HPC & CFD a personal perspective from the origin up to nowdays

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Motivations for CFD

- Lecture based on incompressible flows
 - Solve non-linear equations
 - Euler inviscid
 - Navier-Stokes viscous
- Atmosphere NCAR
- Nuclear Los Alamos
- Finite differences (easy)
- In the 70th psudospectral (complex)
- Finite elements complex geometries
- From continuous to discrete space
- Compact operators staggered variables
- High Reynolds conservation properties

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- Absence of teaching in 60th and 70th
- Few groups
- Torino (compressible) linked to Moretti
- Roma (incompressible) isolated
- Bari (compressible and incompressible)
 - Laminar 2D flows no HPC
 - Attempts to turbulence RANS
 - No classes in turbulence
 - Absence of interaction among groups
 - Absence of contacts with foreign groups

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CFD in the world

- HPC available at NCAR, NASA, Los Alamos ...
- England Germany RANS
- France spectral closures
 - CFD for LES and DNS
 - Large use of pseudospectral (Orszag)
 - Competition MIT (Orszag) Stanford, NASA (Reynolds)
- Luck to be in Stanford, NASA for one year
- Moin, Kim, Mansour ... Ph.D students
- Rogallo , Wray, researchers
- I learnt and enjoyed the physics of turbulence
- For lack of HPC in Italy I worked on RANS
- In 1981 I attended the OLYMPIC in turbulence

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- RANS unable to be universal
- An efficient interpolation scheme (several constants)
- Unsatisfactory to homogeneous turbulence
- At the Stanford OLYMPICS Rogallo presented
- 128³ DNS homogeneous turbulence
- Possible with ILLIAC IV
- Vectoral compiler (Rogallo Wray)
- Decrease interest in LES (constant adjustable)

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Stanford cultural revolution

Proof N-S solves turbulence

A Simulation Milestone

Until around 1980, few researchers attempted to simulate even very simple turbulent flows in their entirety. That year we and our co-workers at the NASA Ames Research Center used a pioneering parallel computer, the ILLIAC-IV, to perform the largest turbulence simulations achieved until then. The work was well received; soberingly enough, however, it was not the

quality of the data that won over many of our colleagues but rather a five-minute motion picture of the simulated flow. The movie showed trajectories of marker particles in a turbulent flow between parallel plates (*left*); remarkably, it resembled similar visualizations made two decades earlier, by filming actual water flow in a laboratory at Stanford University (*inft*). — *PM*, and *JK*.

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- For lack of HPC in Italy I did not enter in LES or DNS
- Frustration to play with constants
- Impossibility to enter in RANS community (England Germany)
- Crocco offered me to enjoy spectral closures
- Crocco transformation for EDQNM
- Difficulty to apply spectral to homogeneous flows
- Crocco died 1985
- From this I learnt physics of turbulence

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CFD of flows past complex geometries

- With Cunsolo N-S in general curvilinear coordinates (2D)
- Flow past airfoil (1977)
- Flow in a 2D elbow

$$\frac{\partial \omega}{\partial t} + \frac{1}{\sqrt{a}} \frac{\partial q^{i} \omega}{\partial x_{i}} = \frac{1}{Re} \frac{1}{\sqrt{a}} \left(\frac{\partial}{\partial x_{k}} \alpha^{kl} \frac{\partial \omega}{\partial x_{l}} \right)$$
$$q^{1} = \frac{\partial \psi}{\partial x_{2}} , \quad q^{2} = -\frac{\partial \psi}{\partial x_{1}}$$
$$\omega = -\frac{1}{\sqrt{a}} \left(\frac{\partial}{\partial x_{k}} \alpha^{kl} \frac{\partial \psi}{\partial x_{l}} \right)$$

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Flow in a 2D elbow



Fig. 2 Steady state stream function at Re = 1,000; elbow having a nondimensional internal radius equal to 1 (a) and equal to 0.5 (b)

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Complex boundaries

- NASA was interested in drag reduction by riblets
- Invited me to spend summers to develop
- 3D code for flows past complex 2D bodies
- Four years struggling with iterative methods
- General curvilinear coordinates
- The code was later on used by several scholars at the CTR
- I was again frustrated
- In Stanford by pseudospectral DNS of
- Channel KMM
- Minimal channel Jimenez
- Boundary layers Spalart
- Mixing layers Moser Rogers
- Wakes Rogers Moser
- Was the center of the world for turbulence
- Moin and Reynolds created the Center for Turbulence
 Research

Vortex dynamics

- In Roma interaction with Carnevale and van Heijst
- 2D dipole rebound Orlandi rebound
- Physics of Fluids A 1990 218 citations



FIG. 5. Flow visualization of experiment in Ref. 4 compared with the contour plot of vorticity of numerical simulation.

