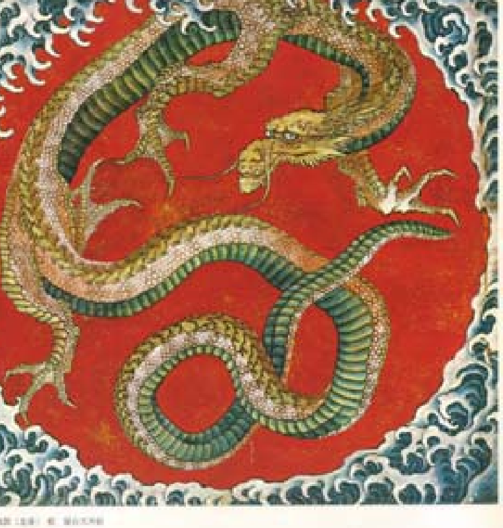
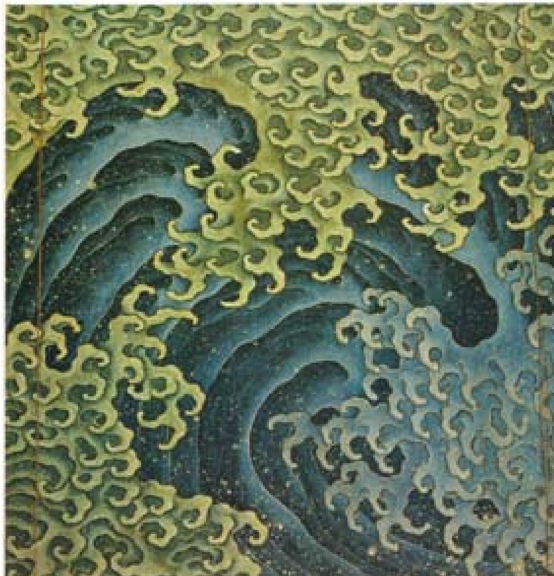


June 23, 2003

Computing Turbulence in the 4096^3 Range



Y. Kaneda

Nagoya University

Collaboration with

Ishihara T. （Nagoya Univ.)

Yokokawa M. (Grid Center)

Itakura K. （Earth Simulator Center)

Uno A. (Earth Simulator Center)

Outline of Talk

I) Overview of DNS on the Earth Simulator and VPP

II) Visualization

III) Some DNS Results

I) Overview of DNS
on the Earth Simulator and VPP

Computational Facilities & Performance

★ **1 (512^3) & ★ 2 (1024^3)**

- Fujitsu vpp500/42, VPP5000/56 （Nagoya UCC)

  0.5TFLOPS(peak), Memory 0.9TB

★ **3 (2048^3) & ★ 4 (4096^3)**

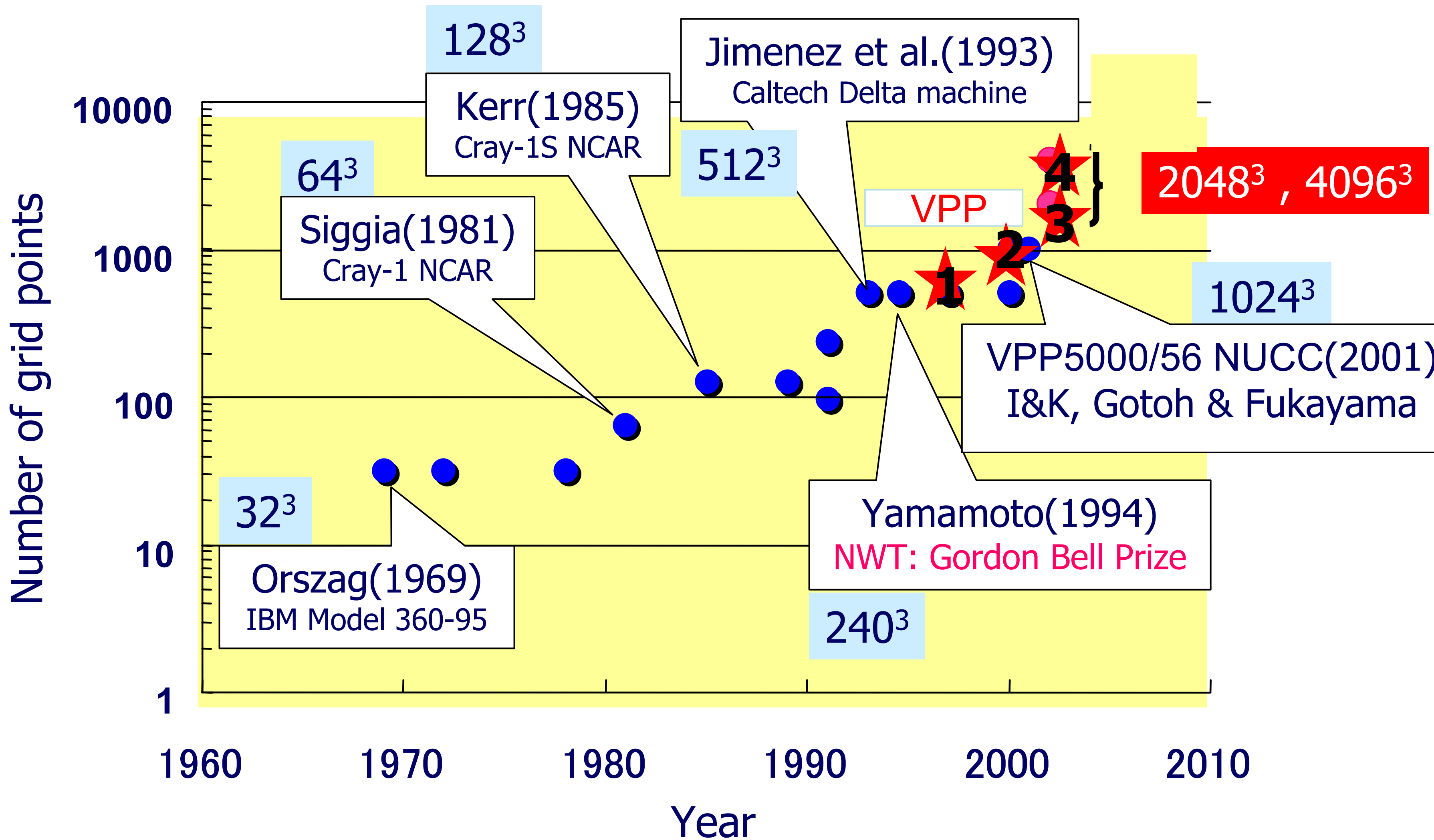
- Earth Simulator (2002)

