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Numerical simulation of subsonic turbulent viscous compressible flows using quasi-gas dynamic equations

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Outline

- **1. Introduction: context of the work**
- **2. Quasi-Gas Dynamic (QGD) equations as an extention of Navier-Stokes system**
- **3. Discretization and numerical algorithm**
- **4. Laminar-turbulent transition in Taylor-Green vortex simulation. Isotropic flow**
- **5. Laminar and turbulent regimes in Couette flow simulation. Boundary layer flow**
- **6. Conclusions**

- **The objective of the present work is to show the possibilities of the so-called Quasi-Gas Dynamic (QGD) equations for laminar-turbulent transition in compressible heat-conducting gas flow simulations.**

- **These equations were developed by Chetverushkin, Elizarova, Sheretov and co-workers and were nicely presented in the talk of B.N. Chetverushkin in the morning session**

- **QGD equations can be obtained basing on Navier-Stokes Eqs. They have additional smoothing or regularization.**

- **QGD equations can be used in different areas, including Rarefied Gas Dynamics, shock-wave flow simulations and in turbulent flow simulations**

Quasi-gas-dynamic equations as an extension of Navier-Stokes system

Navier-Stokes equations

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial \rho u_i}{\partial x_i} = 0, \\ \dfrac{\partial \rho u_i}{\partial t} + \dfrac{\partial \rho u_k u_i}{\partial x_k} + \dfrac{\partial p}{\partial x_i} = \rho F_i + \dfrac{\partial \Pi_{ki}}{\partial x_k}, \\ \dfrac{\partial}{\partial t} \rho \left(\dfrac{u^2}{2} + \varepsilon \right) + \dfrac{\partial}{\partial x_i} \rho u_i \left(\dfrac{u^2}{2} + \varepsilon + \dfrac{p}{\rho} \right) + \dfrac{\partial q_i}{\partial x_i} = \rho u_i F_i + \dfrac{\partial}{\partial x_i} \Pi_{ik} u_k + Q \end{cases}$$

Averaging of Navier-Stokes system over a small time interval $(t, t+\Delta t)$

$$\left\langle f(x,t)\right\rangle = \frac{1}{\Delta t}\int_{t}^{t+\Delta t} f(x,t')\,dt'$$

$$\begin{cases}
\dfrac{\partial\langle\rho\rangle}{\partial t} + \dfrac{\partial\langle\rho u_i\rangle}{\partial x_i} = 0, \\[2ex]
\dfrac{\partial\langle\rho u_i\rangle}{\partial t} + \dfrac{\partial\langle\rho u_k u_i\rangle}{\partial x_k} + \dfrac{\partial\langle p\rangle}{\partial x_i} = \langle\rho F_i\rangle + \dfrac{\partial\langle\Pi_{ki}\rangle}{\partial x_k}, \\[2ex]
\dfrac{\partial}{\partial t}\left\langle\rho\left(\dfrac{u^2}{2}+\varepsilon\right)\right\rangle + \dfrac{\partial}{\partial x_i}\left\langle\rho u_i\left(\dfrac{u^2}{2}+\varepsilon+\dfrac{p}{\rho}\right)\right\rangle + \dfrac{\partial\langle q_i\rangle}{\partial x_i} = \langle\rho u_i F_i\rangle + \dfrac{\partial}{\partial x_i}\langle\Pi_{ik}u_k\rangle + \langle Q\rangle
\end{cases}$$

$$\left\langle f(x,t)\right\rangle = f(x,t) + \tau\frac{\partial f(x,t)}{\partial t} \qquad O(\tau^2), O(\mu\tau), O(\kappa\tau), \frac{\partial^2}{\partial t^2}$$

Example – continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i + \tau \frac{\partial \rho u_i}{\partial t} \right) = 0$$

$$\frac{\partial \rho u_i}{\partial t} = -\frac{\partial}{\partial x_j}\left(\rho u_i u_j + p\delta_{ij} \right)$$

Here we introduce the notations for the additional velocity and mass flux:

$$w_i = \frac{\tau}{\rho}\frac{\partial}{\partial x_j}\left(\rho u_i u_j + p\delta_{ij} \right) \qquad j_i = \rho\left(u_i - w_i \right)$$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial j_i}{\partial x_i} = 0}$$

For momentum and total energy equations additional τ -terms are calculated using Euler equations and differential identities

$$\tau \frac{\partial}{\partial t}\frac{1}{\rho} = -\tau\left(u_i \frac{\partial}{\partial x_i}\frac{1}{\rho} - \frac{1}{\rho}\frac{\partial u_i}{\partial x_i} \right)$$

$$\tau \frac{\partial}{\partial t} u_i = -\tau\left(u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - F_i \right)$$

$$\tau \frac{\partial}{\partial t}\varepsilon = -\tau\left(u_i \frac{\partial \varepsilon}{\partial x_i} + \frac{p}{\rho}\frac{\partial u_i}{\partial x_i} - \frac{Q}{\rho} \right)$$

$$\tau \frac{\partial}{\partial t} p = -\tau\left(u_i \frac{\partial p}{\partial x_i} + \gamma p \frac{\partial u_i}{\partial x_i} - (\gamma - 1) Q \right)$$

QGD equations

$$\frac{\partial}{\partial t}\rho + \nabla_i j_m^i = 0$$

$$\frac{\partial}{\partial t}\rho u^j + \nabla_i \left(j_m^i u^j \right) + \nabla^j p = \nabla_i \Pi^{ij}$$

$$\frac{\partial}{\partial t}E + \nabla_i \left(j_m^i H \right) + \nabla_i q^i = \nabla_i \left(\Pi^{ij} u_j \right)$$

$$\tau = ?$$

$$j_m^i = \rho(u^i - w^i), \quad w^i = \frac{\tau}{\rho}\left(\nabla_j \rho u^i u^j + \nabla^i p \right)$$ mass flux

$$\Pi^{ij} = \Pi_{NS}^{ij} + \tau u_i \rho \left(u_k \nabla^k u_j + (\nabla_j p)/\rho \right)$$

$$+ \tau \delta^{ij} \left(u_k \nabla^k p + \gamma p \nabla^k u_k \right)$$ shear-stress tensor

$$\Pi_{NS}^{ij} = \mu \left(\nabla^i u^j + \nabla^j u^i - (2/3)\nabla^k u_k \right) + \varsigma \delta^{ij} \nabla^k u_k$$

$$q^i = q_{NS}^i - \tau u_i \rho \left(u_j \nabla^j \varepsilon + p u_j \nabla^j (1/\rho) \right)$$ heat flux, $$q_{NS}^i = -\kappa \nabla^i T$$

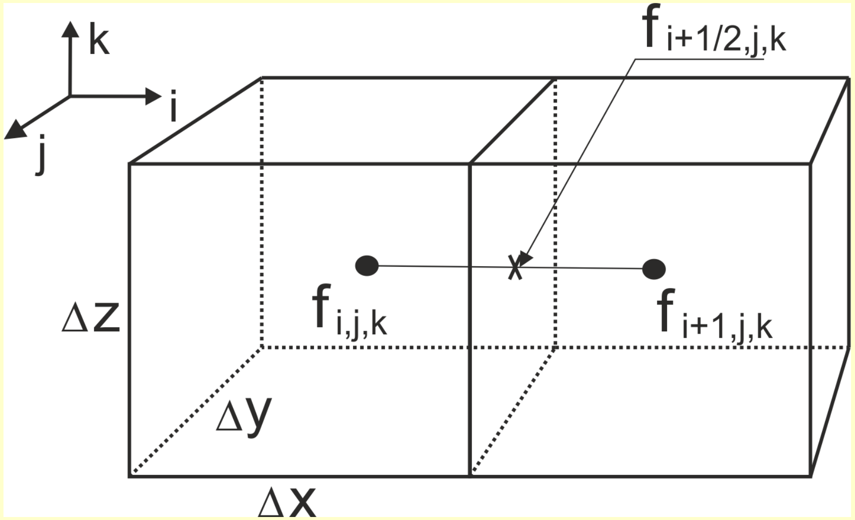
Properties of QGD equations

- QGD Eqs have the form of conservation laws, including entropy theorem and angular momentum conservation.
- Prandtl boundary layer limit is obtained.
- Common exact solutions with the NS system for a number of classical problems (e.g., Couette flow, barometric distribution).
- A number of theoretical results – Petrovski parabolicity, linearased stability of equilibrium solutions, ets.. (Yu.V. Sheretov,

A.A. Zlotnik,..)

Discretization and numerical algorithm

Explicit-in-time finite-difference scheme with central differences approximation for all space derivatives



$$f_{i+1/2,j,k} = \frac{f_{i+1,j,k} + f_{i,j,k}}{2}$$

$$\frac{\partial f}{\partial t} \rightarrow \frac{\hat{f}_{i,j,k} - f_{i,j,k}}{\Delta t} \qquad \frac{\partial f}{\partial x} \rightarrow \frac{f_{i+1/2,j,k} - f_{i-1/2,j,k}}{\Delta x}$$

$$\left.\frac{\partial f}{\partial x}\right|_{i+1/2,j,k} = \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x}$$

Benefits of QGD equations

- **Additional dissipative τ -terms act as a “built in” regularization that contributes to the stability of the algorithms.**
- **Allows using simple and efficient algorithms for computing liquid and supersonic-subsonic gas flows:**
  - Space-derivatives, including those appearing in convective terms, are approximated by centered finite differences
  - Suited to unstructured grids
  - Explicit-in-time (conditionally stable)
  - Suited to unsteady flows
  - Facility of parallelization

- regularization parameter is related with grid step h and local sound velocity c
- $\tau = \alpha\, h/c$

Parallel computing

- **Computations were carried out on highly-parallel computers Keldysh-100 and BlueGene/P of the Russian Academy of Sciences.**

- **A parallel variant of the numerical algorithm was based on a decomposition of the computational domain by planes x = cste.**

- **MPI standard was used to allow portability between computers.**

- **For the problem under consideration, parallelization results in a linear efficiency increase with increasing the number of nodes.**

- **Computer Keldysh-100 is approximately 10 times more efficient than BlueGene/P for an identical number of active nodes.**

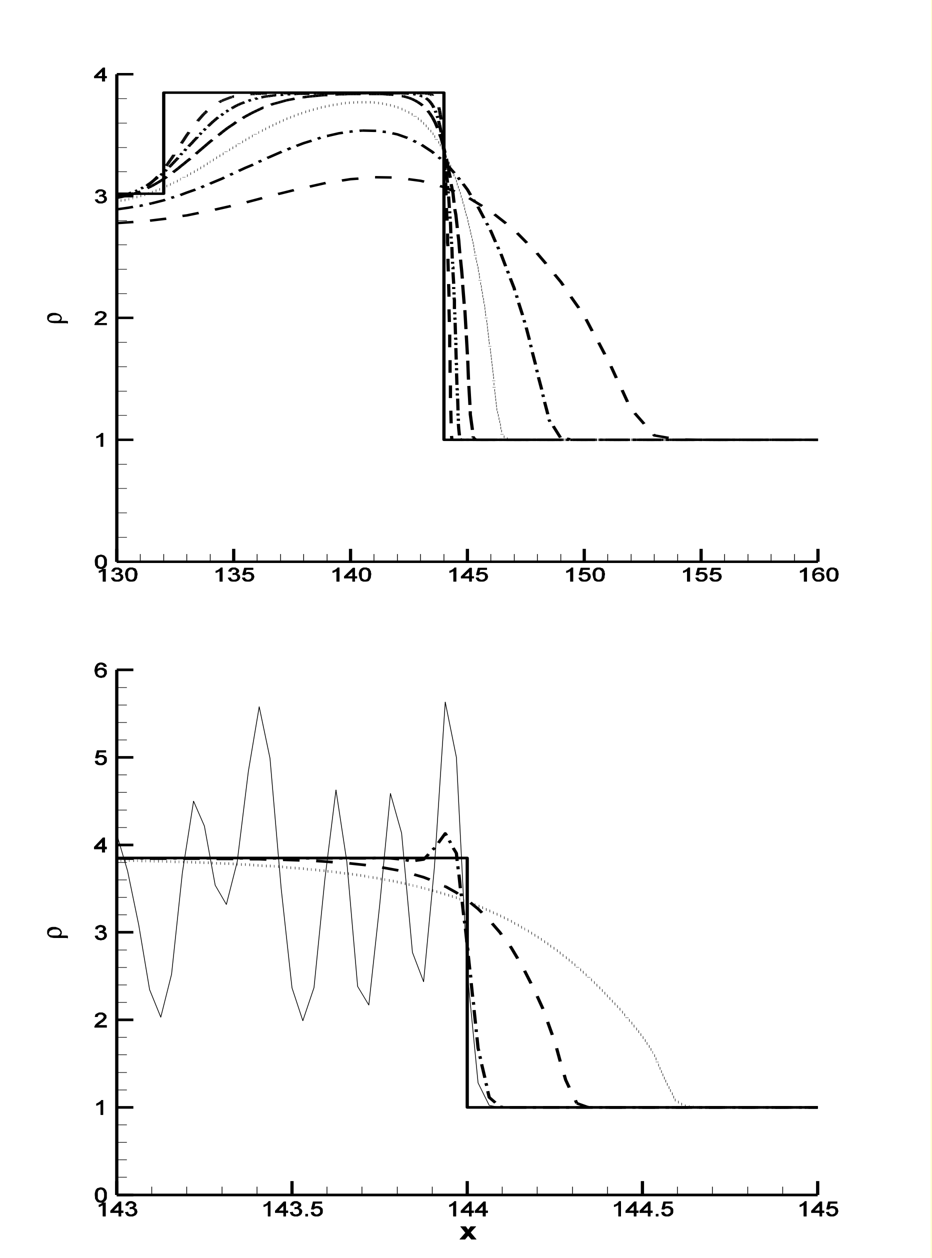
Sod problem, strong discontinuity decay

Grid step h, number of points N:

1	200
0.5	400
0.25	800
0.125	1600
0.0625	3200
0.03125	6400

Coefficient α:

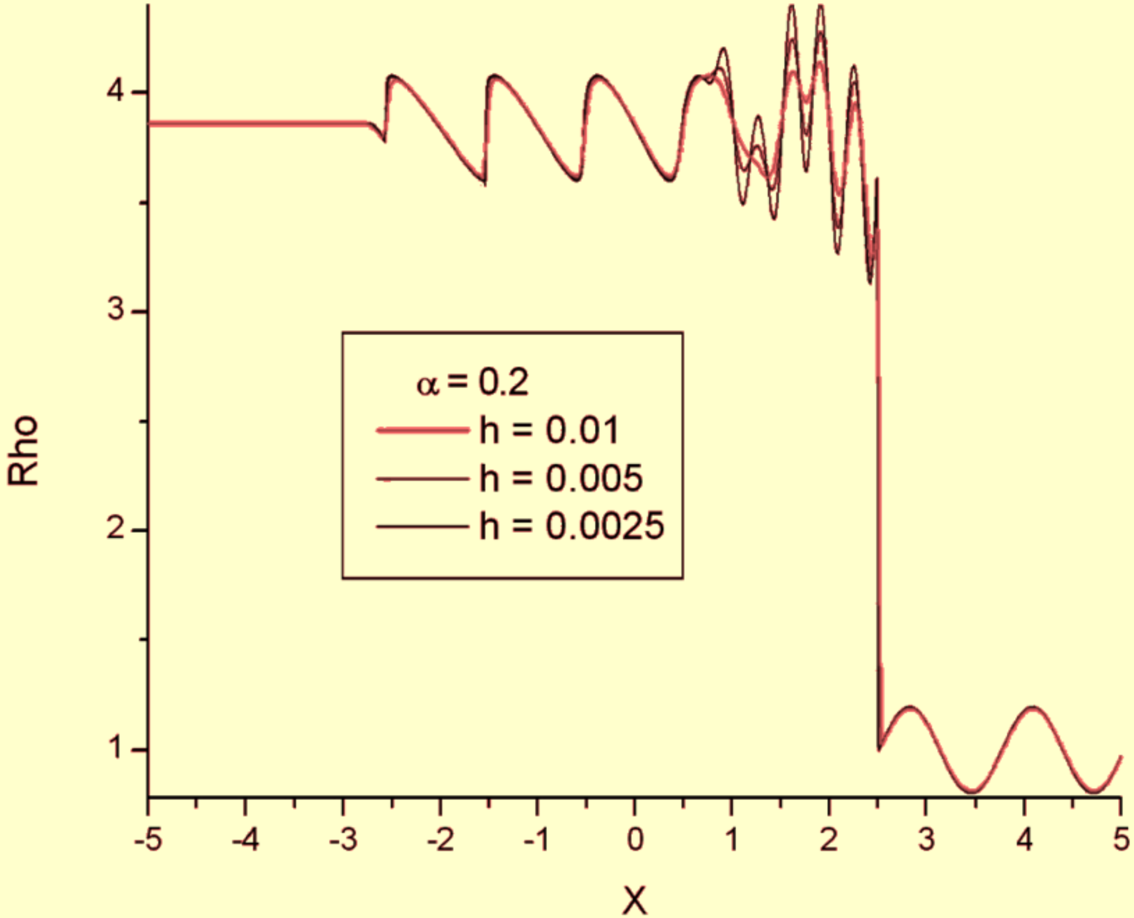
0.02
0.10
0.50
1.00



Shu-Osher problem

Interaction of shock and entropy waves, grid convergence

$$\gamma = 1.4, \quad \alpha = 0.2, \quad \beta = 0.4$$



Quasi-Gas Dynamic equations for turbulent flows

- **Relating the value of τ to the space-grid step h as $\tau \sim h / c$, where c is the local sound velocity, we can consider the associated viscosity as an original variant of sub-grid dissipation in LES models, that averages the fluctuations of flow parameters on a time-space scale depending on discretization.**
- **This sub-grid dissipation differs from the Smagorinsky viscosity, as the τ-terms have another mathematical structure and additional terms appear not only in the momentum and energy equations, but also in the continuity equation. This latter property models the turbulent mass-diffusion, which is inherent to turbulent mixing.**
- **Along a wall, the τ-terms vanish.**

- $\tau = \alpha\, h/c$
- accounts for subgrid dissipation
- sound velocity c is estimated locally
- h is the grid resolution
- α is an empirical coefficient

Numerical simulation of Taylor-Green flow

The evolution of the single-vortex flow, defined at the initial time as the Taylor-Green vortex may be one of the simplest flow for which a laminar-turbulent transition can be observed numerically. This process includes two stages

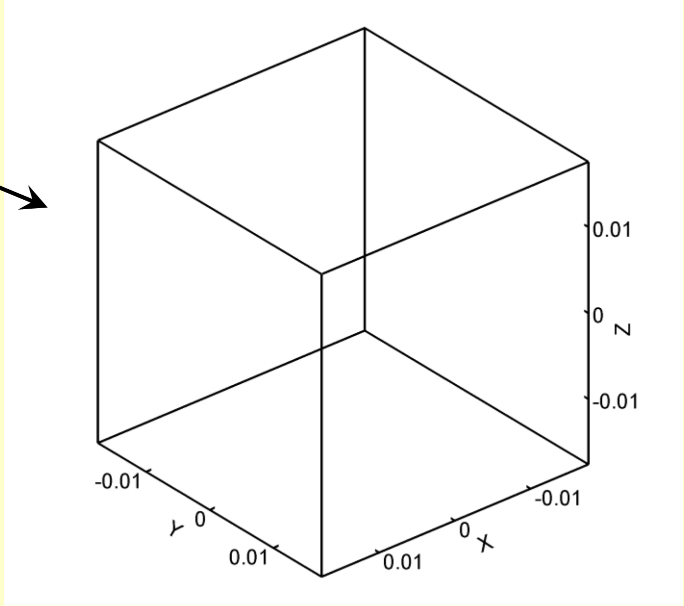
– large scale vorticities break into smaller ones in laminar regime

- after the time point corresponding to the maximum dissipation rate vortex decay leads to a turbulent energy cascade

Taylor-Green flow: problem formulation

Computational domain: $-\pi L \le x, y, z \le \pi L$

$\pi L = 0.016$ м



Working gas is nitrogen N_2 with initial temperature $T = T_0 = 273$

Boundary conditions are periodic for X, Y, Z

Mach number: $Ma = U_0 / c_{S0} = 0.1$

c_{S0} - sound velocity in nitrogen with initial temperature

Innitial conditions : Teylor-Green vortex

$$u_x = U_0 \sin(x/L)\cos(y/L)\cos(z/L)$$

$$u_y = -U_0 \cos(x/L)\sin(y/L)\cos(z/L)$$

$$u_z = 0$$

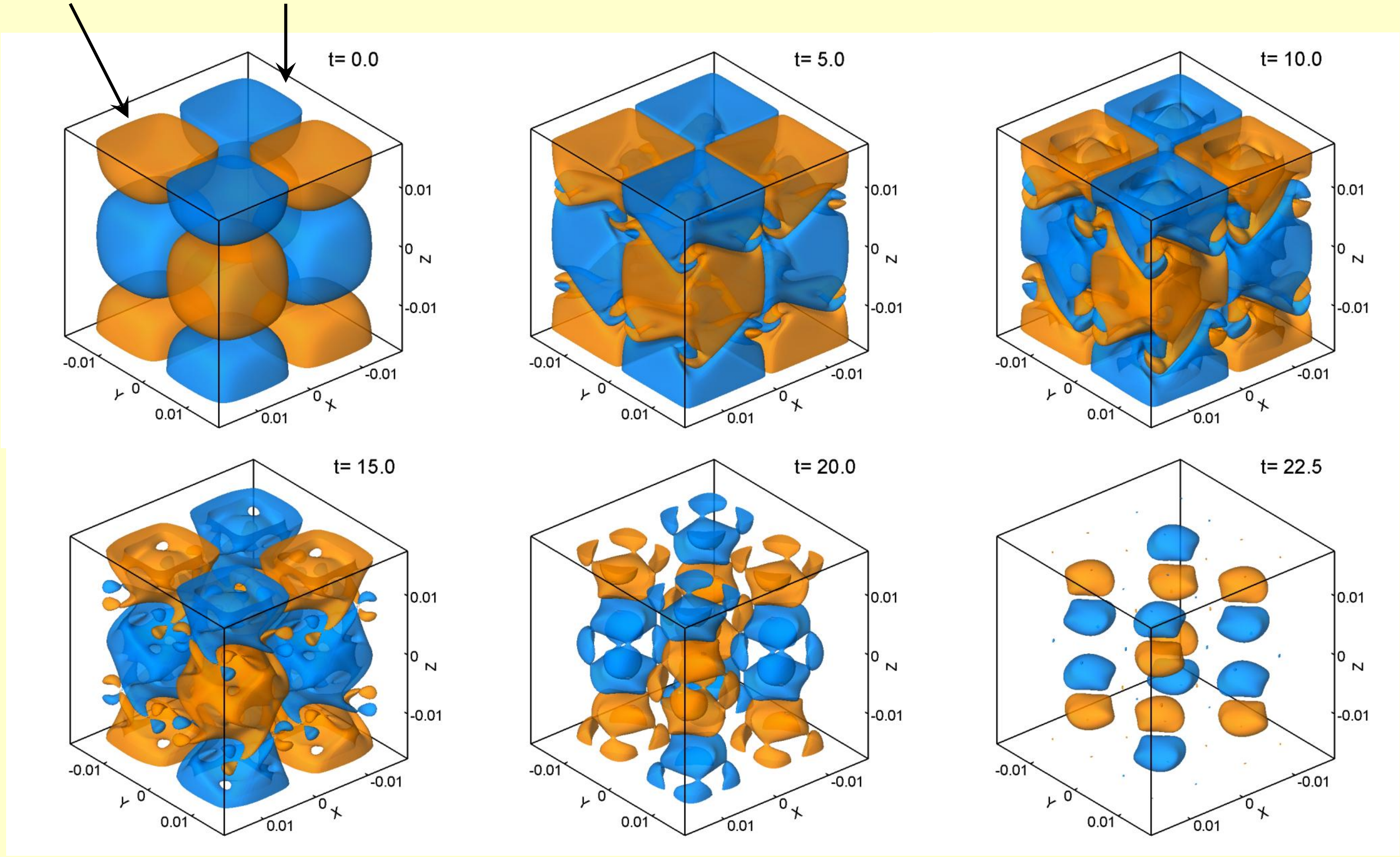
Reynolds number: $\mathrm{Re} = \rho_0 U_0 L / \mu_0$

μ_0 - viscosity of the nitrogen for initial temperature

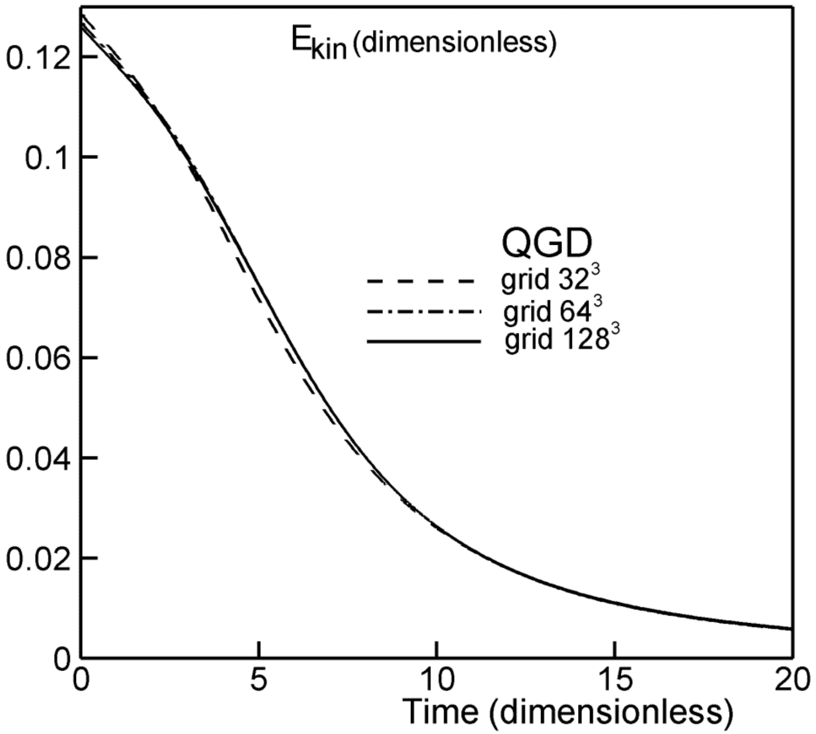
$$p = p_0 + (\rho_0 U_0^2 / 16)(\cos(2x/L) + \cos(2y/L))(\cos(2z/L) + 2)$$