Dipole and walls



Cylindrical coordinates

- The frustration with iterative schemes
- The use of FFT to solve elliptic equations
- The interest for vortex rings
- The use of staggered variables
- The trick to treat the geometrical singularity at r = 0
- Good students (Verzicco, Fatica)

JOURNAL OF COMPUTATIONAL PHYSICS 123, 402–414 (1996) ARTICLE NO. 0033

A Finite-Difference Scheme for Three-Dimensional Incompressible Flows in Cylindrical Coordinates

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Use of cylindrical coordinates

- Large number citations of JCP 496
- Today adapted to HPC
- Turbulent rotating pipe
- 3D tripole formation
- Stability vortex rings
- Vortex rings interacting walls
- DNS of transitional circular jets
- Thermal convection in cylindrical cells
- Drag reduction turbulent MHD pipes
- Code available in
- Fluid Flow Phenomena: a numerical toolkit

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Comments of finite differences

- Widely accepted for cylindrical
- Criticised several paper rejected
- Large effort for validation
- Spectral and finite difference solutions of the Burgers equation
- Isotropic turbulence decay
- Statistics of KMM and Jimenez channel
- Time-reversibility of the Euler equations
- Turbulent channel flow simulations in convecting reference frames
- Appreciated
- More paper accepted

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Burgers equation

Computers & Fluids \/nl 14 Nn l nn 23-41 1986

Table 3. Maximum absolute value of the slope at the origin and time t_{max} at which this maximum value occurs for all the numerical algorithms and for the analytical solution.

Method	Interval	lau laxi max	π•t _{max}	N/M	Δt·π
- Fourier Galerkin	[-1,1]	151.942	1.6035	682/1024	5.10-4
		142.665	1.60	682/1024	10-2
		148.975	1.603	170/256	5.10-4
		142.313	1.60	170/256	10-2
-Fourier Pseudospectral	[-1,1]	142.606	1.60	256/256	10-2
		144.237	1.60	128/128	10-2
- ABCN collocation	[-1,1]	145.877	1.60	512	5.10-3
+coordinate transform.	[-1,1]	152.123	1.60	64	10-2
Spectral Element	[-1,1]	152.04	1.6033	16 x 4	10 ⁻² /6
PD	[-1,1]	150.1	1.63	81	10-2
Chebyshev					
ABCN spectral	[0,1]	152.05	1.60	64	1/300
Rosenbrock spectral	[0,1]	151.998	1.60	64	10-2
	[0,1]	150.144	1.60	32	10-2
ABCN collocation	{0,1}	152.126	1.60	64	10-2
Analytical		152.00516	1.6037		
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• FFP (Pg.160)



Fig. 8.5 Time history of \mathcal{E} and Ω for finite difference symbols and pseudospectral (Wray) lines; b) Energy spectra (Kolmogorov units) at moderate Reynolds number, —— initial spectrum, —— present simulation $R_{\lambda} = 54.3$, …… Mansour & Wray $R_{\lambda} = 56.2$, \square Compte Bellot & Corrsin $R_{\lambda} = 60.7$

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Validation turbulent channel vorticity rms

- Results for $R_{\tau} = 900$
- Comparison with pseudospectral DNS by Jimenez's group



Improvement turbulent channel

Laboratory and convective frame Bernardini (JCP 2012)



Small effect on the statistics profiles

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Inviscid Energy Conservation

- Resolution 96³
- Time reversibility forward up to t = 10

• At
$$t = 20 V(20, X) = V(0, X)$$

• Isosurface of $\lambda_2 = -0.025$



t = 0 t = 10 t = 20 t = 20

Validation inviscid

- Comparison for unresolved Taylor Green Duponchel et al. (2008)
- Comparison FD2, FD4, Pseudospectral