  40TFlops (peak), **16.4TFlops**(sustained),

  Memory:10TB

History of representative DNS

Incompressible Homogeneous Isotropic Turbulence under periodic BC



16.4 Tflops Direct Numerical Simulation of Turbulence by a Fourier Spectral Method on the Earth Simulator

Mitsuo Yokokawa

Ken'ichi Itakura, Atsuya Uno

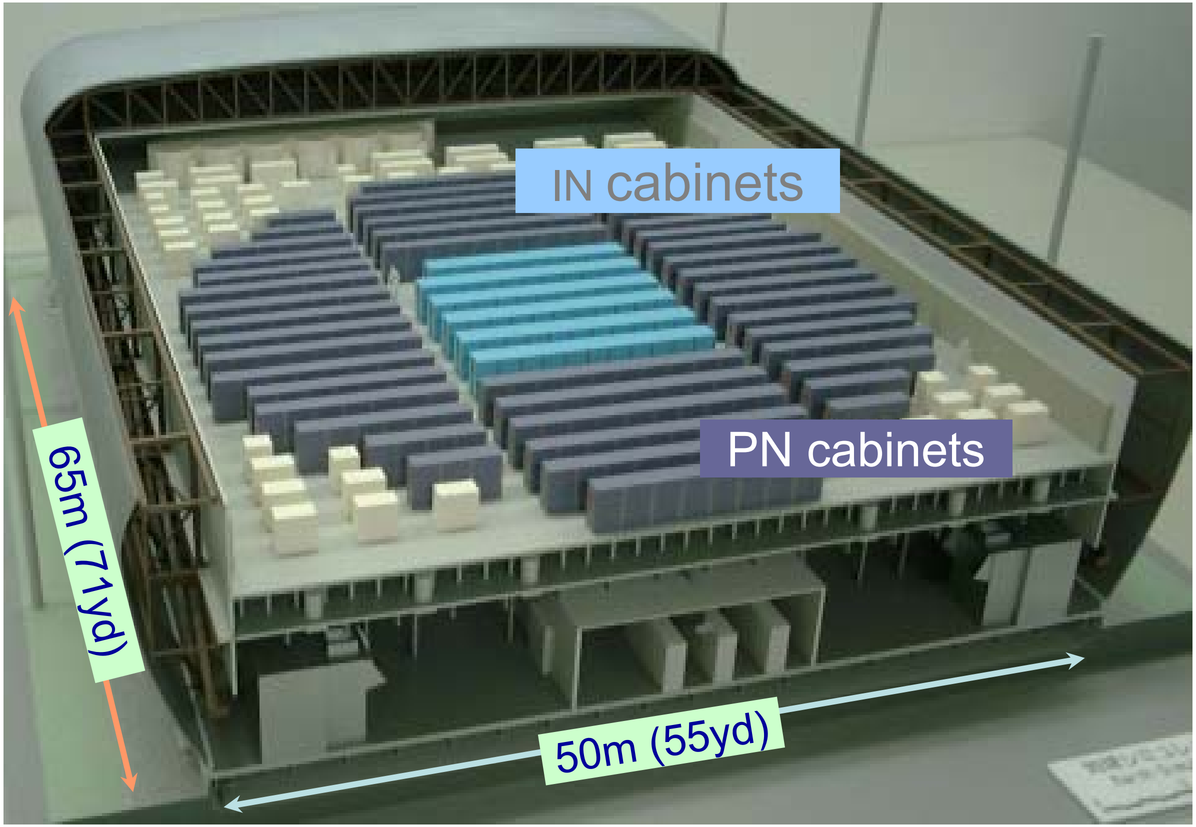
Takashi Ishihara and Yukio Kaneda

See: Yokokawa, Itakura, Uno, Ishihara & Kaneda (SC2002)[YIUYK(SC2002)]
http://www.sc-conference.org/sc2002/
& also http://www.ultrasim.info