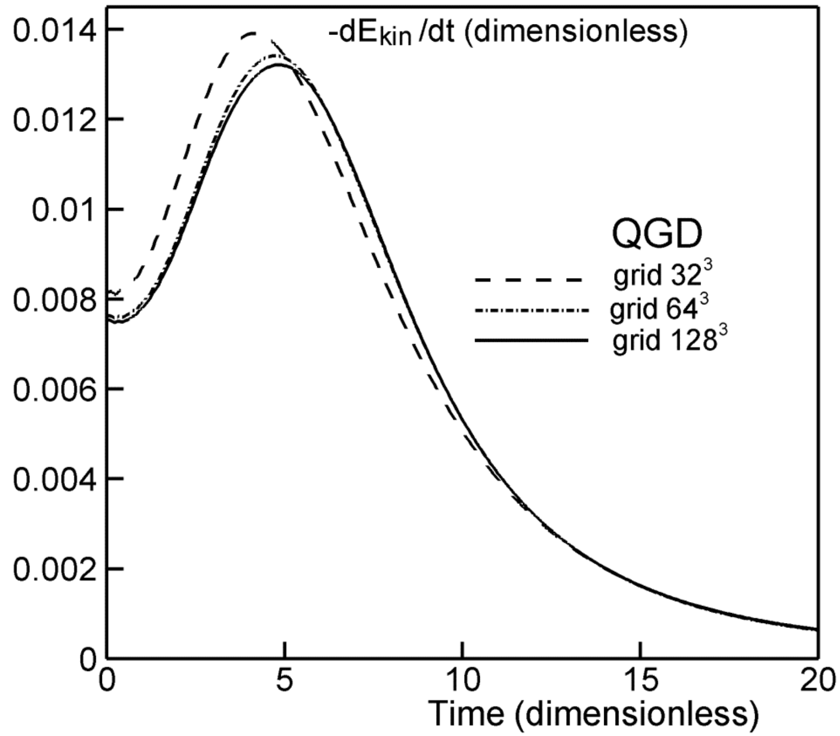
Re=100 evolution of iso-surfaces of z-component of vorticity

$Vz = 0.2$ $\quad$ $Vz = -0.2$ $\qquad$ $Vz = \partial u_y / \partial x - \partial u_x / \partial y$



Re=100, kinetic energy and dissipation rate, grid convergence

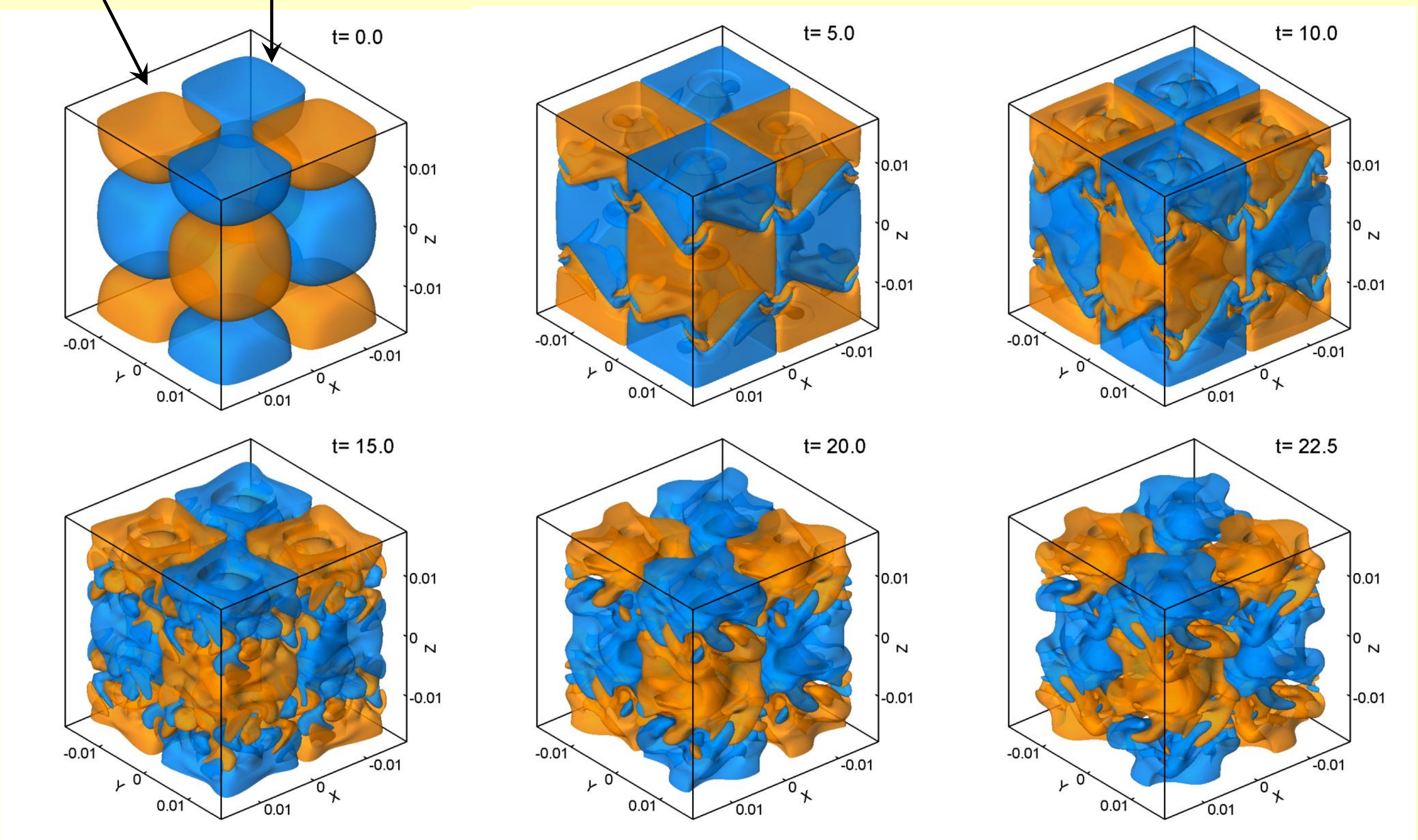




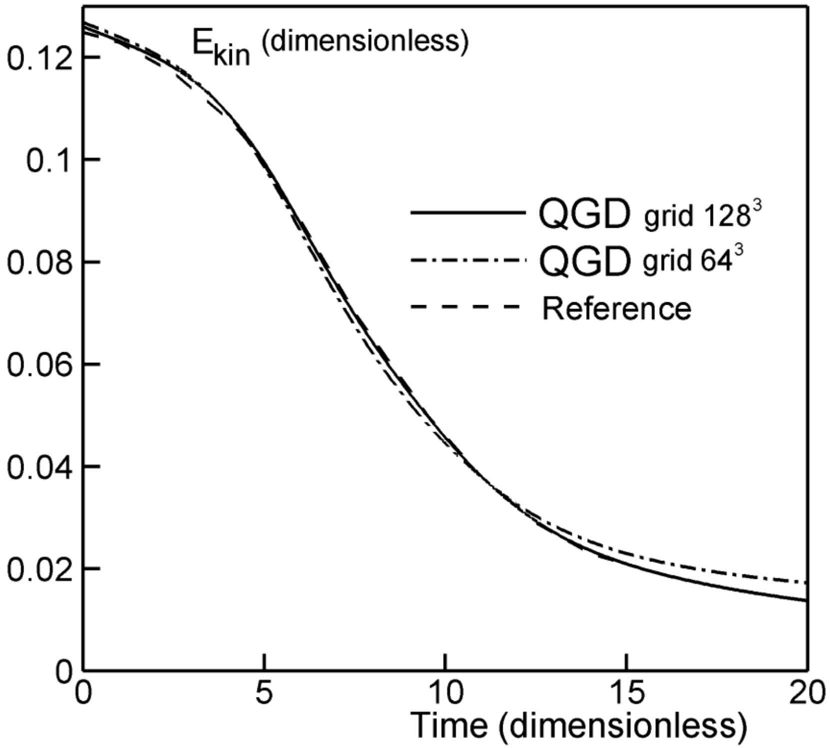
Re=280 evolution of iso-surfaces of z-component of vorticity