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Numerics on FTS Taylor-Green

- Pseudospectral Cichowlas & Brachet (2006)
- Pile-up can be eliminated by exponential filters (Hou & Li)
- Second order finite difference FD2 Orlandi & Carnevale (2008)
- Simulations at 256³ and 512³



t = 3.5 t = 4.0

FTS Taylor-Green E(k) t = 4.5



● FD2 symbols 512 lines 1024 4.0 < *t* < 4.5 black *t* = 4.35

By FD2 YES but difficult to establish

• whether for
$$t \to t_s$$
, $\delta(t) \to 0$

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Cartesian HPC FD for Clay prize

- Finite Time Singularity from smooth I.C.
 - Euler equations
 - Navier-Stokes equations
- Transition from Vortex Dynamics to Turbulence
- Link between Vortical Structures and
- Power Spectra
- Give insights to mathematician to prove
- Existence of FTS
- Insert passive scalar
- Look at the difference between
 - Energy and scalar spectra
 - Vortical and scalar structures

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Euler

- FTS does exist if
- $|\omega|_{max} \propto (t_{
 m s}-t)^{-1}$
- $E(k) \propto k^{-3}$ at t_s infinite enstrophy
- other requirements in Kerr (2006)
 - I.C. and numerics important
 - Lamb dipoles Orlandi & Carnevale (2008)

•
$$t = 0 E(k) = k^{-6}$$

- Lamb vortex solution Euler
- for $t \to t_s$, $|\omega|_{max} \propto |\widetilde{\omega}_2|_{max}$, $\widetilde{\omega}_2 \propto S_2$

•
$$\frac{\partial \widetilde{\omega}_2}{\partial t} = \mathbf{S}_2 \widetilde{\omega}_2 = \widetilde{\omega}_2^2$$

- Having a FTS
- Close to FTS investigate
- Differences in the spectra between scalars and velocity
- Differences in the structures

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- FTS does not exist
- Interest to understand
- Turbulence from Vortex Dynamics
- Evolution of energy spectrum
- Different from forced DNS
- Evolution of spectra and tendency to equilibrium range

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Inviscid energy spectra

10 1 0.1 0.01 t=2.75 0.001 t=0t=0.05 0.0001 t=1 t=1.5 1e-05 t=2.0 t=2.5 1e-06 10 100 1000 k

 $E(k)k^3$

• 2048³

Profs of FTS easier for persistence k⁻ⁿ up to t_s

Inviscid Scalar spectra



 $E_{\theta}(k)k^2$

• 2048³

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Viscous Flows

- Energy $q = \langle u_i^2 \rangle$ equation
- $\frac{\partial q}{\partial t} = \frac{\Omega}{Re}$
 - Kolmogorov at large $t \ q \propto t^{-m}$
 - m does not depend on ν
 - If Re increases Ω increases
- Enstrophy equation

•
$$\frac{\partial\Omega}{\partial t} = P_{\Omega} - \frac{D_{\Omega}}{Re}$$

- D_{Ω}/Re rate enstrophy dissipation
- $D_{\Omega}/Re = \langle (\frac{\partial \omega}{\partial x_i})^2 \rangle/Re; P_{\Omega} = \langle \omega_i \omega_j S_{ij} \rangle$
 - Opposite effects of P_{Ω} and D_{Ω}/Re
 - However at high Re initially P_{Ω} strong
 - To create Ω at intermediate scales
 - Later on D_{Ω}/Re grows preventing FTS
- Scalar equation

•
$$\frac{\partial \theta_l}{\partial t} + \frac{\partial u_i \theta_l}{\partial x_i} = \frac{1}{RePr} \frac{\partial^2 \theta_l}{\partial x_i^2}$$

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Enstrophy evolution



- For *t* < 1 Ω = *const*
- For 1.8 < *t* < 2.4 exp. growth
- For 2.6 < t < 2.7 FTS for ν = 0</p>
- For $\nu \neq 0$ there is Ω_{max} tendency
- FTS Impossible to prove by DNS

