The database analysis consits in analysing a time-discrete series of instantaneous space-discrete velocity and pressure fields

Numerical requirements for physically relevant flow simulations

- High order temporal accuracy effectively reached for (u,p)
- Long-time integration (for statistics)
- Good high wave number resolution (spectral method)
- Consistency with (Navier-) Stokes i.e.
  - no spurious boundary layers in (u,p)
  - no spurious space-time operators
- No spurious pressure modes

Current capabilities of direct numerical simulation

<u>Grid size for higher-order methods</u>

- 3D-homogeneous : $\approx 600^3$ (no special symmetries)
- 2D-homogeneous : $\approx 300^3$
- 1D-homogeneous : $\approx 240^3$
- 3D-inhomogeneous : $\approx 170^3$ (in simple geometries)

- Re_λ from ~10 (driven cavity) to ~250 (3D homogeneous)
- Physical-time span of simulation : tens of minutes
- Flow sample requirements increases with degree of inhomogeneity
- Length of sample also depends on type of statistics required
- Costs may escalate if large time-space scales exist
- typical cost on vector/parallel machines :

  Nec-Sx4/5 : 2000-4000 CPU hours/run (Lid Driven Cavity)
  Origin 3800 : 2000 Real time hours/run (4 processors)(Duct, rotating duct)

Direct numerical simulation at LIN-EPFL

- Forced homogeneous isotropic (Fourier-3D, grid=**256x256x256**)
- Straight square duct (finite difference-2D/Fourier-1D, **768x127x127**)
- Straight rectangular duct (spectral element-2D/Fourier-1D, **250x271x151**)
- Strg. duct with rotation (spectral element-2D/Fourier-1D, **256x169x169**)
- Lid driven cavity (Chebyshev-3D, 129^3 upto 169^3)

Computing ressources used : parallel/vector computers

- Cray-YMP, 4-processors, 512Mw of core
- Origin 3800, 128 processors (500MHZ, 512Mb, tot=65GB)
- Nec-Sx4, 12 processors, (2Gflops, 4Gb)
- Nec-Sx5, 10 processors, (8Gflops, 20Gb)

Most costly simulation undertaken so far is the lid driven cavity

Post-processing of DNS data

Because the flow sample is relatively short in the physical time, the simulated flow field must be sampled at intervals of the order of the smallest significant time scale. This is between the 1/40th and 1/30th of the large-scale turnover time.

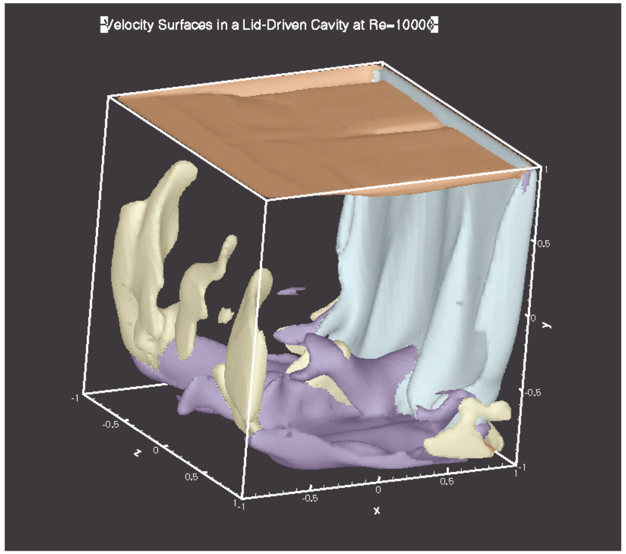
- Data visualisation and animation : partial/complete scan
- Simple statistics : mean fields, rms, skewness, flatness
- Reynolds stress equations terms
- Conditional sampling of energy dissipation/production events
  - more costly with inhomogeneity
  - scanning the whole database for every diss./prod. term and threshold
  - storage requirements : 3D velocity-pressure fields surrounding the events
- Proper orthogonal decomposition (POD)
  - cost of calculating the cross spectral density tensor (complete scan)
  - cost of solving eigenvalues problems for each wavenumber
- A priori test of turbulence models