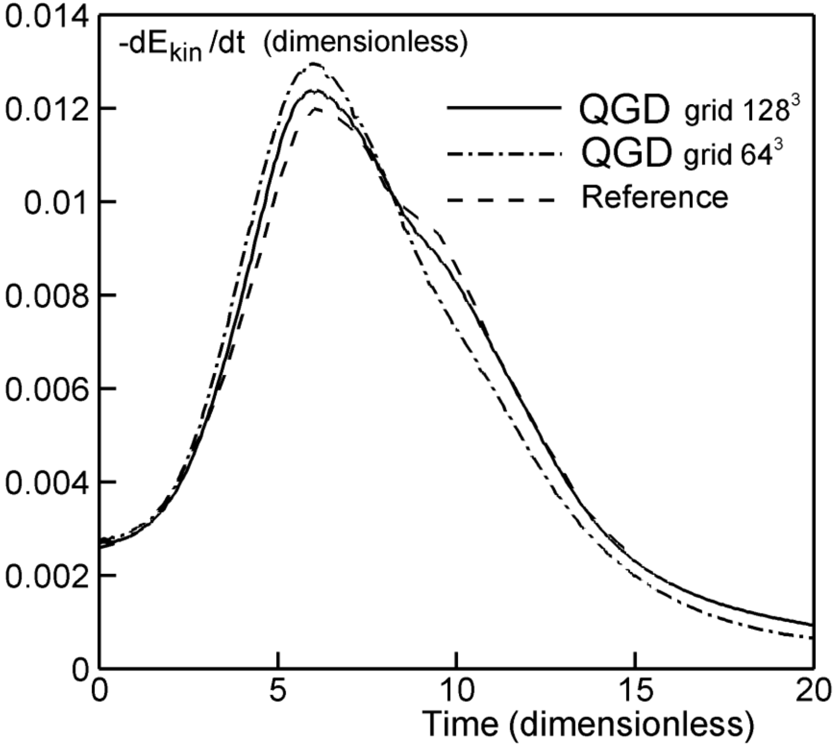
$Vz = 0.2$ $Vz = -0.2$

$$Vz = \partial u_y / \partial x - \partial u_x / \partial y$$



Re=280, kinetic energy and dissipation rate, grid convergence

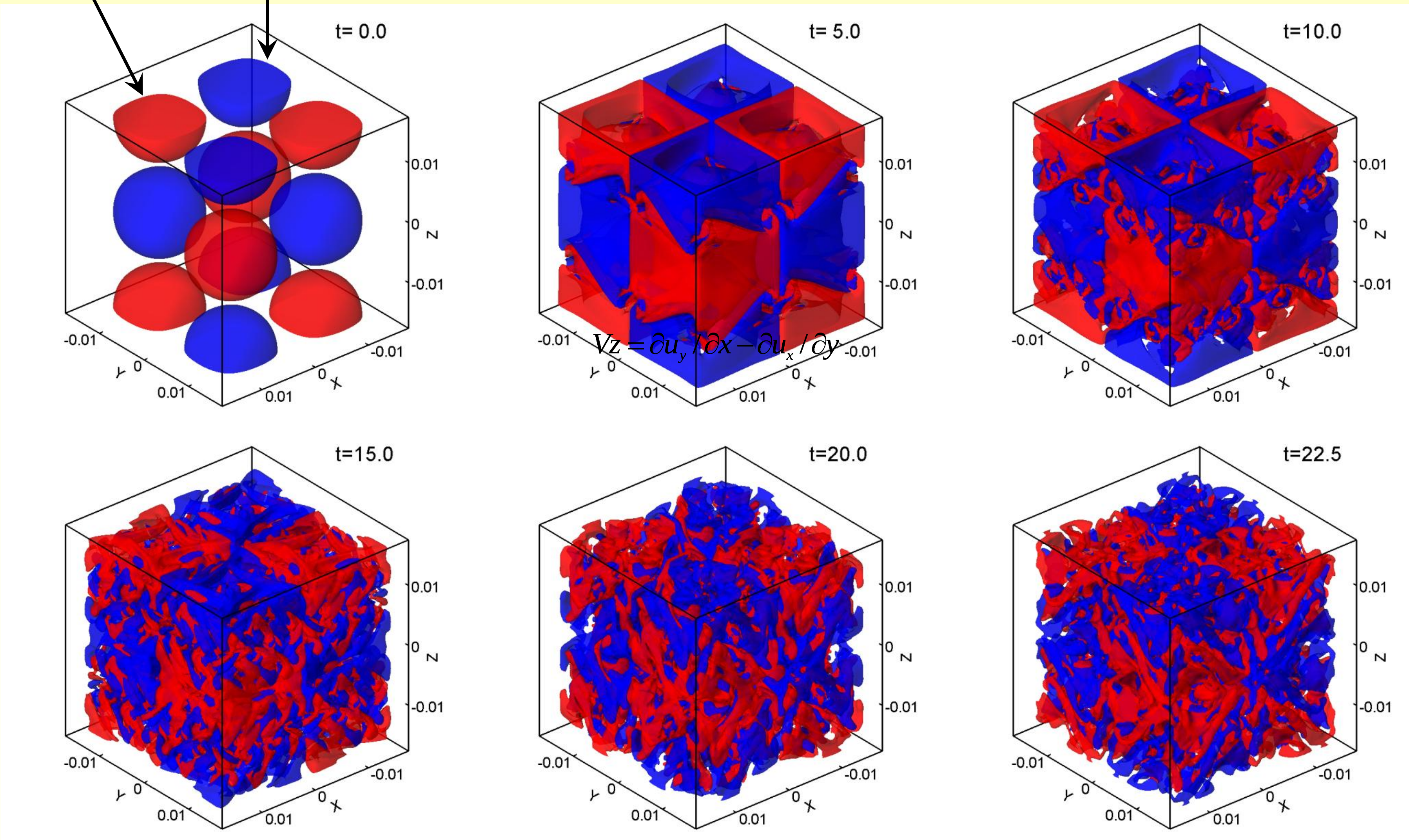




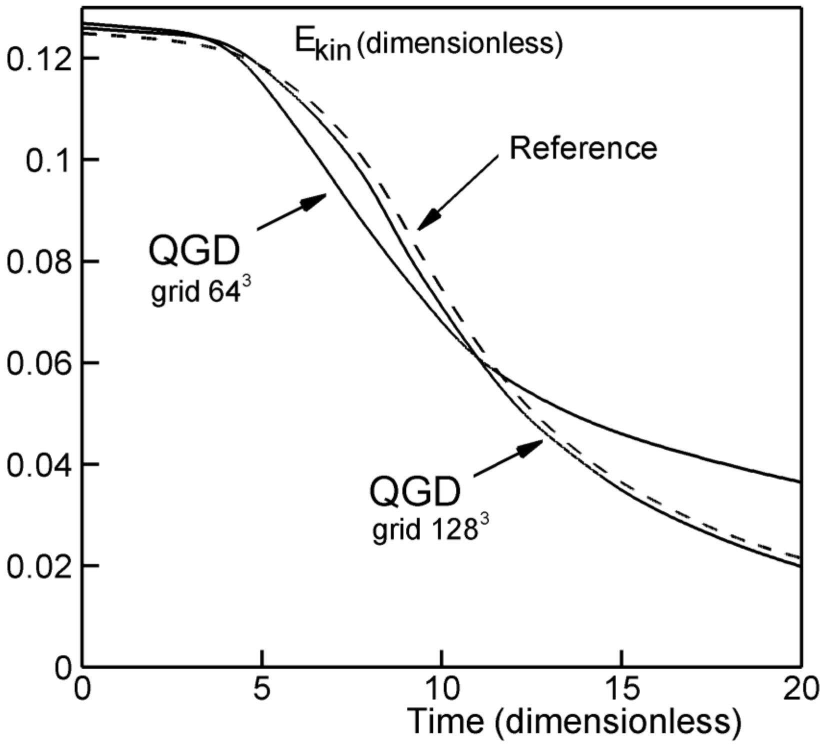
Re=1600, evolution of iso-surfaces of z-component of vorticity

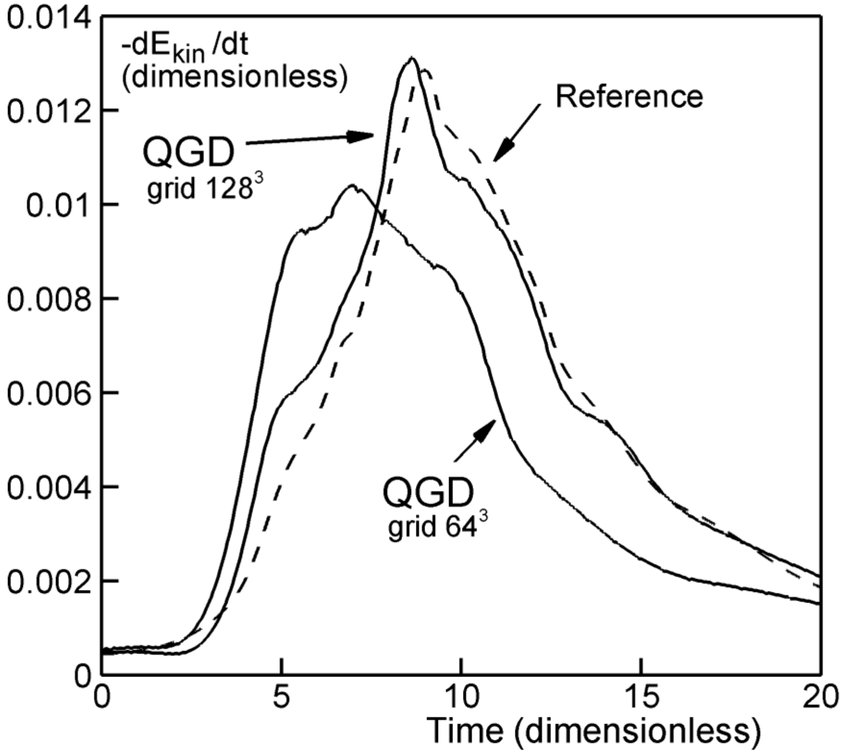
$$Vz = \partial u_y / \partial x - \partial u_x / \partial y$$

$Vz = 0.7$ $\quad Vz = -0.7$

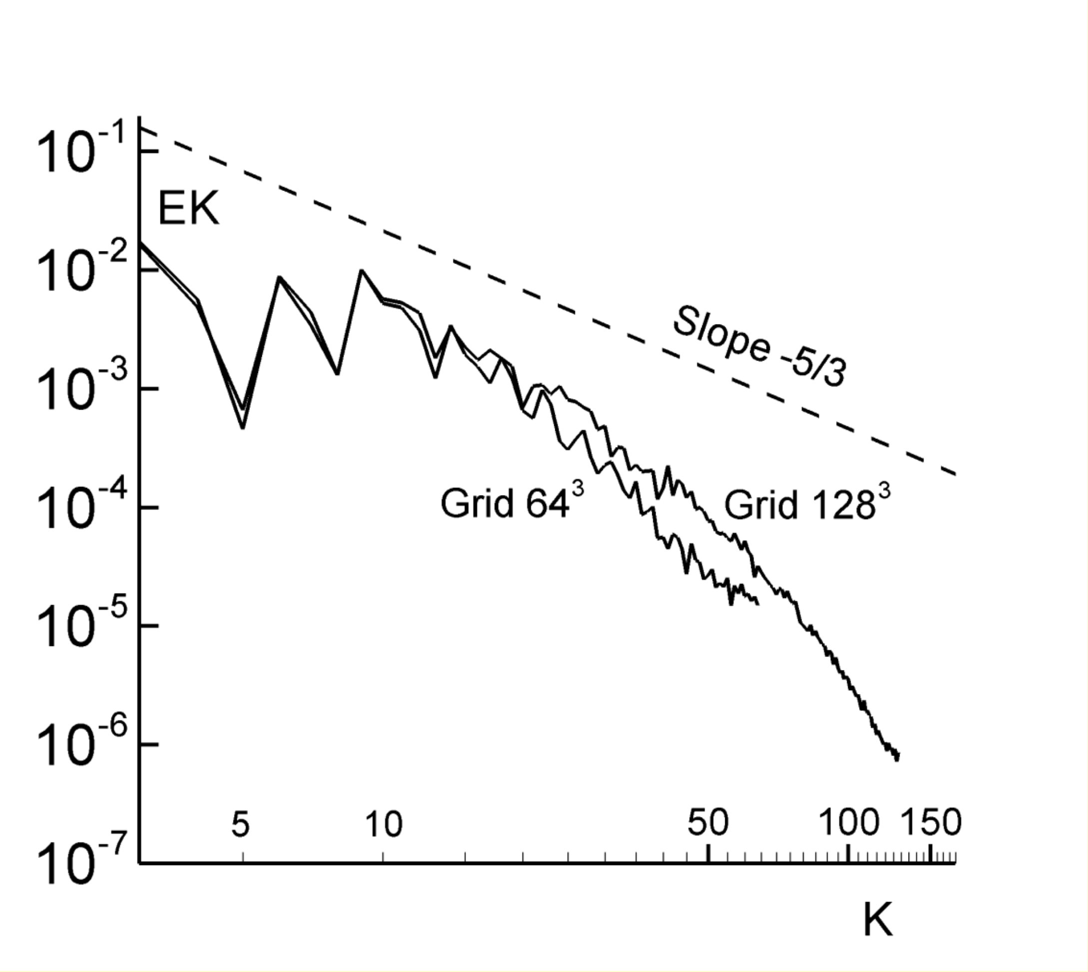


Re=1600, kinetic energy and dissipation rate, grid convergence

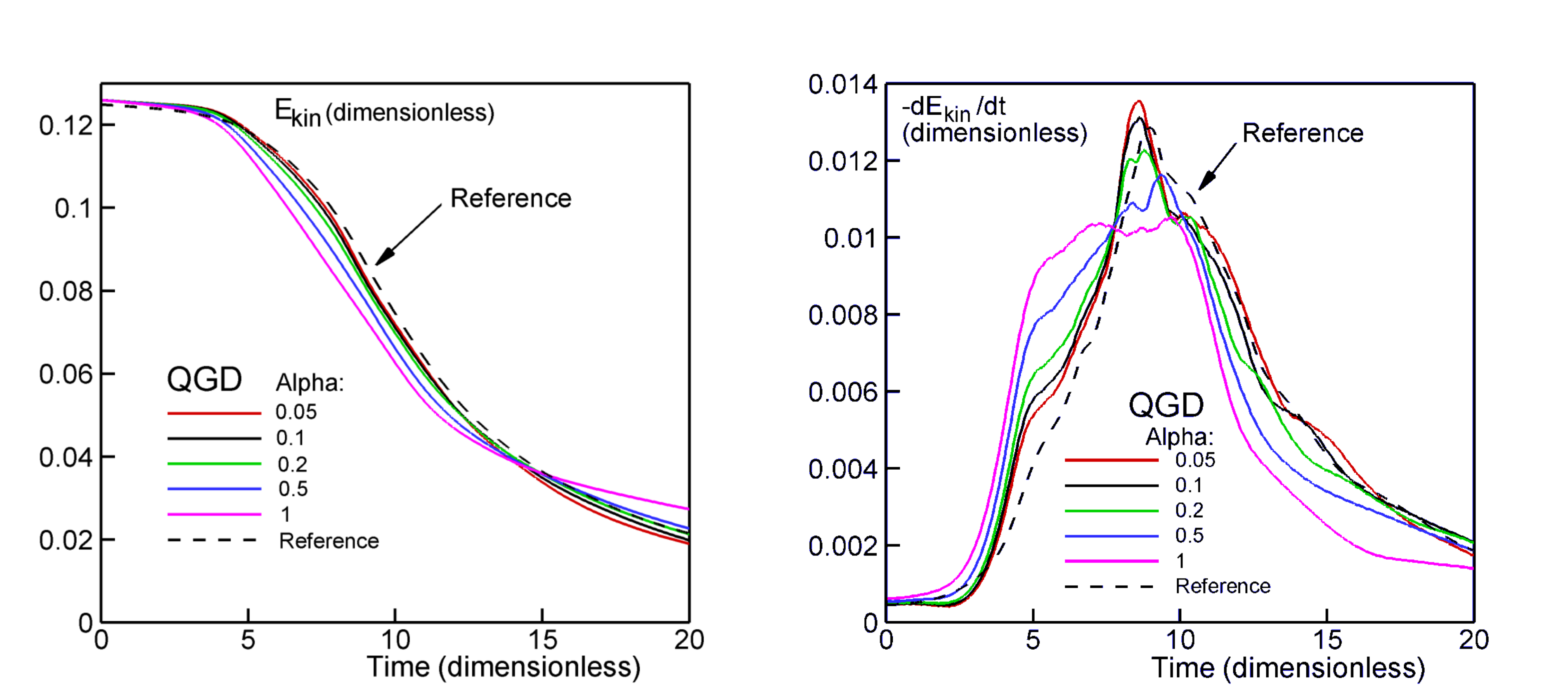




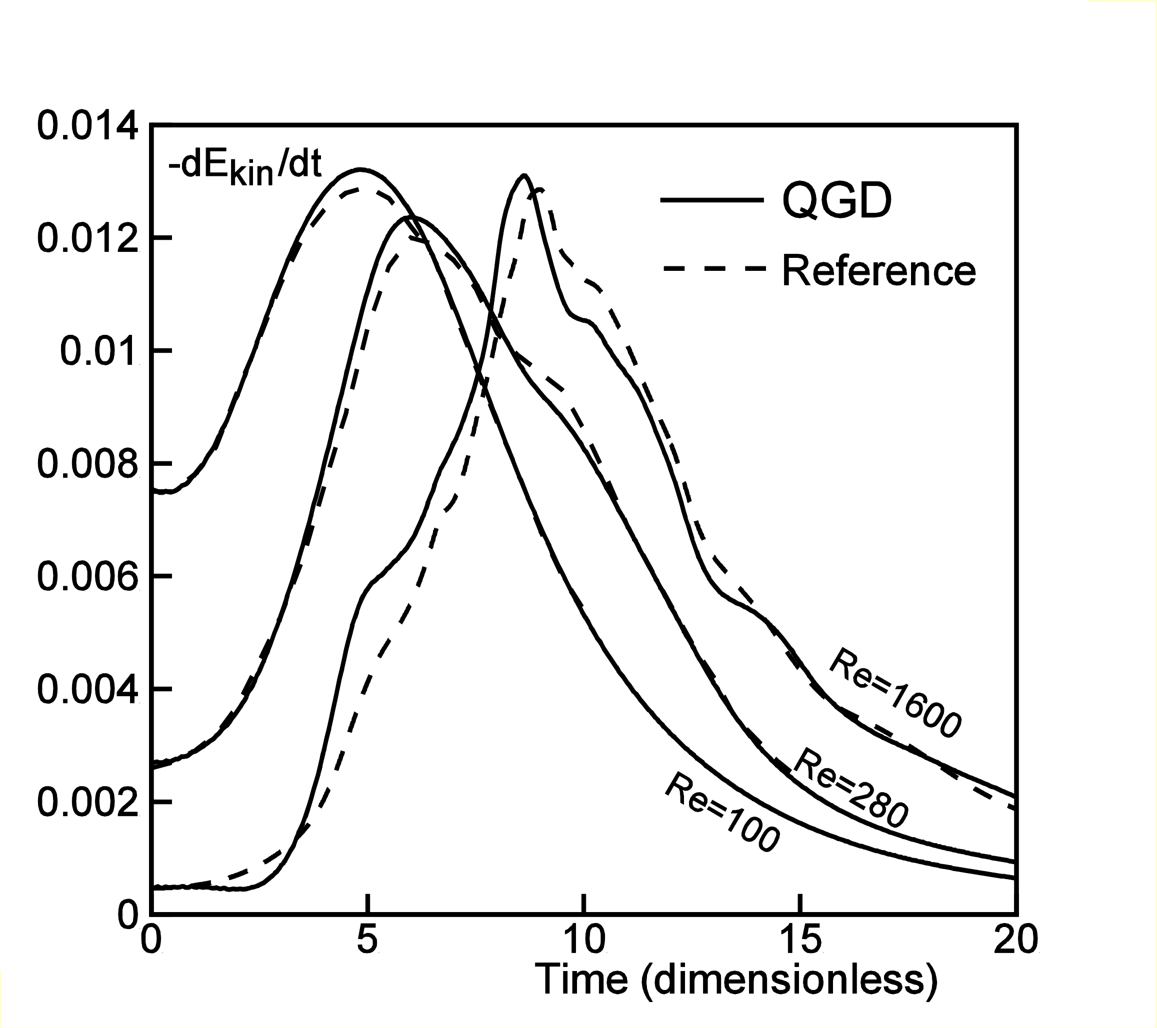
Spectrum of kinetic energy, Kolmogorov-Obukhov law