Enstrophy production

•
$$\frac{\partial\Omega}{\partial t} = \langle \omega_i \omega_j S_{ij} \rangle + \frac{1}{Re} \langle \omega_i \nabla^2 \omega_i \rangle, \quad P_{\Omega} = \langle \omega_i \omega_j S_{ij} \rangle$$

• $\tilde{P}_{\Omega I} = \tilde{\omega}_I^2 \tilde{S}_I$



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Spectra and Structures

- Inviscid t = 2.75 filtered 1536^3
- Viscous *t* = 3.0 *Re* = 10000 1024³ , *Re* = 2500 768³



Spectra and Structures from Vortex to Turbulence

• t = 3.0 t = 3.5 t = 4.0



t = 4.5

t = 5.0



Scalar gradient variance and enstrophy evolution

- Scalar dissipation $\chi = <(\frac{\partial \theta}{\partial x_i})^2 > = < G_i^2 >$
- $\frac{\partial \chi}{\partial t} = \langle G_i G_j S_{ij} \rangle + \frac{1}{RePr} \langle G_i \nabla^2 G_i \rangle$ $P_G = \langle G_i G_j S_{ij} \rangle$ • $\tilde{P}_{G_I} = \tilde{G}_I^2 \tilde{S}_I$



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Rate of energy and scalar dissipation

• $\epsilon = \nu \Omega$ • $\epsilon_{\theta} = \alpha \chi$



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Difference between χ and Ω



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t = 3.00

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t = 4.00

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t = 6.00

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- Comparison with forced isotropic turbulence
- Jimenez at $R_{\lambda} = 168$ Donzis & Sreenivasan $R_{\lambda} = 1100$



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Conclusions MFU Velocity

- DNS allow to establish
 - Euler has FTS
 - I.C. important for the best trend $(t_s t)^{-1}$
 - Flows with power laws (Lamb) k⁻ⁿ more efficient
 - Numerical methods affect the trend
- Navier-Stokes do not have FTS
- Depending on *Re* earlier deviation from $(t_s t)^{-1}$
- Varying Re finite rate of energy dissipation ϵ
- In time Ω amplification $P\Omega > D_{\Omega}$
- Constant $\epsilon P\Omega \approx D_{\Omega}$
- *n* varies from n = -3 (FTS) to n = -5/3 Kolmogorov
- Formation of exponential range
- More on JFM Vol.690 280-320.

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Conclusions Scalar

Inviscid

- Passive scalar at $t = 0 E_{\theta} \approx k^{-4}$
- at FTS $t = 0 E_{\theta} \approx k^{-2}$ sheets
- Growth of χ similar to Ω
- $< G_i G_j S_{ij} >$ not too different from $< \omega_i \omega_j S_{ij} >$

Viscous scalar

- Maximum of *χ* and Ω at same *t*
- Dependence on Re
- Power law decay with t^{-n}
- E(k) and E_{θ} reach $k^-5/3$
- Large differences in $\langle G_i G_j S_{ij} \rangle$ and $\langle \omega_i \omega_j S_{ij} \rangle$
- More on JOT Vol.15 No. 11 731-751.

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- Large interest in wall-bounded flows
- Boundary layers, circular pipes and plane channels
- Theoretical arguments
- Log-law for U⁺ Prandtl
- Attached eddies (Townsend)
- Very high Re superstructures

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- Channel Bernardini JFM 742, Orlandi JFM 770
- Superstructures at high Re
 - del Alamo *et al.* up to $Re_{\tau} = 2000$ not wide log-law
 - at $Re_{\tau} > 10^4$ very satisfactory for many question
 - at $Re_{ au} \approx$ 4000 crossover prod. at $y^+ \approx$ 100
 - at $Re_{\tau} = 4000$ some answer
 - $Re_{\tau} = 4000$ Bernardini $8192 \times 1024 \times 4096$ in $12\pi \times 2\pi$
- Couette Pirozzoli JFM 758
- Production at centerline
- Superstructures at low Re
 - $\textit{Re}_{ au}$ up to 1000 5120 imes 512 imes 1536 in 12 π imes 2 π

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$\overline{u_2'^2}$ stress

• Townsend (attached eddies) $\overline{u_2'^2}/u_{\tau}^2 = C_2$



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$\overline{u_1'u_2'}$ stress