Post-processing of DNS data (ctd)

- Overall, the cost of post-processing phase is unbounded
- In practice, the cost of data analysis could exceed that of simulation
- Near solid boundaries, accuracy achieved up to 2nd derivatives

- **The only cost-effective archiving medium is magnetic tape**
- **Automatic tape loader give 24h access to databases**
- **Data set migration facilities : « direct » file access on tape**
- Optical disks not very competitive for rates Gbytes/min

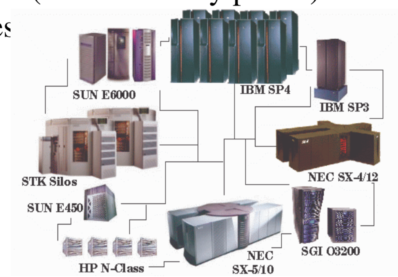
Lid Driven Cavity (3D inhomogeneous Chebyshev)



E. Leriche

DNS in the lid-driven cavity

- Reynolds (based on the lid velocity) : 12000
- Mesh (Chebyshev-3D) : **129x129x129** (=2.15 millions nodes)
- Time Step : 0.0025
- Sample span : 125 turnover times
- Sampling rate : every 0.031 turnover times
- Number of flow samples : 4000
- Stored quantities : (u,v,w) and p
- Size of database dump : 68.7 Mbytes (with boundary points)
- Total data held in store : 275 Gbytes
- Cartridges : CSCS (Manno)