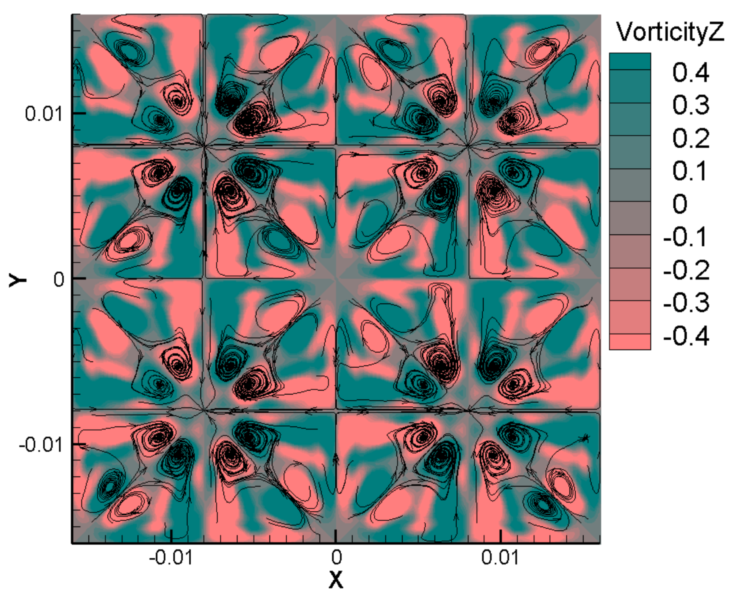
Kinetic energy and dissipation rate, tuning coefficient convergence (Re=1600)

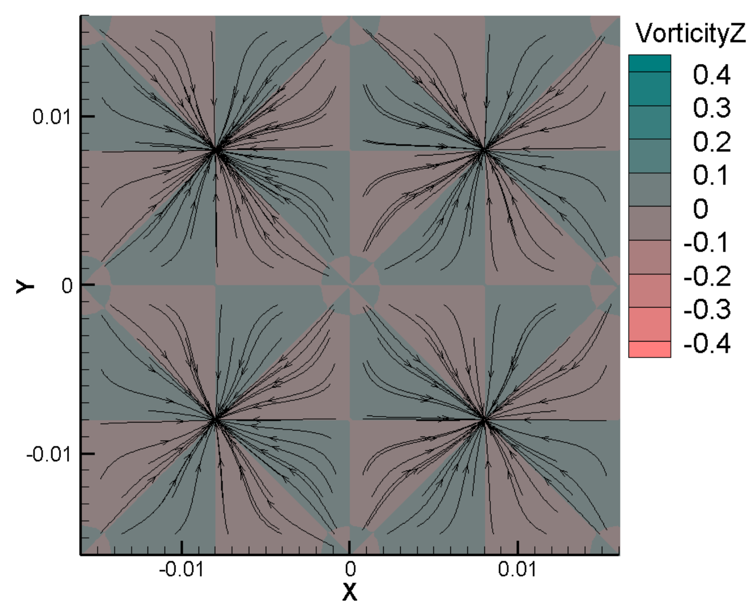


Comparison of dissipation rate evolution for Re=100, 280 and 1600



Symmetry of the numerical solution the conservation of the flow symmetry is related with the conservation of the invariants – helicity (in 3D) and enstropy (2D), that are fundamentaly related with the symmetry of the flow





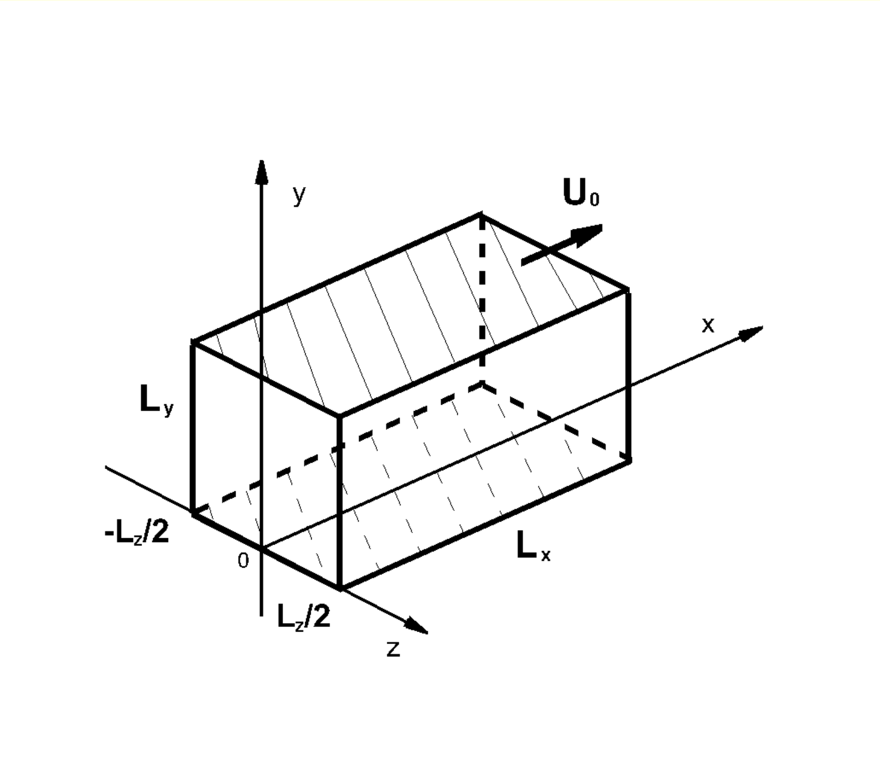
Re=1600 **Re=100**

[1] M. Brachet, D. Meiron, S. Orszag, B. Nickel, R. Morf, U. Frisch.
Small-scale structure of the Taylor-Green vortex. J. Fluid Mech., 1983, vol. 130, pp. 411–452.

[2] Wim M. van Rees, Anthony Leonard, D.I. Pullin, Petros Koumoutsakosa. A comparison of vortex and pseudo-spectral methods for the simulation of periodic vortical flows at high Reynolds numbers. J. of Computational Physics, 2011, vol. 230, pp. 2794–2805

[3] J.B. Chapelier, M. De La Llave Plata, F. Renac, E. Martin. Final abstract for ONERA Taylor-Green DG participation. 1st International Workshop On High-Order CFD Methods. January 7-8, 2012 at the 50th AIAA Aerospace Sciences Meeting, Nashville, Tennessee

Couette flow: problem formulation



Initial conditions

$u_x = U_0 y / L_y$

Initial disturbance: $u_y = u_z = 0.2\ U_0 \sin(8\pi x / L_x)$

$T = T_0 = 273\ K$

p and ρ are defined by Reynolds number

Boundary conditions

Solid walls, $y = 0$: $u_x = u_y = u_z = 0$

$y = L_y$: $u_x = U_0, u_y = u_z = 0$

$$y = 0,\ y = L_y: \begin{cases} \partial p / \partial n = 0 \\ \partial \rho / \partial n = 0 \\ \partial T / \partial n = 0 \end{cases}$$

Periodic boundary conditions in the streamwise (X) and the spanwise (Z) directions

Couette flow, gas-dynamic parameters for nitrogen

$R = 297$ J/(kg·K).	Gas constant
$\gamma = 7/5$	specific heat ratio for nitrogen
$\Pr = 14/19$	Prandtl number
$T_0 = 273$ K	Initial temperature
$\mu = \mu_0 (T / T_0)^{\omega}$	Temperature power-law
$\mu_0 = 1.67 \cdot 10^{-5}$ kg/(m·s)	Viscosity coefficient for $T_0 = 273$
$\omega = 0.74$	Coefficient in temperature power-law
$U_0 = 168.5$ m/s	Velocity of the upper wall
$c_S = \sqrt{\gamma R T}$	Sound velocity
$c_{S0} = \sqrt{\gamma R T_0} = 337$ m/s	Sound velocity for initial conditions
$Ma = U_0 / c_{S0} = 0.5$	Mach number for initial conditions

Couette flow: computational parameters

$L_x = 0.16$ м	Channel length
$L_y = 0.08$ м	Channel height – the distance between solid walls
$L_z = 0.08$ м	Channel width
$N_x = 162$ $N_y = 82$ $N_z = 82$	Space computational grid
$h = 0.001$ м	Computational grid step
$h_t = \beta h / c_{S0} = 5.936 \cdot 10^{-7}$ с	Time step
$\beta = 0.2$	Courant number
$\tau = \alpha h / c_s$	Parameter of relaxation
$\alpha = 0.1$	Tuning coefficient

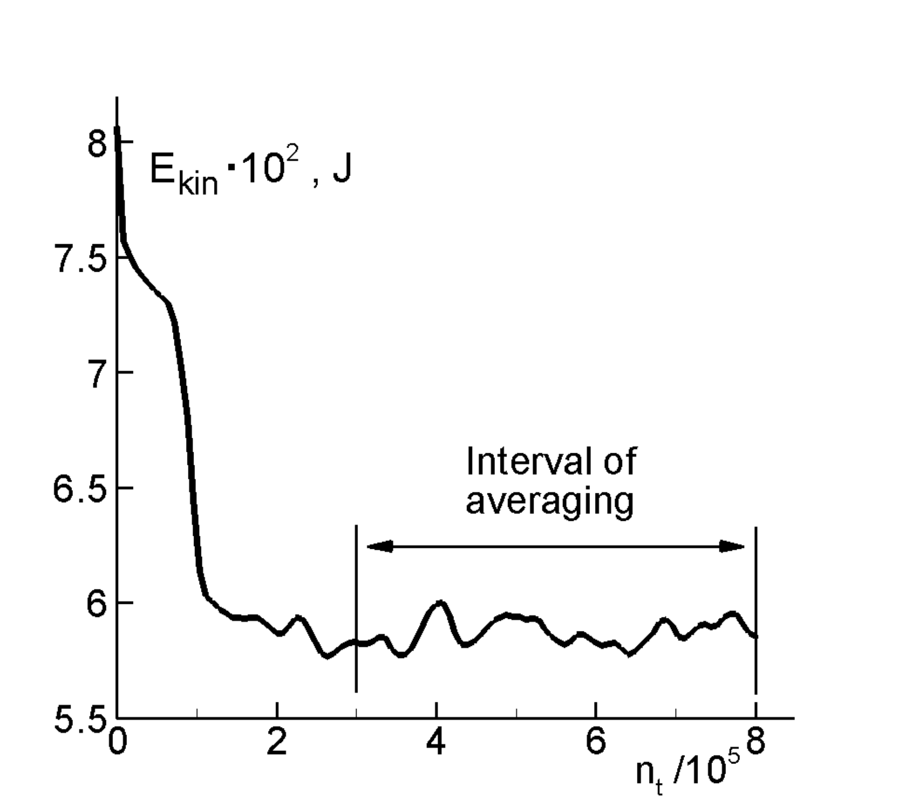
Couette flow: mean (averaged) and friction (wall) values

$\mathrm{Re} = \rho_0 (U_0/2)(L_y/2)/\mu_0$	Reynolds number for initial cond.
$\mathrm{Re}^m = (\rho^m (U_0/2)(L_y/2)/\mu^m)\big\|_{y=0}$	Averaged Reynolds number
$\mathrm{Re}_\tau = (\rho^m u_\tau (L_y/2)/\mu^m)\big\|_{y=0}$	Wall Reynolds number
$\mu^m \quad u_x^m \quad \rho^m$	Time-averaged viscosity, velocity and density
$u_\tau = ((\tau_\omega/\rho^m)^{1/2})\big\|_{y=0}$	Wall velocity
$l_\tau = (\mu^m/(\rho^m u_\tau))\big\|_{y=0}$	Wall length
$\tau_w = (\mu^m (du_x^m/dy))\big\|_{y=0}$	Shear stress on the wall
$u_+ = u_x^m/u_\tau$	Non-dimensional velocity
$y_+ = y/l_\tau$	Non-dimensional (wall) coordinate
$C_f = 2\tau_w/(\rho^m (U_0/2)^2)$	Friction coefficient

Couette flow: laminar and turbulent cases

Regim	Re	Re^m	Re_τ	C_f
Laminar	300	286	17	0.007
Turbulent	3000	2804	153	0.0059
Turbulent	4250	3994	198	0.0049