The slides (No.8-19) are made from this presentation

The Earth Simulator

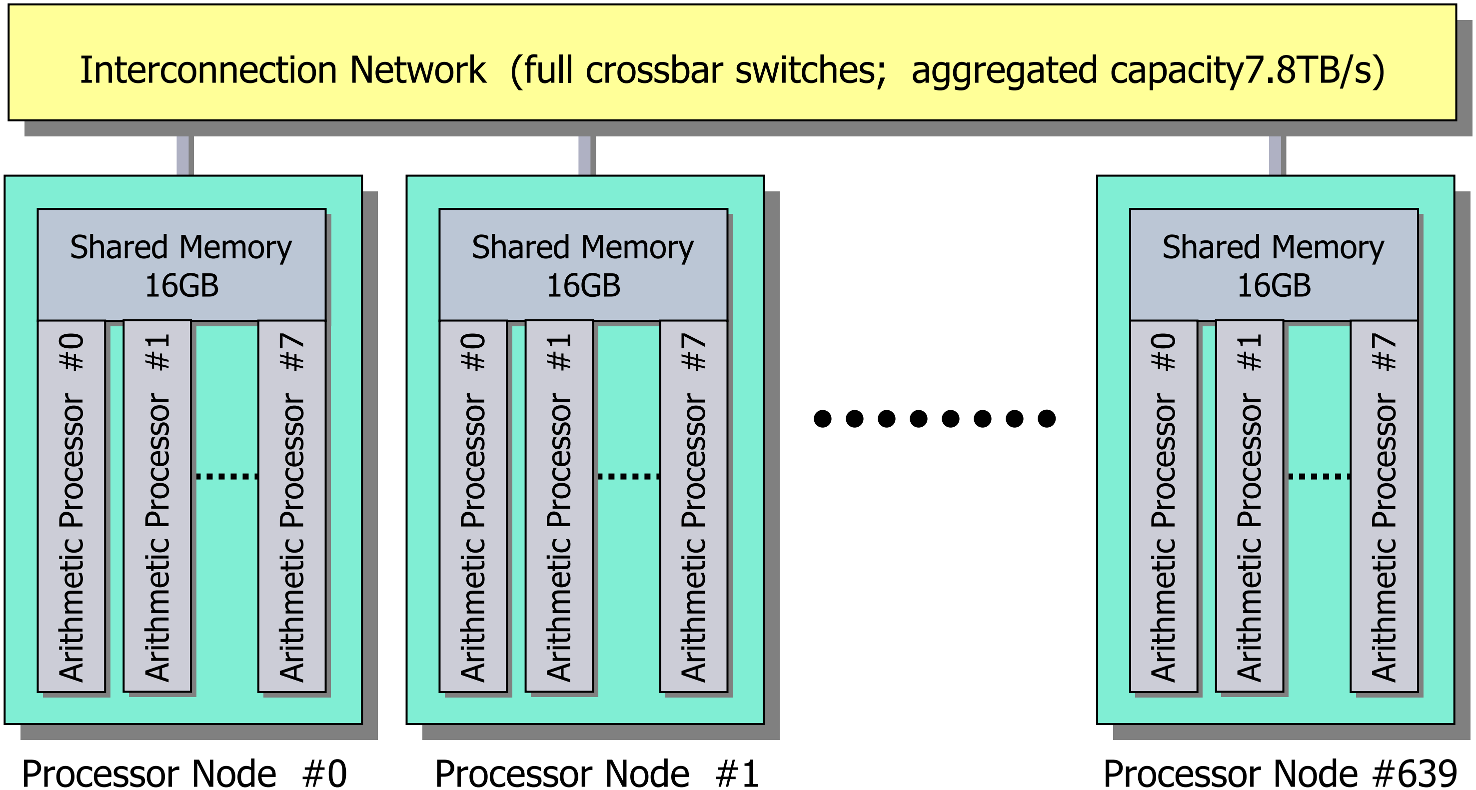
- 35.86Tflops sustained in Linpack benchmark was achieved.
- It's actually the world fastest supercomputer.
- "TIME" chose it as one of 2002 world inventions



Configuration of the Earth Simulator

- Total number of PNs : 640
- Peak performance/AP : 8Gflops
- Peak performance/PN : 64Gflops
- Shared memory/PN : 16GB

- Total peak performance : 40Tflops
- Total main memory : 10TB



Features of the Earth Simulator

- One chip vector processor of 8 Gflops
  - 0.15 μm CMOS LSI technology with Cu wiring
  - Large size LSI of 20.79mm x 20.79mm
  - Vector pipeline units at 1GHz and other parts at 500MHz
- SMP cluster
  - High bandwidth memory access of 256 GB/s
- High-bandwidth and non-blocking interconnection crossbar network
  - Aggregate switching capacity of 7.8 TB/s

Overview of DNS code

- Forced incompressible Navier-Stokes equations under periodic BCs.