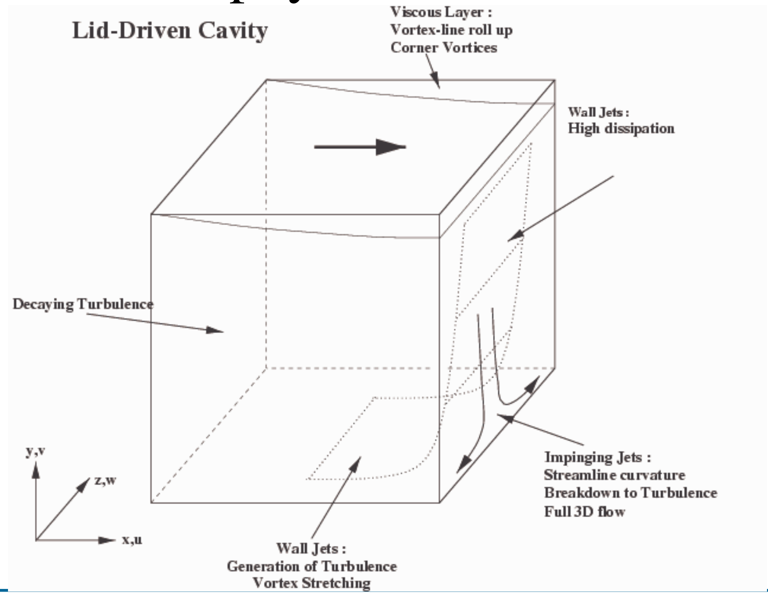


Visualisation from the database

The animation is available at

http://www.cscs.ch/expertise/vis/projects/Leriche.html

Flow physics in the LDC



Ensemble Averaged Navier-Stokes Equations

Reynolds decomposition : Mean + fluctuating : $u = U + u'$

$\langle u' \rangle = 0$

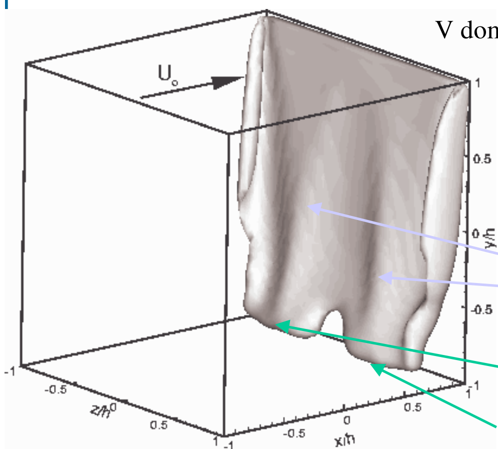
$$\begin{cases} \dfrac{\partial U_i}{\partial t} + U_k \dfrac{\partial U_i}{\partial x_k} = \dfrac{1}{Re} \dfrac{\partial^2 U_i}{\partial^2 x_k} - \dfrac{\partial P}{\partial x_k} + \dfrac{\partial}{\partial x_k} \langle u'_i u'_k \rangle \\ \dfrac{\partial U_i}{\partial x_i} = 0 \end{cases}$$

Interaction between mean and fluctuating flieds :

- **Reynolds stress tensor :**$\langle u'_i u'_k \rangle$

- Trace of the Reynolds stress tensor : **turbulent kinetic energy k**

Mean Field : isosurface of V=0.1 U_0



V dominant near the downstream wall

Wall jets with variable thickness

Wall jets separation

Two higher speed regions (thickest)

Impingement of two elliptical jets on the bottom wall

Impingement region : high turbulent production

Reynolds Stress Equations

$$\left(\frac{\partial}{\partial t}+U_k\frac{\partial}{\partial x_k}\right)\langle u_i'u_j'\rangle = P_{ij}+\Phi_{ij}+T_{ij}+D_{ij}^p+D_{ij}^v-\varepsilon_{ij}$$

$$P_{ij}=-\langle u_j'u_k'\rangle\frac{\partial U_i}{\partial x_k}-\langle u_i'u_k'\rangle\frac{\partial U_j}{\partial x_k} \quad \text{(Production)}$$

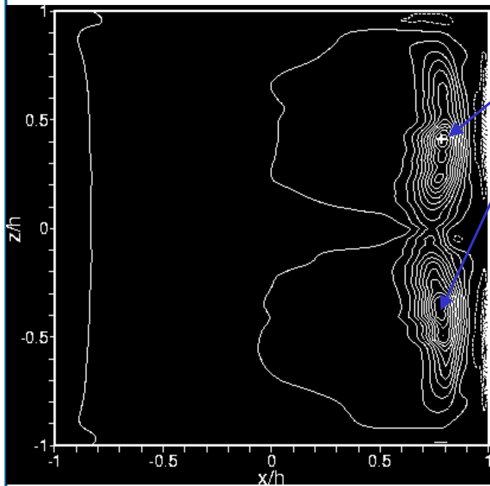
$$\Phi_{ij}=-\left\langle p'\left(\frac{\partial u_i'}{\partial x_j}+\frac{\partial u_j'}{\partial x_i}\right)\right\rangle \qquad T_{ij}=-\frac{\partial}{\partial x_k}\langle u_i'u_j'u_k'\rangle$$

$$D_{ij}^v=\frac{1}{\mathrm{Re}}\frac{\partial^2}{\partial^2 x_k}\langle u_i'u_j'\rangle \qquad D_{ij}^p=-\frac{\partial}{\partial x_j}\langle p'u_i'\rangle-\frac{\partial}{\partial x_i}\langle p'u_j'\rangle$$

$$\varepsilon_{ij}=\frac{2}{\mathrm{Re}}\left\langle\frac{\partial u_i'}{\partial x_j}\frac{\partial u_j'}{\partial x_i}\right\rangle \quad \text{(Dissipation)}$$

Reynolds stress equation : production P_{22}

Production P_{22} on a plane parallel to the bottom wall (y/h0-0.924)