Turbulent Couette flow, Re=3000: temporal evolution of gas kinetic energy



$$E_{kin}(t)=\sum_{i=1}^{Nx-2}\sum_{j=1}^{Ny-2}\sum_{k=1}^{Nz-2}\frac{1}{2}\rho_{ijk}(t)(u_{x\,ijk}^{2}(t)+$$

$$+u_{y\,ijk}^{2}(t)+u_{z\,ijk}^{2}(t))\cdot h^{3}$$

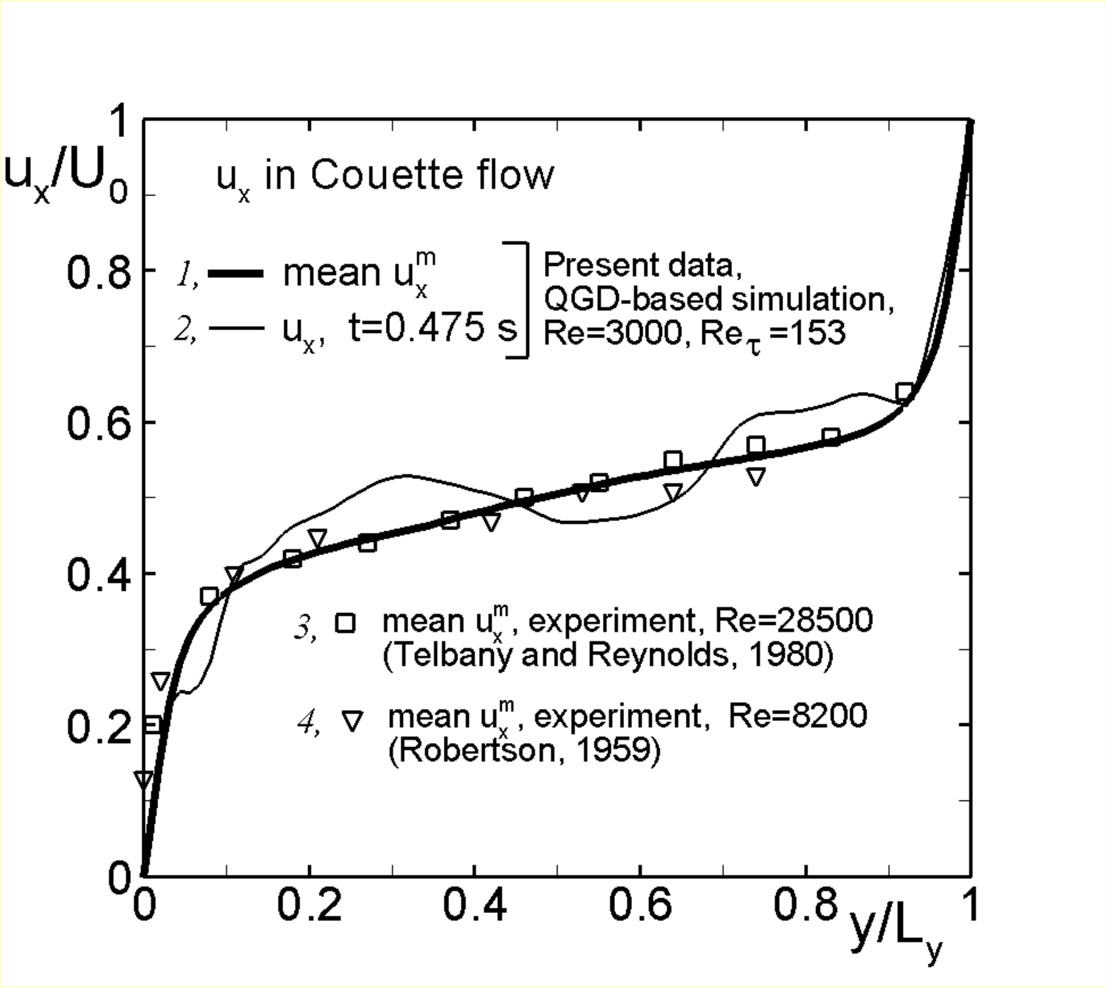
Total number of time steps: $n_t = 8\cdot 10^5$

Total physical time: $t = 0.475\ s$

Total machine time: 160 hours

32 processing nodes of K-100
(Intel Xeon X5670)

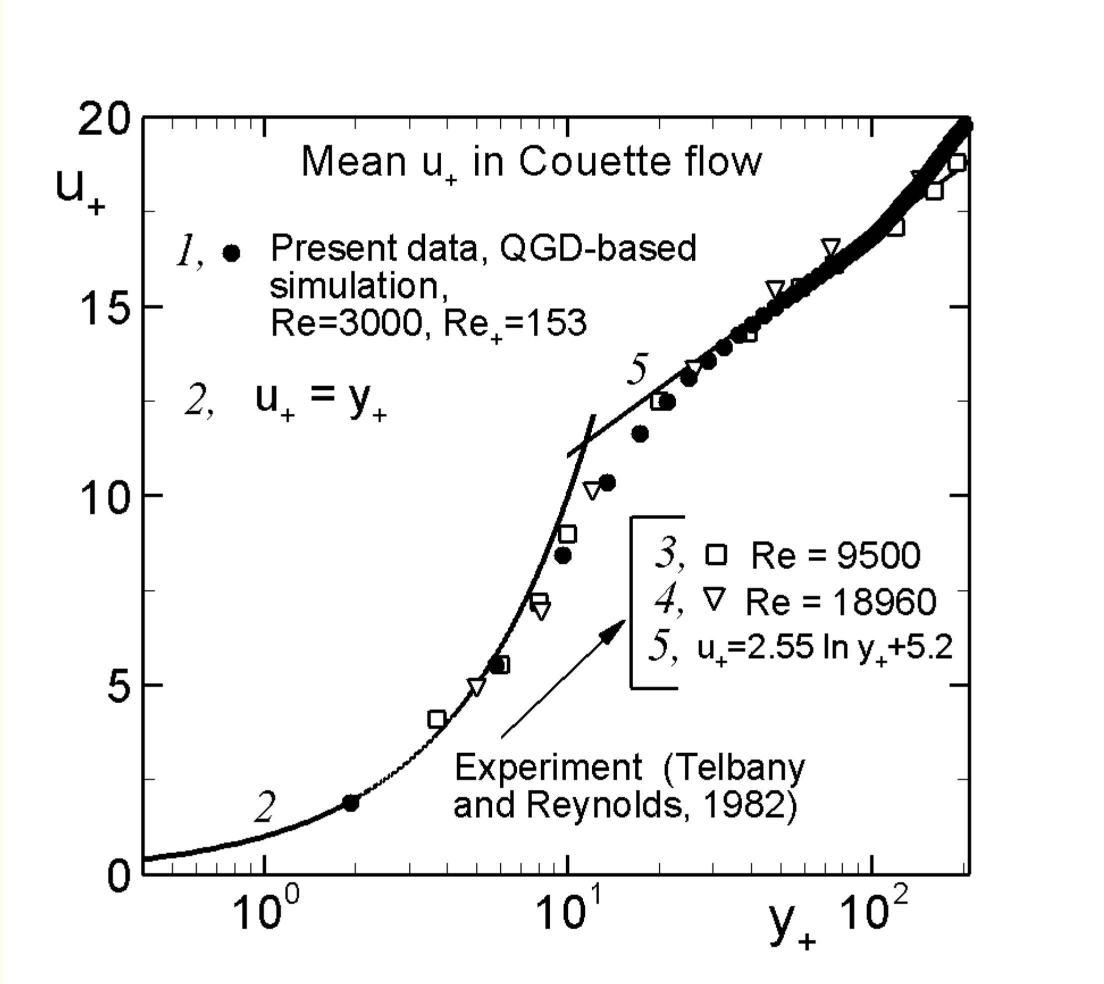
Turbulent Couette flow, Re=3000: downstream velocity profile



Mean downstream velocity:

$$u_x^m = \frac{1}{n_{t2} - n_{t1} + 1} \left(\sum_{n_t = n_{t1}}^{n_{t2}} u_x \right)$$

Turbulent Couette flow, Re=3000: mean downstream velocity profile in wall coordinates



Non-dimensional mean velocity:

$$u_+ = u_x^m / u_\tau$$

Wall friction velocity:

$$u_\tau = ((\tau_w / \rho^m)^{1/2})\Big|_{y=0}$$

Non-dimensional length:

$$y_+ = y / l_\tau$$

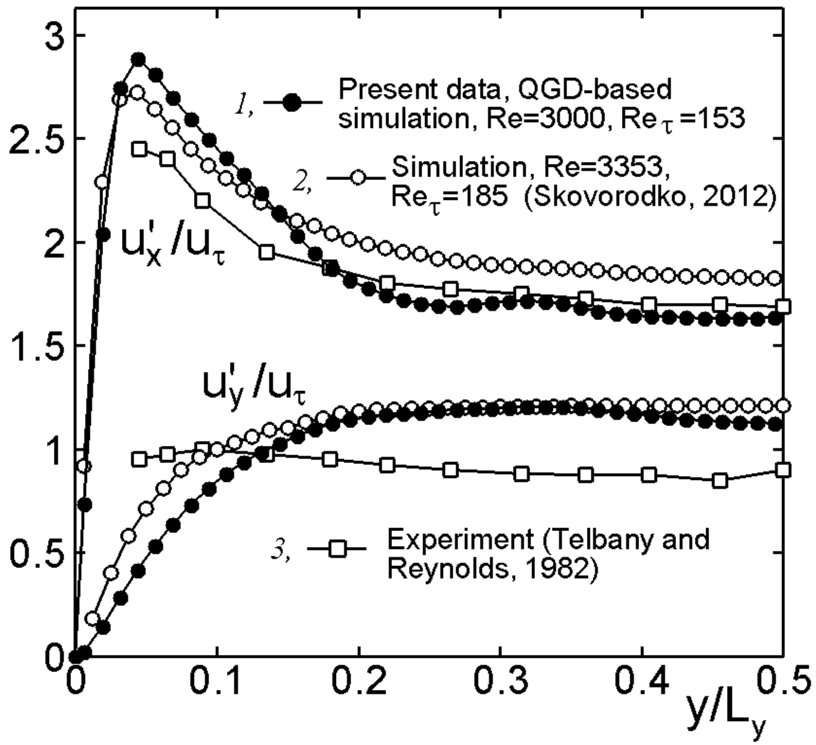
Wall friction length:

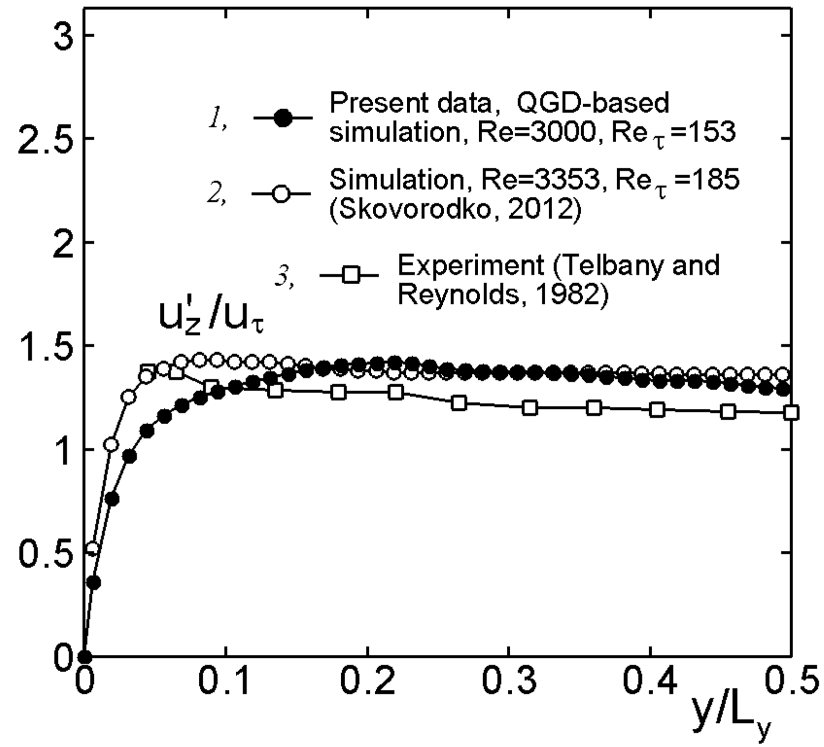
$$l_\tau = (\mu^m / (\rho^m u_\tau))\Big|_{y=0}$$