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{t}} = \boldsymbol{u} \times \boldsymbol{\omega} - \nabla \Pi + \nu \, \Delta \boldsymbol{u} + \boldsymbol{f} \quad \text{(Rotational form)} \qquad \nabla \cdot u = 0$$

- Fourier spectral method
- Alias error removed by mode truncation & phase shift
- Fourth-order Runge-Kutta method for time advancing

Implementation of DNS code

- written in Fortran90.

- Eighteen 3D-FFTs are required for evaluations of the right hand side of O.D.E.'s in 1 time step of R-K time advancing

  ⇨ FFT can be carried out efficiently on vector processors, or on the Earth simulator.

- Memory size is increased as $O(N^3)$, where N is a number of grid points in one-direction.

Memory capacity required for a sequential version = $25N^3$

N^3	$25N^3$
512^3	25 GB
1024^3	200 GB
2048^3	1.6 TB
~~4096^3~~	~~12.8 TB~~
~~8192^3~~	~~102 TB~~

possible on ES !!

Double precision for Nonlinear term, but single for the linear term & R-K integration

7.2TB in Total

4096^3 DNS is possible on 512 nodes of ES

Implementation of a DNS code

- written in Fortran90.

- Eighteen 3D-FFTs are required for evaluations of the right hand side of O.D.E.'s in 1 time step of R-K time advancing

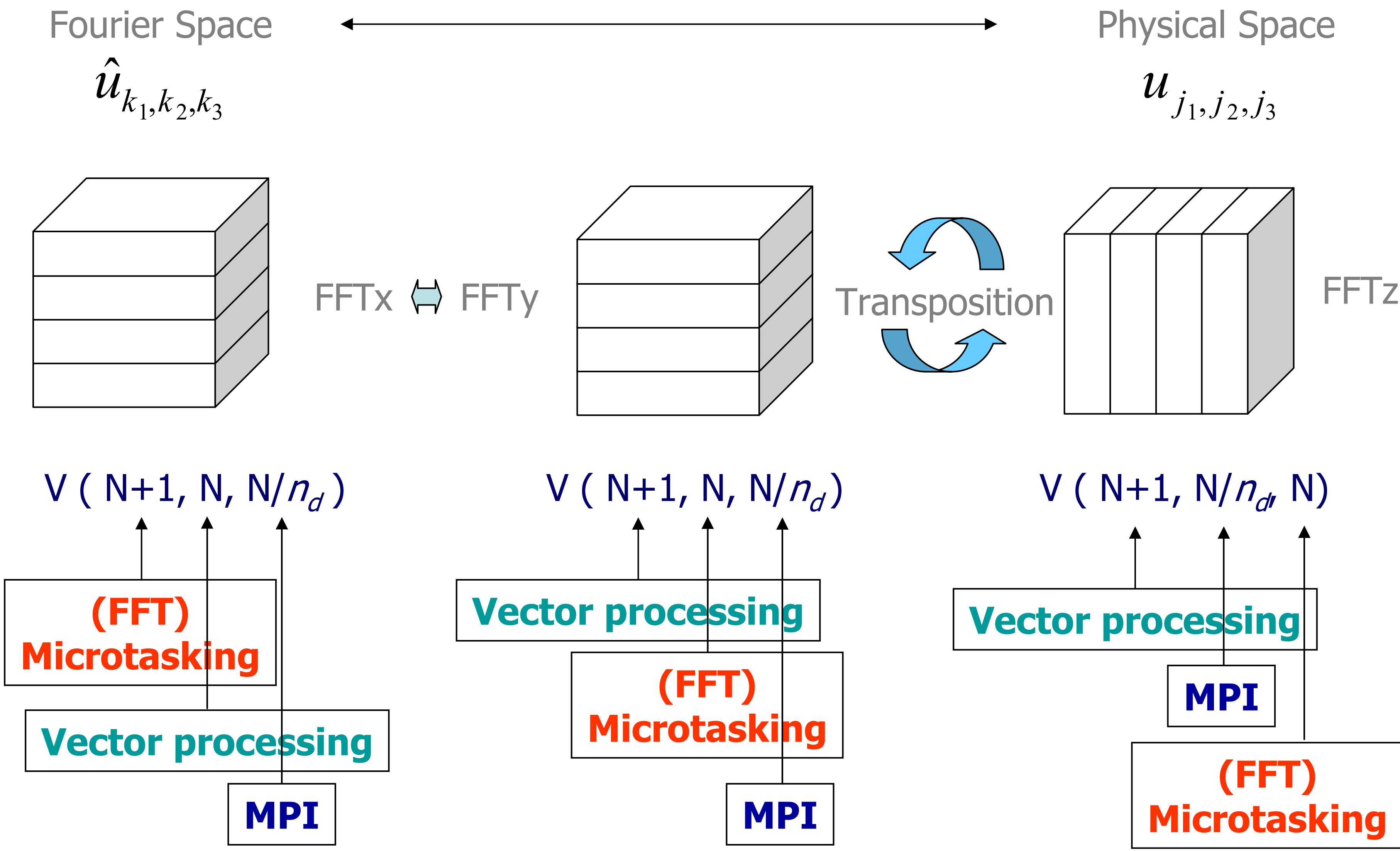
  ➡ FFT can be carried out efficiently on vector processors, or on the Earth simulator.