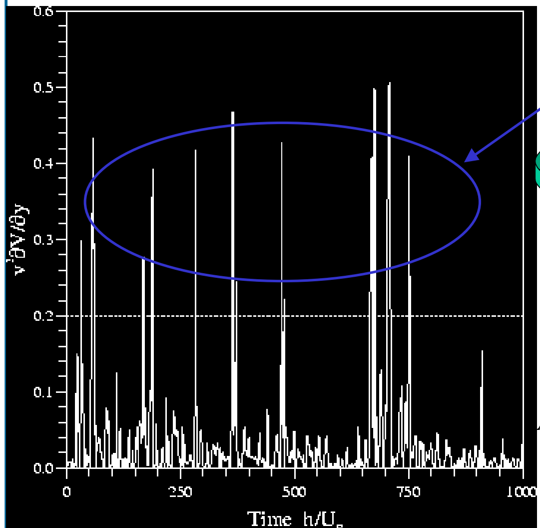


Maximum Production at the Impingement point

Near the maximum $P_{22}\approx-\langle v'^2\rangle\frac{\partial V}{\partial y}$

Dominant flow structure attached to the maximum of P_{22}?

Reynolds stress equations : P_{22} near impingement point



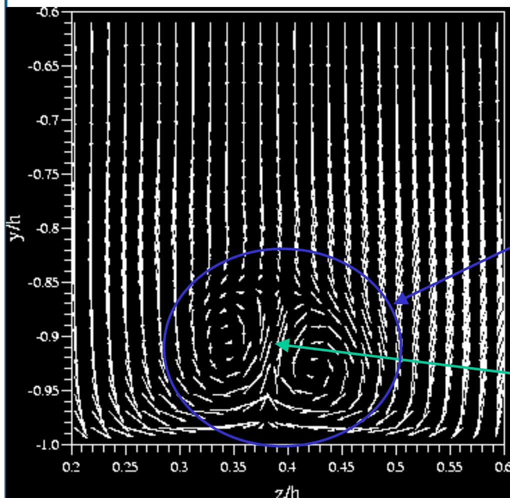
Subset : $P_{22}(t)\approx-v'^2\frac{\partial V}{\partial y}\geq 0.2\ \frac{U_0^3}{h}$

Contribution of 0.3 P_{22}

Time history of $-v'^2\frac{\partial V}{\partial y}$ at the maximum of P_{22}

Location : (x/h=0.773, y/h=-0.924, z/h=0.388)

Conditional sampling according to $-v'^2\frac{\partial V}{\partial y}\geq 0.2\ \frac{U_0^3}{h}$



Plane normal to the bottom wall & parallel to the downstream wall

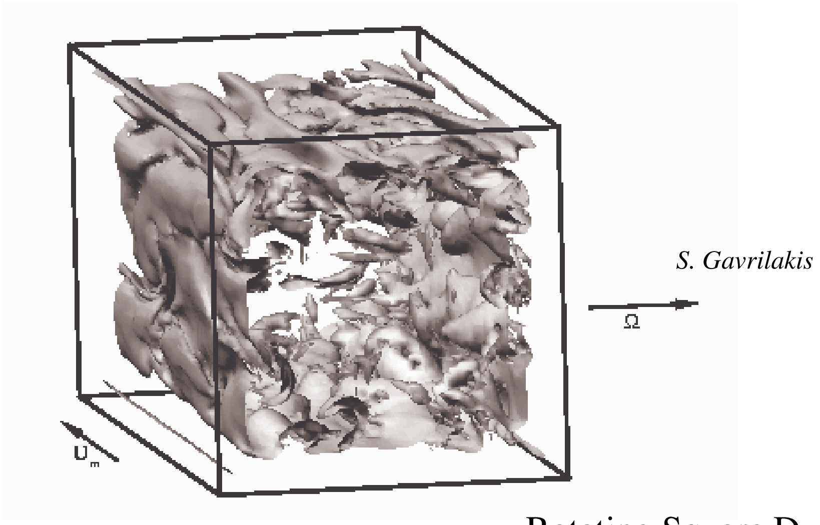
Location : x/h=0.773

Pair of conter-rotating vortices

Maximum of production at the Center of the pair

Location : (x/h=0.773, y/h=-0.924, z/h=0.388)

DNS in the Square Duct (2D inhomegeneous / 1D Fourier)



Rotating Square Duct

DNS in a square duct (without rotation)