• Townsend (attached eddies) $\overline{u'_1 u'_2}/u_{\tau}^2 = 1$





• Townsend (attached eddies) $\overline{u_3'^2}/u_{ au}^2 = C_3 + klog(h/y)$



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$\overline{u_1^{\prime 2}}$ stress

• Townsend (attached eddies) $\overline{u_1'^2}/u_{ au}^2 = C_1 + klog(h/y)$



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Transport of TKE

- Balance of production and ϵ
- In the outer region $y^+P^+ = y^+\epsilon^+$



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$\langle u_2^{\prime 2} \rangle$ and N-S equations

- $\langle \textit{u}_2'^2 \rangle$ difficult to measure small dependence on Re
- $ilde{u}_2|_{max} pprox u_{ au}$ then $ilde{u}_2^+ pprox 1$
- From u_2 equation $\langle p \rangle + \langle u_2'^2 \rangle = P_0$
- From pressure equation

•
$$-\nabla^2 p = s_{ij}s_{ji} - \omega_i\omega_i/2 = -Q$$

- Q > 0 tube-like
- Q < 0 ribbon-like</p>

$$-\frac{\partial^2 \langle \boldsymbol{p} \rangle}{\partial x_2^2} = -\langle \boldsymbol{Q} \rangle = \langle \boldsymbol{s}_{ij} \boldsymbol{s}_{ji} \rangle - \langle \omega_i \omega_i / \boldsymbol{2} \rangle = \frac{\partial^2 \langle \boldsymbol{u}_2^2 \rangle}{\partial x_2^2}$$
(1)

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$$\frac{\partial^2 \langle u_2^2 \rangle}{\partial x_2^2}$$
 accounts for structures

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Production and structures



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\boldsymbol{q} and ϵ



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• $Sq/\epsilon > 5$ formation longitudinal structures

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Superstructures and drag Control

- Smits & Marusic Physics Today (2013)
- connection between superstructures and wall structures could plausibly reveal new strategies to reduce drag by manipulating the super structures
- Our view drag Control only by changing wall b.c.



blue 3D staggered cubes red longitudinal 2D triangular

- In Wind Tunnels a clean flow
- Requires an accurate design of
- inlet (contraction)
- test section
- exit (diffuser)
- return
- FOR A NUMERICAL WIND TUNNEL
 - Accurate basic numerical method

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In wind tunnels flows past bodies

- Numerically
 - Body fitted coordinates non-orthogonal
 - Difficulties in numerics
 - Inefficient codes (elliptic equations)
- Orthogonal coordinates body surface discretized
 - Simple numerics
 - Efficient codes direct solver elliptic equations
 - Inaccuracy near walls
 - Small scales generated
 - Dissipated by viscosity

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Early Immersed Boundary Methods

- Vieceli (1969) 2D steady
- Vieceli (1971) 2D unsteady
- Imposition impermeability
- Peskin body forces 1972 2D
- Basdevant , Briscolini & Santangelo Mask method
- Based on impositions of body forces
- Inaccurate near surface
- Small Δt
- Impossibility to deal with turbulence

- Fadlun (JCP 2000 1430 citations) revisited Vieceli approach
 - Zero velocity inside body
 - Interpolation first point external body
 - Large Δt
 - Turbulent flows accessible
- Huge number of versions available

Our immersed boundary methods

- Rough channels
- No constant mass with interpolation
- Interpolation does not give true friction
- No Balance between pressure gradient and wall friction
- Present
- Inside body as Fadlun
- Metric at the first external point
- For viscous terms
- No correction for non-linear
- No correction for pressure
- Impermeability more than sufficient

Validation IBM roughness

- Turbulent flows past circular rods
- Comparison between boundary layers (exp)
- and channels (DNS)



Validation IBM through experiments

- Turbulent flows past square bars
- Experiment ad hoc designed
- Burattini JFM 600

Case	$Re_b = \frac{U_b H}{v}$	$Re_{\tau_r} = \frac{u_{\tau_r}H}{v}$	$Re_{\tau_s} = \frac{u_{\tau_s}H}{v}$	$k^+ = \frac{k u_{\tau_r}}{v}$	y _U /H	u_{τ_r}/U_M	u_{τ_r}/u_{τ_s}
E1	3600	300	230	30	1.24	0.073	1.31
E2	7100	620	430	62	1.32	0.074	1.44
E3	13000	1120	760	112	1.33	0.072	1.48
D1	2800	260	190	26	1.22	0.078	1.38
D2	6900	634	430	63	1.27	0.076	1.46
D3	12000	1094	730	109	1.27	0.076	1.50

TABLE 3. Main results for measurements (E1, E2, E3) and simulations (D1, D2, D3).