- Memory size is increased as $O(N^3)$, where N is a number of grid points in one-direction.

- 3D-FFT parallelized by domain decomposition needs all-to-all communications in transposing data distributed on the system

  ➡ High-speed data transfer is required.

3D-FFT by domain decomposition



Points of Implementation (radix-4 FFT)

- Ratio of memory access to floating point operation is a critical issue on ES to keep performance high enough.
  - Peak performance of vector processor is 8 Gflops.
  - Bandwidth between a VP and main memory is 32 GB/s.
  - The ratio of the number of times memory is accessed to the number of floating point data operations is 0.5.

- Kernel code of radix-2 FFT shows the ratio as 1.

- Radix-4 or more FFT can be achieved higher performance, because the ratio is lower than 0.5.

⇒ Radix-4 FFT is taken in the implementation.

Performance

Table 1: Performance in Tflops of the computations with double [single] precision arithmetic as counted by the hardware monitor on the ES. The numbers in (-) denote the values for computational efficiency, C_E. The number n_p of APs in each PN is a fixed 8.

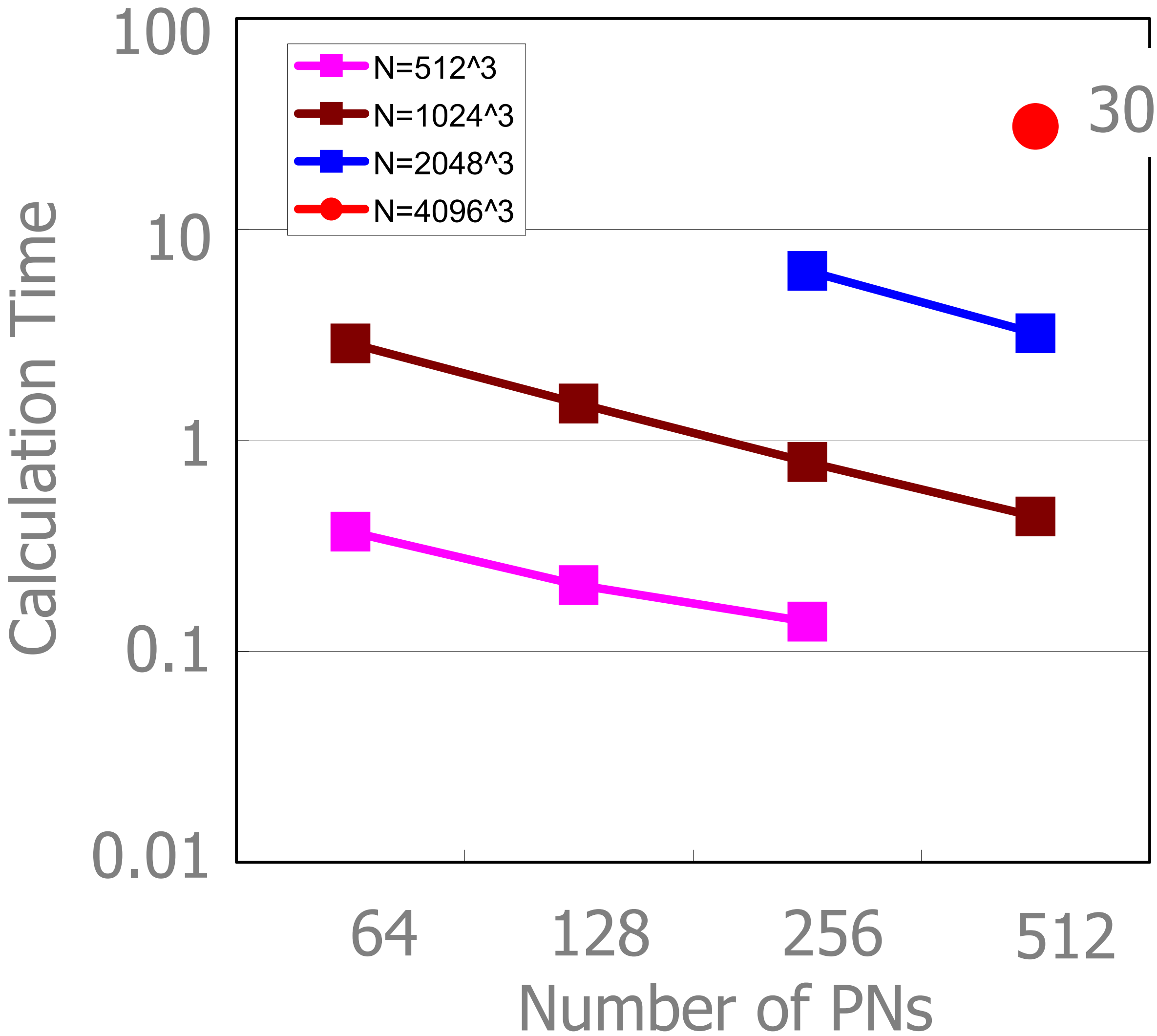
$N^3 \setminus n_d$	512	256	128	64
2048^3	13.7(0.43)[15.3(0.48)]	6.9(0.43)[7.8(0.49)]	–	–
1024^3	11.3(0.35)[11.2(0.35)]	6.2(0.39)[7.2(0.45)]	3.3(0.41)[3.7(0.47)]	1.7(0.43)[1.9(0.48)]
512^3	–	4.1(0.26)[4.0(0.25)]	2.7(0.34)[3.0(0.38)]	1.5(0.38)[1.7(0.43)]
256^3	–	–	1.3(0.16)[1.2(0.15)]	1.0(0.26)[1.1(0.28)]
128^3	–	–	–	0.3(0.07)[0.3(0.07)]