- Reynolds (based on the mean velocity) : 4800
- Reynolds (based on the friction velocity) : 320

- Mesh (Fourier-1D/finite difference-2D) : **768x127x127** (=12.38 millions nodes)
- Time Step : 0.0003

- Sample span : 4.4 turnover times time step : 0.0003
- Sampling rate : every 0.022 turnover times
- number of flow samples : 200
- stored quantities : (u,v,w) and p

- Size of database dump : 410 Mbytes (with boundary points)
- Periodic full dumps : 717 Mbytes each
- total data held in store : 96 Gbytes

A priori test of turbulence models

2 equations $k-\varepsilon$ model : turbulent kinetic energy and dissipation

⇨ Closure assumption to model the Reynolds stress tensor :

$$-\langle u_i' u_j' \rangle = f\left(\frac{\partial U_i}{\partial x_j}, k, \varepsilon, D_{ij}, W_{ij}, \frac{\partial D_{ij}}{\partial x_k}, \frac{\partial W_{ij}}{\partial x_k}\right)$$

where

$$k = \langle u_i' u_i' \rangle,\ \varepsilon = \frac{2}{\mathrm{Re}}\left\langle \frac{\partial u_i'}{\partial x_j}\frac{\partial u_j'}{\partial x_i}\right\rangle,\ D_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \text{ and } W_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i}\right)$$

- The left hand side $\langle u_i' u_j' \rangle$ is evaluated directly from DNS database
- Each term in the RHS is coming from the turbulence model but is evaluated from DNS database
- The difference between the LHS and RHS quantifies the «quality» of the turbulence models

A priori test : Speziale turbulence model

$$-\langle u_i' u_j' \rangle = -\frac{2}{3}k\delta_{ij} + c_\mu \frac{k^2}{\varepsilon} 2D_{ij} + c_d c_\mu^2 \frac{k^3}{\varepsilon^2}\left(D_{im}D_{mj} - \frac{1}{3}D_{mn}D_{mn}\delta_{ij}\right) + c_E c_\mu^2 \frac{k^3}{\varepsilon^2}\left(\overset{\nabla}{D}_{ij} - \frac{1}{3}\overset{\nabla}{D}_{mm}\delta_{ij}\right)$$

where

$$D_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \quad \text{and} \quad \overset{\nabla}{D}_{ij} = \frac{\partial D_{ij}}{\partial t} + U_k \frac{\partial D_{ij}}{\partial x_k} - \frac{\partial U_i}{\partial x_k} D_{kj} - \frac{\partial U_j}{\partial x_k} D_{ki}$$

with $c_d = c_E = 1.68$ and $c_\mu = 0.09$

A priori turbulence models test

$$-\langle u_i' u_j' \rangle = -\frac{2}{3}k\delta_{ij} + c_\mu \frac{k^2}{\varepsilon} 2D_{ij}$$

$$- F_1 \frac{k^3}{\varepsilon^2}\left(\frac{\partial U_i}{\partial x_n}\frac{\partial U_n}{\partial x_j} + \frac{\partial U_j}{\partial x_n}\frac{\partial U_n}{\partial x_i} - \frac{2}{3}\frac{\partial U_m}{\partial x_n}\frac{\partial U_n}{\partial x_m}\delta_{ij} \right)$$

$$- F_2 \frac{k^3}{\varepsilon^2}\left(\frac{\partial U_i}{\partial x_n}\frac{\partial U_j}{\partial x_n} - \frac{1}{3}\frac{\partial U_n}{\partial x_m}\frac{\partial U_n}{\partial x_m}\delta_{ij} \right)$$

$$- F_3 \frac{k^3}{\varepsilon^2}\left(\frac{\partial U_n}{\partial x_i}\frac{\partial U_n}{\partial x_j} - \frac{1}{3}\frac{\partial U_n}{\partial x_m}\frac{\partial U_n}{\partial x_m}\delta_{ij} \right)$$