FIGURE 6. RMS turbulence intensities. (a) E1 and D1; (b) E2 and D2; (c) E3 and D3. (b) and (c) are shifted upwards by 0.1 and 0.2. Symbols: experiments; lines simulations. Filed symbols: X-wire; empty symbols: single wire. $\Phi, O, -, u; \blacksquare, -, v; A, --, w$. Arrows indicate y_0/H from experiments. Repeated symbols are for different streamwise positions (MW and

Isotropic turbulence decay

- Grid turbulence in wind tunnels
- Intermediate solidity



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Laminar-turbulent b.l. transition

- Orlandi (arXiv.1503.08614.pdf 2015)
- Paper rejected twice for numerics
- Solid element



Figure 6: Surface contours of surface contour of $\lambda_2 = 1$ a) cube Re = 5500, a) SU at Re = 5500.

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2D trip

• Transverse square bar



Bluff bodies

- Two cylinders
- Vorticity at Re = 600



- Darcy (1857) resistance function of friction factor $C_f(V, D, \epsilon, \nu)$
- Several exp. performed to find C_f
 - Pigott (1933) real pipes fully rough
 - Nikuradse (1933) fully rough sand-grain
 - Schlichting (1936) roughness elements spheres cones etc.
 - Colebrook (1938) sand-grain + large elements
 - Moody (1944) produced a diagram of practical interest

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- Three regimes
 - Laminar independent from surface depends on Re
 - Fully turb. depends on surface indep. from Re
 - Transitional depends on surface and Re

Roughness description

• U contours in a z - y plane





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Time evolution of components flow resistance



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U^+ profiles definition



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U^+ profiles



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Total stress



Roughness parametrization for channel

• Roughness function ΔU_W^+ vs $\tilde{u}_2'^+|_w$

•
$$ilde{U}^+ - ilde{U}^+_w = \kappa^{-1}\ln(ilde{y}^+) + B(1-rac{ ilde{u}_2'^+|_w}{\kappa})$$

- Roughness classified by $\tilde{u}'_2|_w$
- Holds for any kind of rough surface



Eguivalent roughness height and $\tilde{u}_2^{\prime+}|_w$

• 8.48 +
$$\frac{1}{\kappa} \ln(y^+/Z^+) = \kappa^{-1} \ln(\tilde{y}^+) + B(1 - \frac{\tilde{u}_2'^+|w}{\kappa})$$



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• Based on \tilde{u}'_2 and U_W

•
$$\tilde{U} - \tilde{U_w}^+ = \kappa^{-1} \ln(\tilde{y}^+) + B(1 - \frac{\tilde{u}_2'^+|_w}{\kappa})$$
, $B = 5.0$
• $\tilde{U_H}^+ = \kappa^{-1} \ln(H^+) + B(1 - \frac{\tilde{u}_2'^+|_w}{\kappa})$
• Since $U_H^+ = C + U_{bulk}^+$

• If
$$\lambda = u_{\tau}/U_{bulk}$$
, $C_f = 2\lambda^2$
• $\lambda = \frac{(1.+B/\kappa \tilde{u}'_2|w/U_{bulk}-U_w/U_{bulk})}{[C+ln(Re_b\lambda)]}$

• To fit with $C_f = 0.0725 Re_b^{-.25}$ C = 4.5

The new diagram





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- CFD is a useful toll to explore
 - Vortex dynamics
 - Turbulence
- Lucky to have theoretical models
- Euler and Navier-Stokes equations
- Hard life in the 60th and 70th
- Easy life today HPC and software
- I WAS UNLUCKY
- HOPING MY EFFORT WILL MAKE YOU
- HAPPY

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