Table 2: Performance in Tflops as calculated for the same cases in Table 1 by using the analytical expressions for numbers of operations

$N^3 \setminus n_d$	512	256	128	64
2048^3	14.6[16.4]	7.4[8.4]	–	–
1024^3	12.2[12.1]	6.7[7.7]	3.5[4.0]	1.8[2.1]
512^3	–	4.4[4.3]	3.0[3.3]	1.7[1.9]
256^3	–	–	1.4[1.3]	1.1[1.2]
128^3	–	–	–	0.3[0.3]

From YIUIK(SC2002)

Calculation time of 1 time step



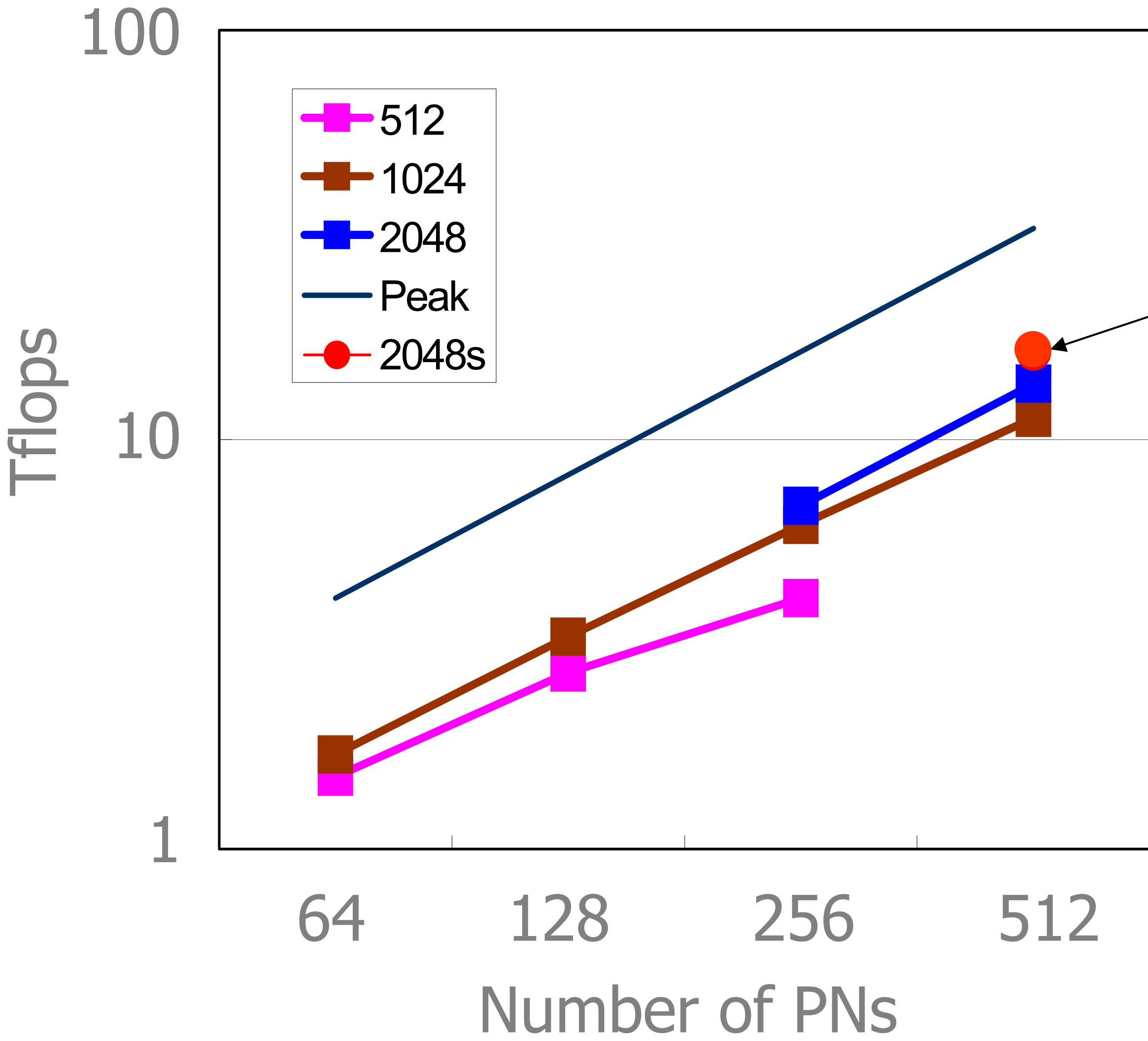
30.7sec

about 3days by

512 PNs for 1T

(about 8400steps)

Performance in Tflops



16.4Tflops

50% of the peak

(single precision &

analytical FLOP number)

Performance by VPP5000

N^3	256^3	512^3	1024^3
# of PE	16(8,4,2)	32(16,8,4)	32
Com. sped [1step]	4.45sec (10,23,48)	17sec (38,94,189)	160sec
Com. time	12h/20T	47h/20T	177h/5T
Required memory	2.7GB	22GB	176GB
I／O (time)	0.4GB (—)	3GB (7／5sec)	24GB (4／1min)

Data Size & Transfer

3D-field, 1snap shot, double(single) precision

N^3	Data-Size
512^3	1 GB
1024^3	8 GB
2048^3	64GB
4096^3	(256GB)

FTP with 10Mbps ~1MB/s

16 min.