where c_μ, F_1, F_2, F_3 are models dependent

A priori turbulence models test

c_μ, F_1, F_2, F_3 are model dependent

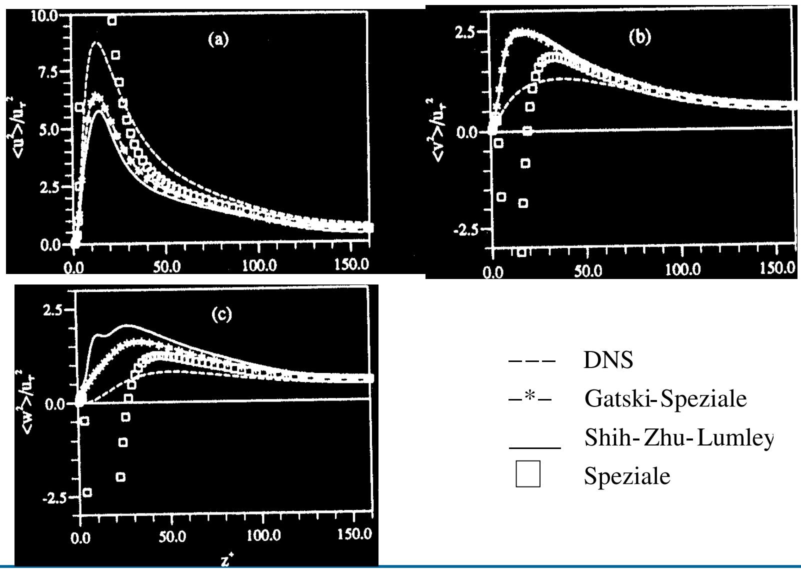
	F_1	F_2	F_3	c_μ
Demuren-Rodi	0.052	0.092	0.013	0.092
Rubinstein-Barton	0.104	0.034	-0.014	0.092
Shih-Zhu-Lumley	-4/A	13/A	-2/A	0.67/(1.25+ η)
Gatski-Speziale	0.030 R	0.093 R	-0.034 R	0.068 R

$A = 1000 + \eta^3,\ R = (1 + 0.0038\,\eta^2)/D$

$D = 3 + 0.0038\,\eta^2 + 0.0008\,\eta^2\varsigma^2 + 0.2\,\varsigma^2$

$$\eta = \frac{k}{\varepsilon}(2D_{ij}D_{ij})^{1/2},\ \varsigma = \frac{k}{\varepsilon}(W_{ij}W_{ij})^{1/2},\ D_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right),\ W_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i}\right)$$

Diagonal term of the Reynolds stress tensor



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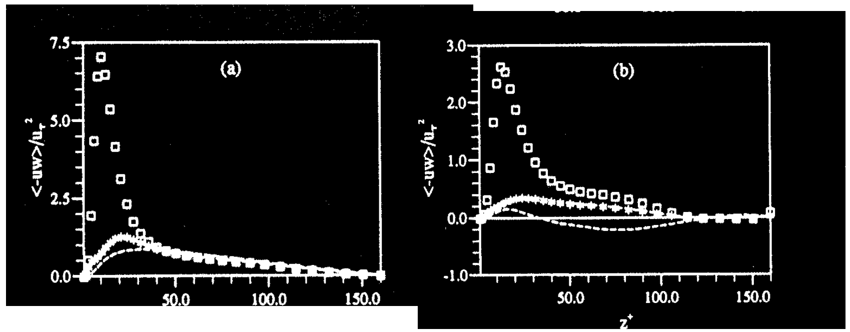
–*– Gatski-Speziale

—— Shih-Zhu-Lumley

□ Speziale

Off-diagonal term of the Reynolds stress tensor



--- DNS

–*– Gatski-Speziale

—— Shih-Zhu-Lumley

□ Speziale

Conclusions

- DNS is nowadays a standard well established tool
- Efficient numerical methods even in complex geometries are still required
- Limiting factor move from CPU to massive storage needs
- Parametric investigation is now possible : Reynolds, rotations
- Additional effect : heat (thermally driven cavity)
- POD analysis in 3D confined geometry

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