Shear stress on the wall:

$$\tau_w = (\mu^m (du_x^m / dy))\Big|_{y=0}$$

Turbulent Couette flow, Re=3000: turbulence intencities

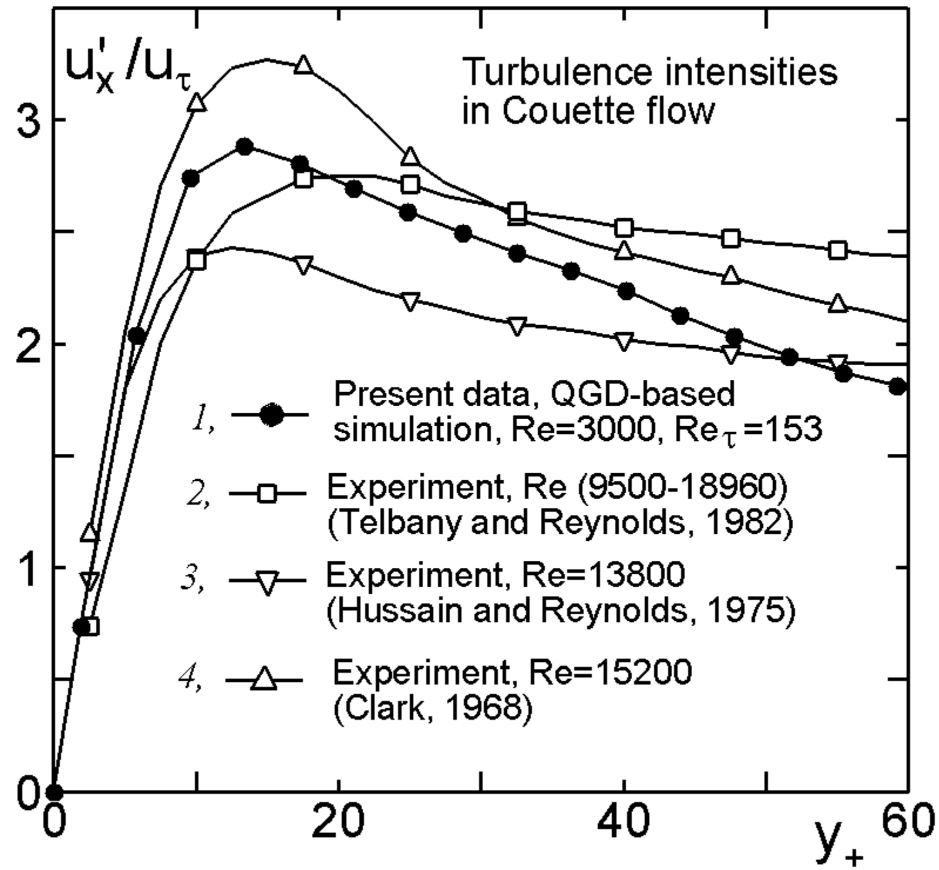




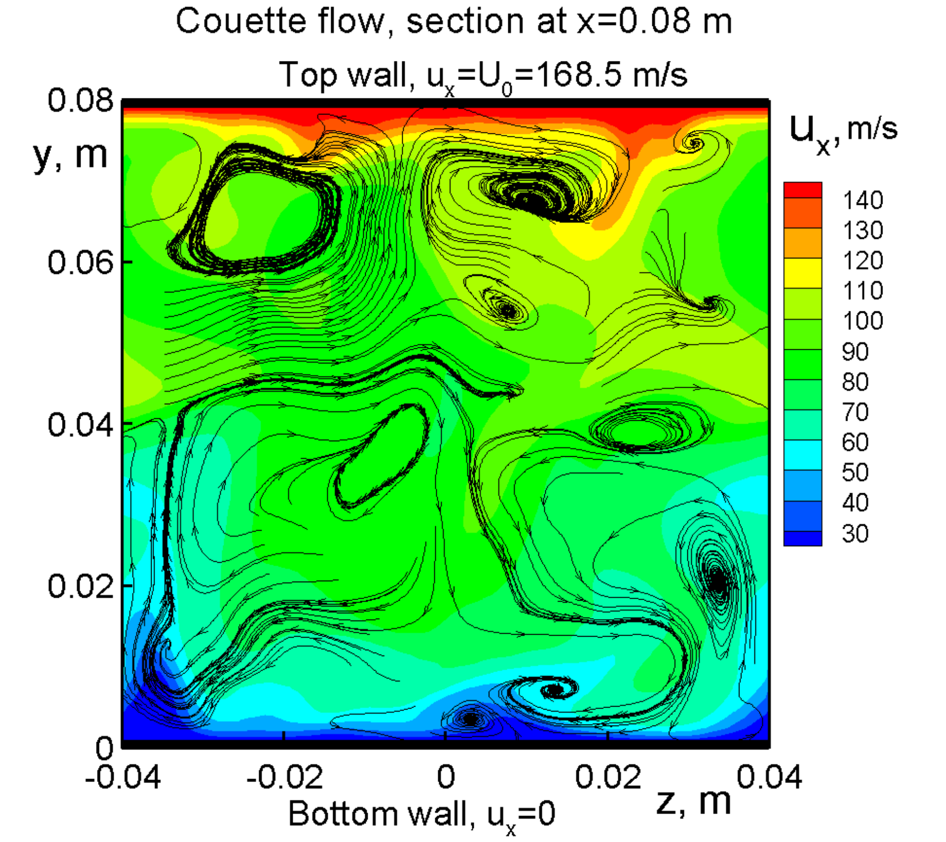
$$u'_x = \left[\frac{1}{n_{t2} - n_{t1} + 1} \left(\sum_{n_t = n_{t1}}^{n_{t2}} u_x^2 \right) - (u_x^m)^2 \right]^{1/2}$$

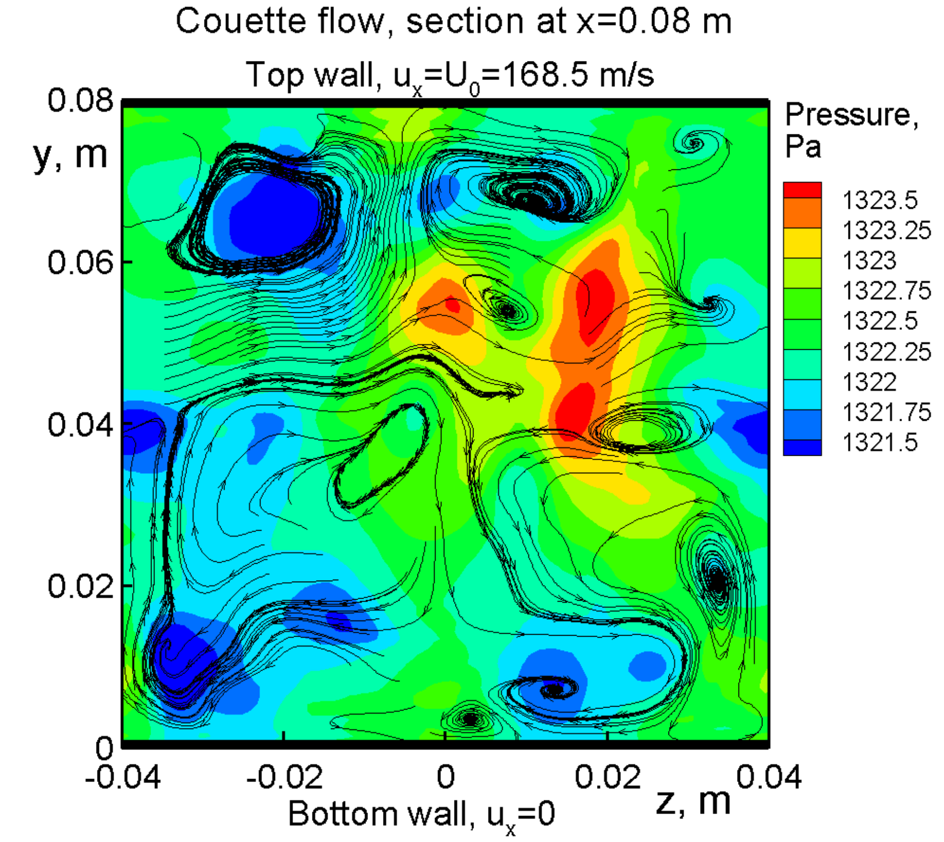
, same for u'_y and u'_z

Turbulent Couette flow, Re=3000: turbulence intencities, wall coordinate

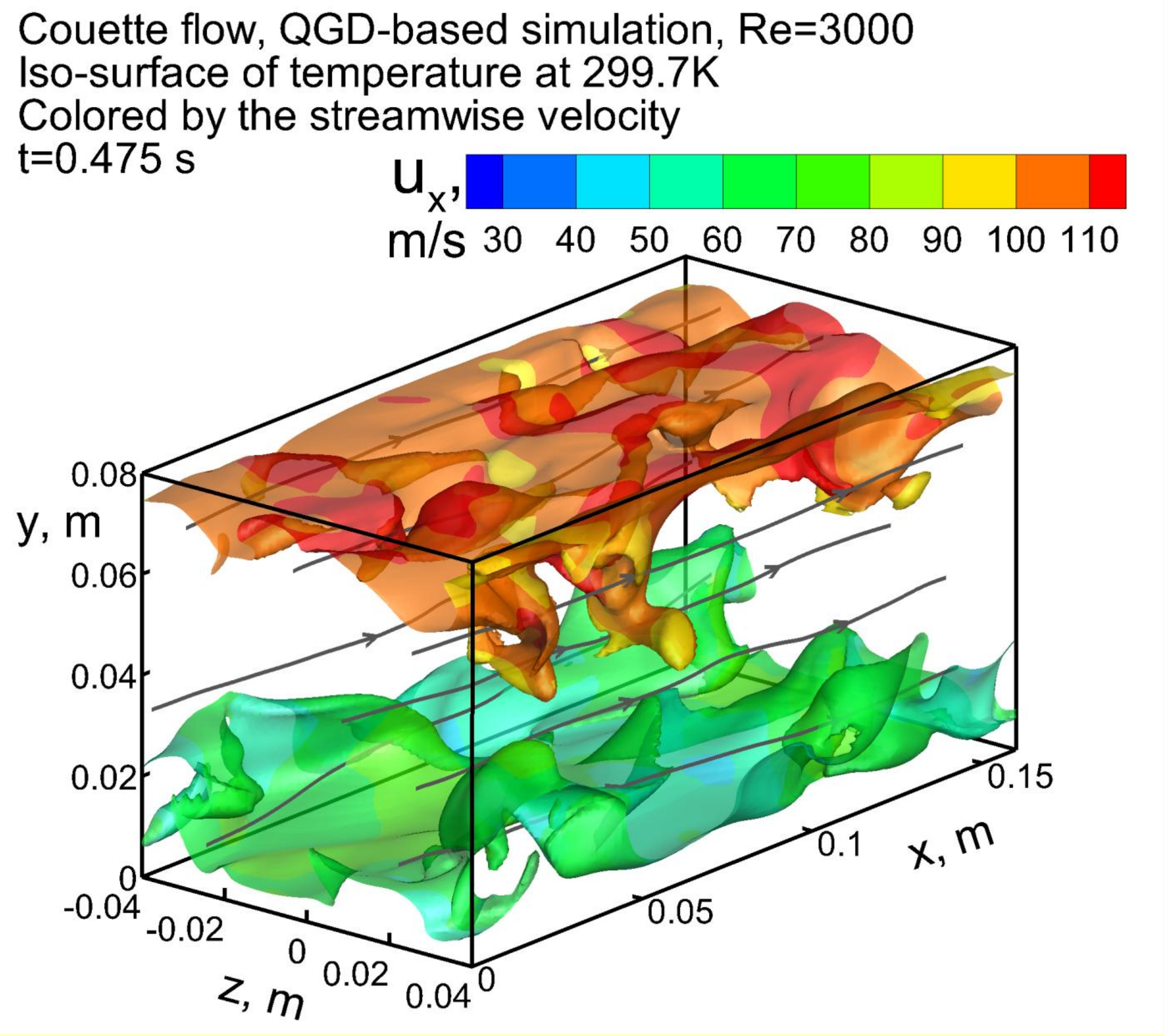


Turbulent Couette flow, Re=3000:
2D cross-section in the middle of domain, downstream velocity and pressure contours, cross velocity streamlines