2.2 h

18 h

3 days

(u,v,w) + etc → 0.8TB

Conclusion I

- High Performance Computing (16.4TFlops) DNS of Turbulence in the 4096^3 range

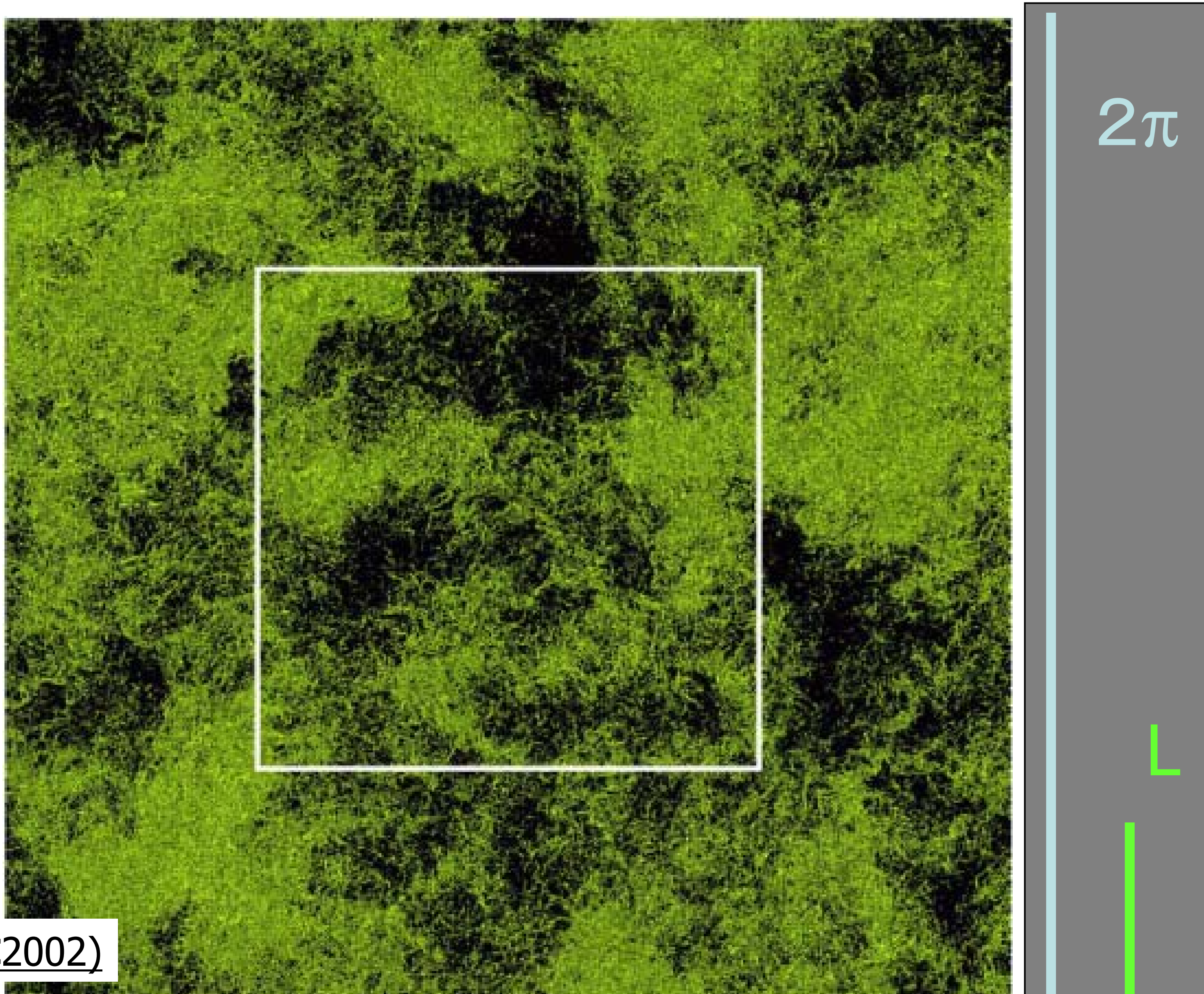