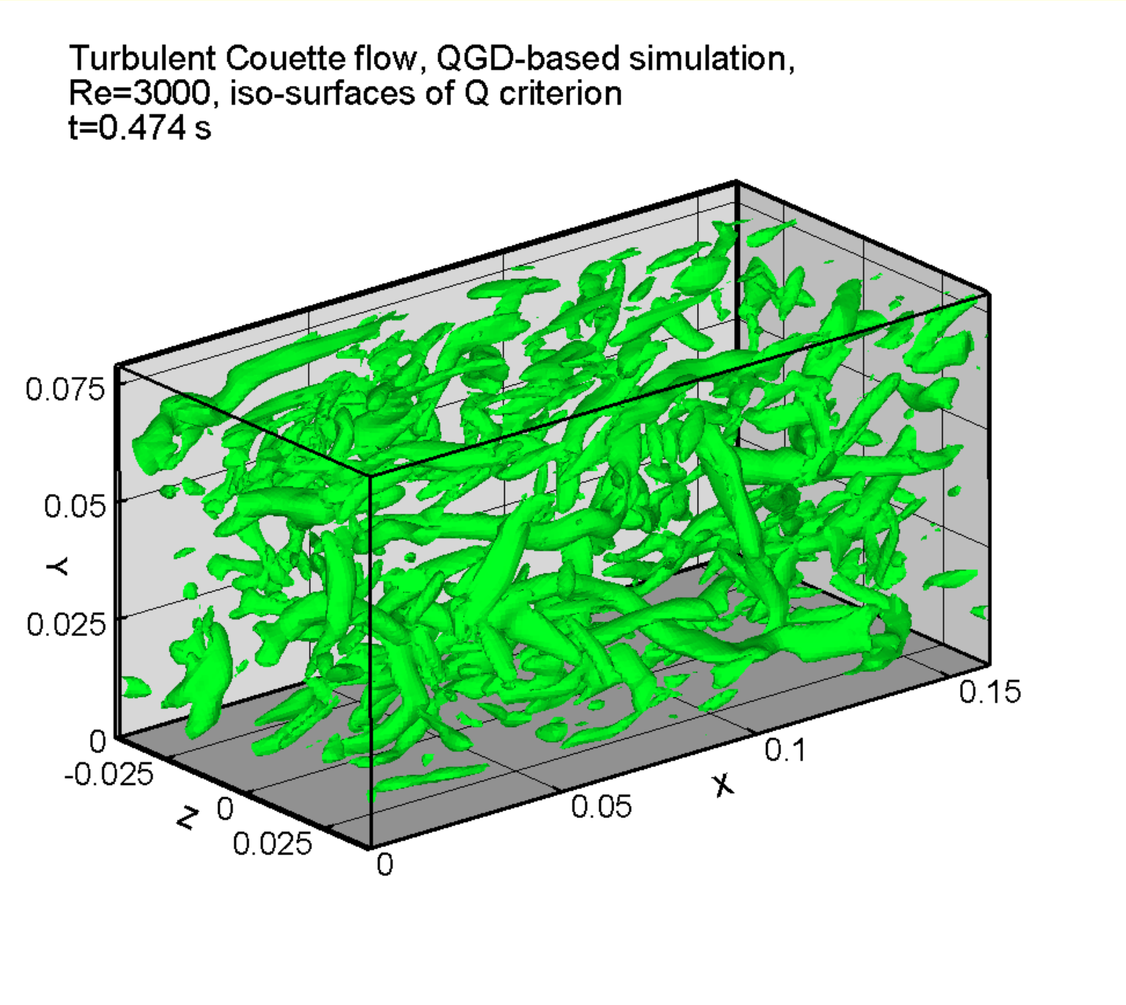




Turbulent Couette flow, Re=3000



Turbulent Couette flow: coherent vortices

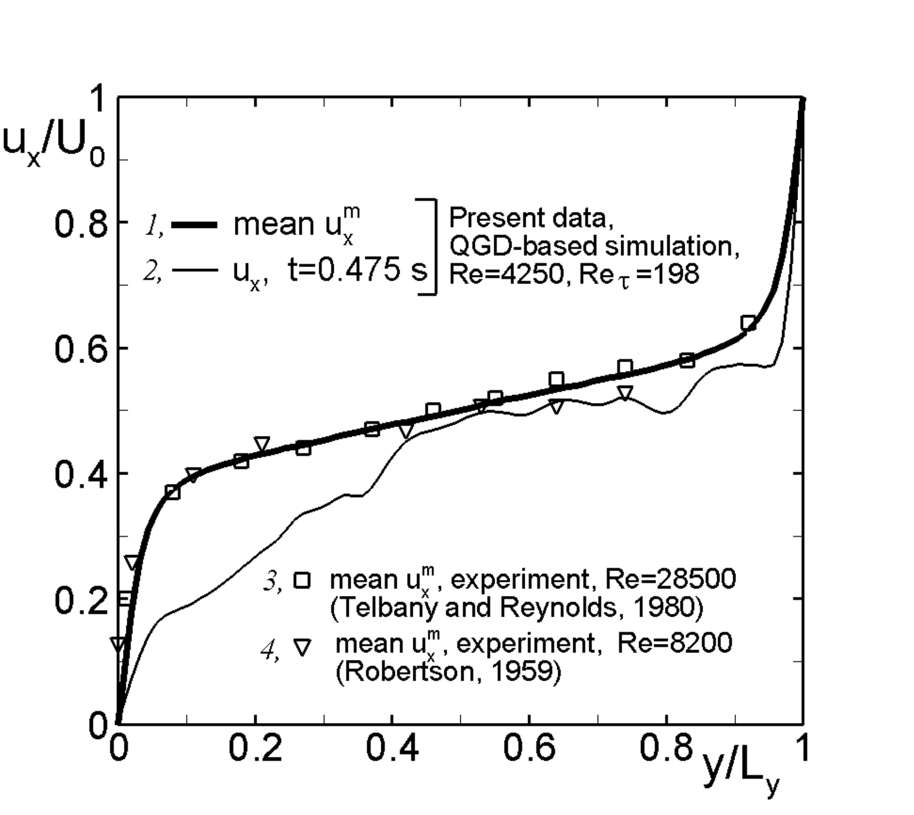


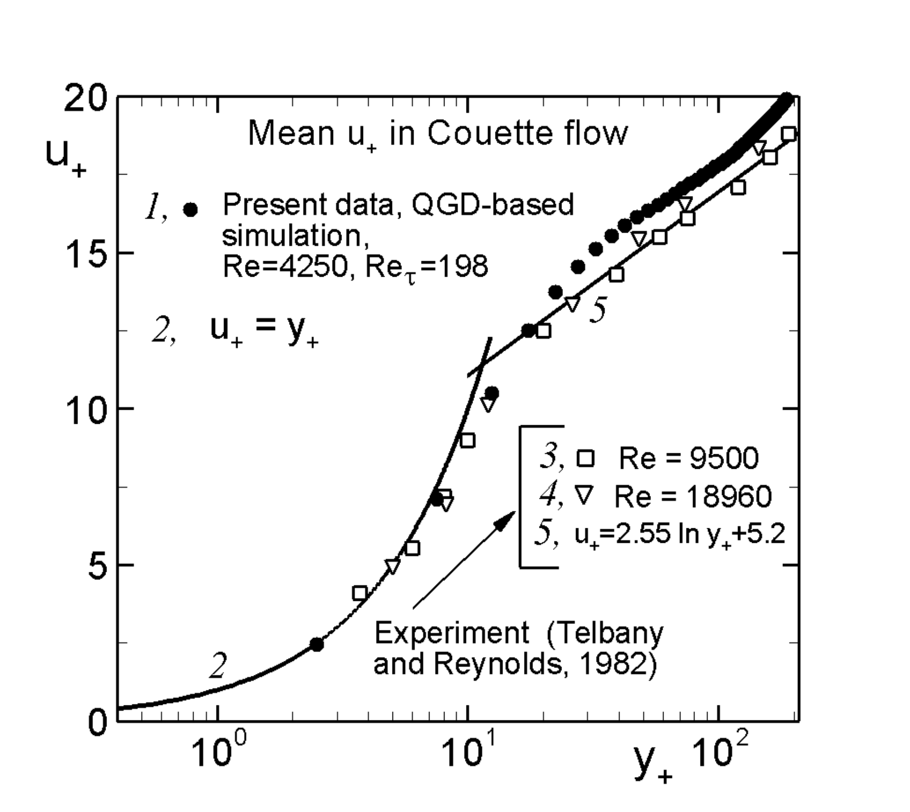
Coherent vortices are visualized by the Q criterion:

$$Q = \frac{1}{2}(\Omega_{ij}\Omega_{ij} - S_{ij}S_{ij})$$

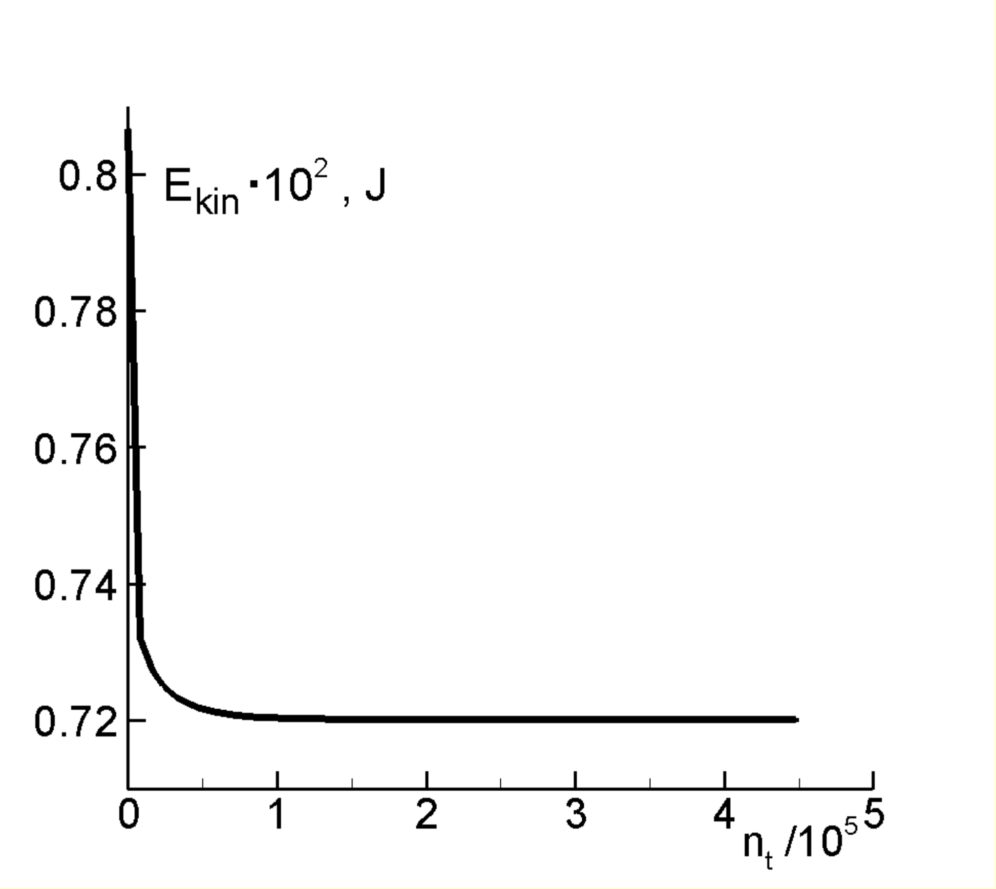
S_{ij} and Ω_{ij} are respectively the symmetric and antisymmetric parts of the velocity-gradient tensor $\partial u_i / \partial x_j$

Turbulent Couette flow, Re=4250: downstream velocity profiles

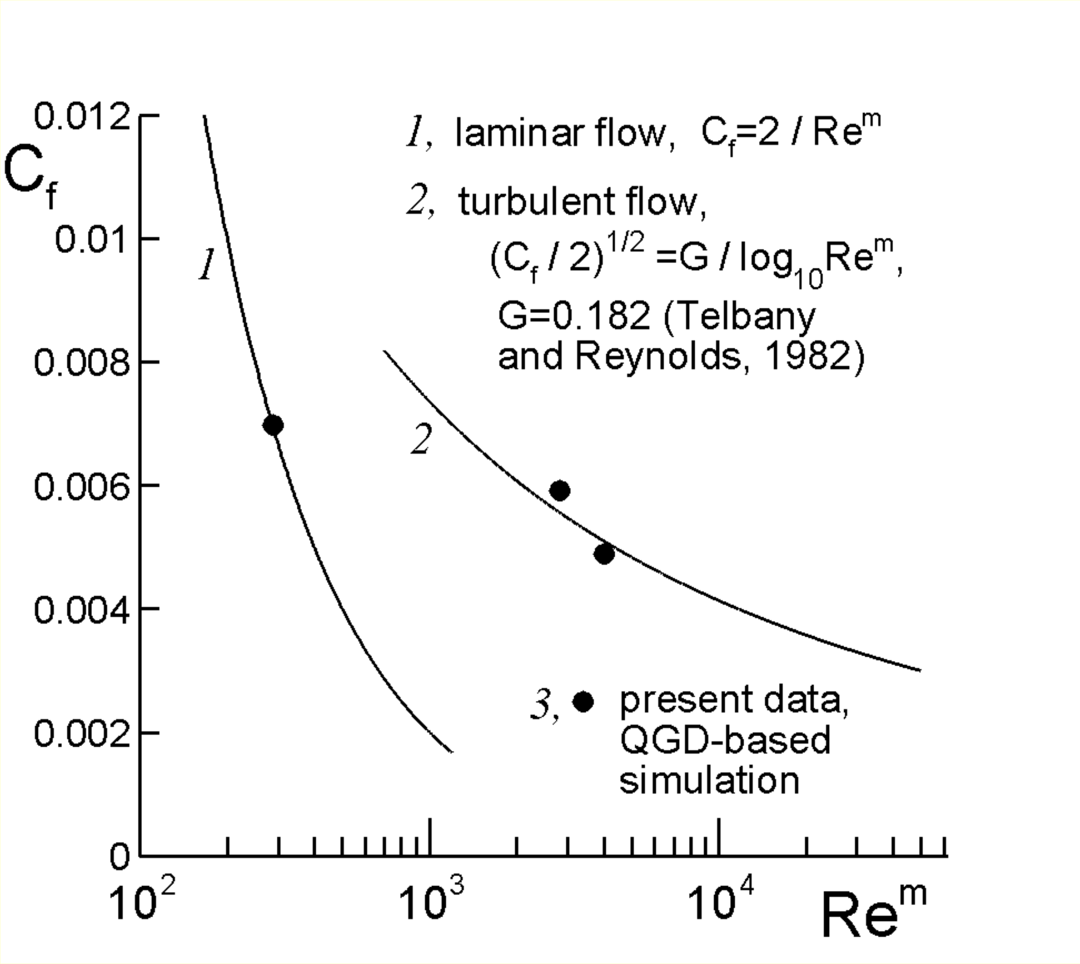




Laminar Couette flow, Re=300:
temporal evolution of gas kinetic energy



Couette flow: skin-friction coefficient as a function of mean Reynolds number



Mean Reynolds number:

$$\mathrm{Re}^m = (\rho^m (U_0/2)(L_y/2)/\mu^m)\big|_{y=0}$$

Skin-friction coefficient:

$$C_f = 2\tau_w/(\rho^m (U_0/2)^2)$$

Shear stress on the wall:

$$\tau_w = (\mu^m (du_x^m/dy))\big|_{y=0}$$

Conclusions

Quasi gas-dynamic (QGD) equations may be regarded as a new approach in simulation of turbulent gas dynamic flows.

The additional dissipative terms in QGD system serve to model the effects of the unresolved subgrid scales.

QGD system provides a uniform simulation of laminar and turbulent regimes in free-stream flows and near-boundary flows.