# of freedom = **2.5×10^11** with

Strong-**Nonlinear**, **Non-Local Interaction**

Dissipative Open system

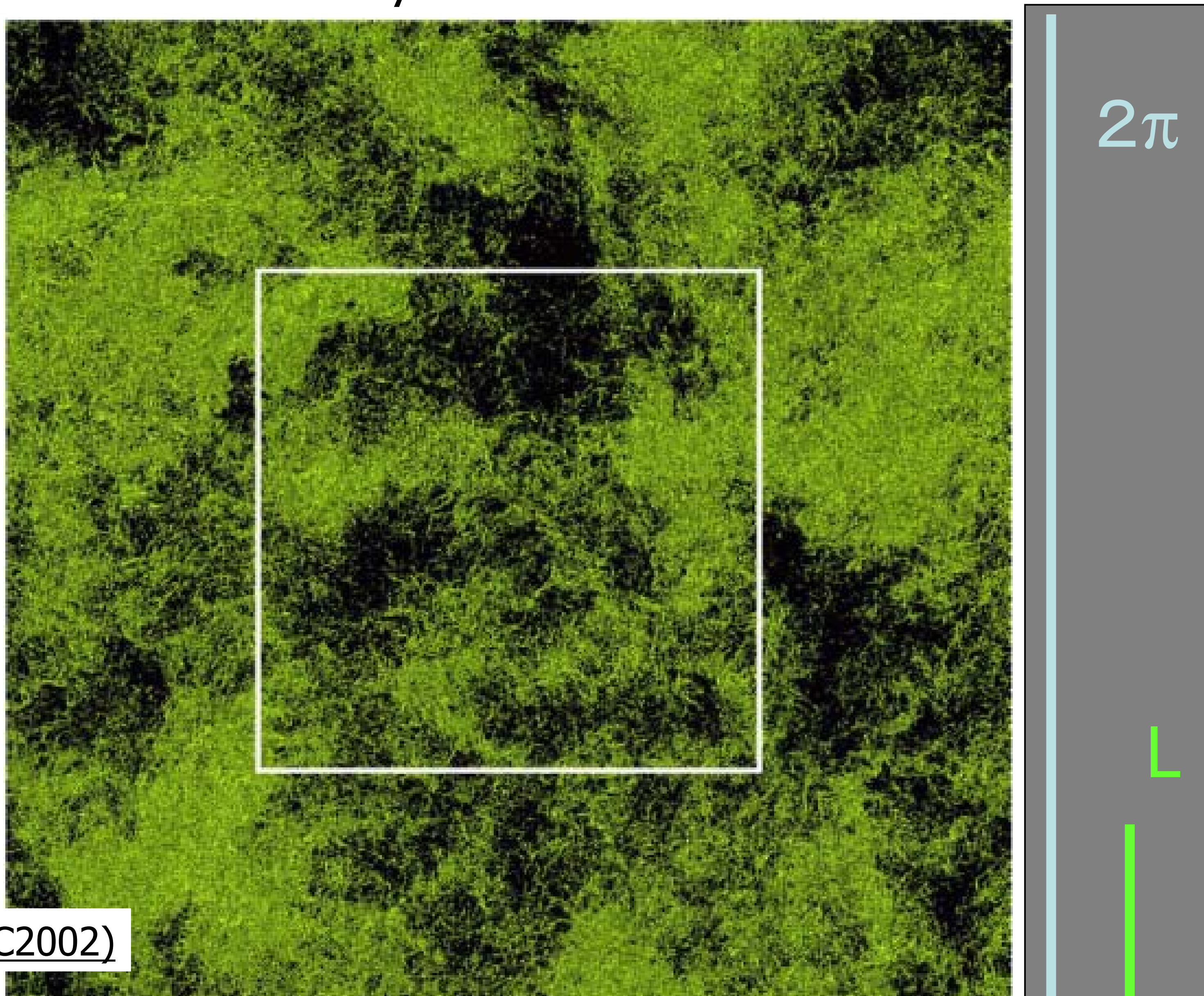
II) Visualization

N=2048



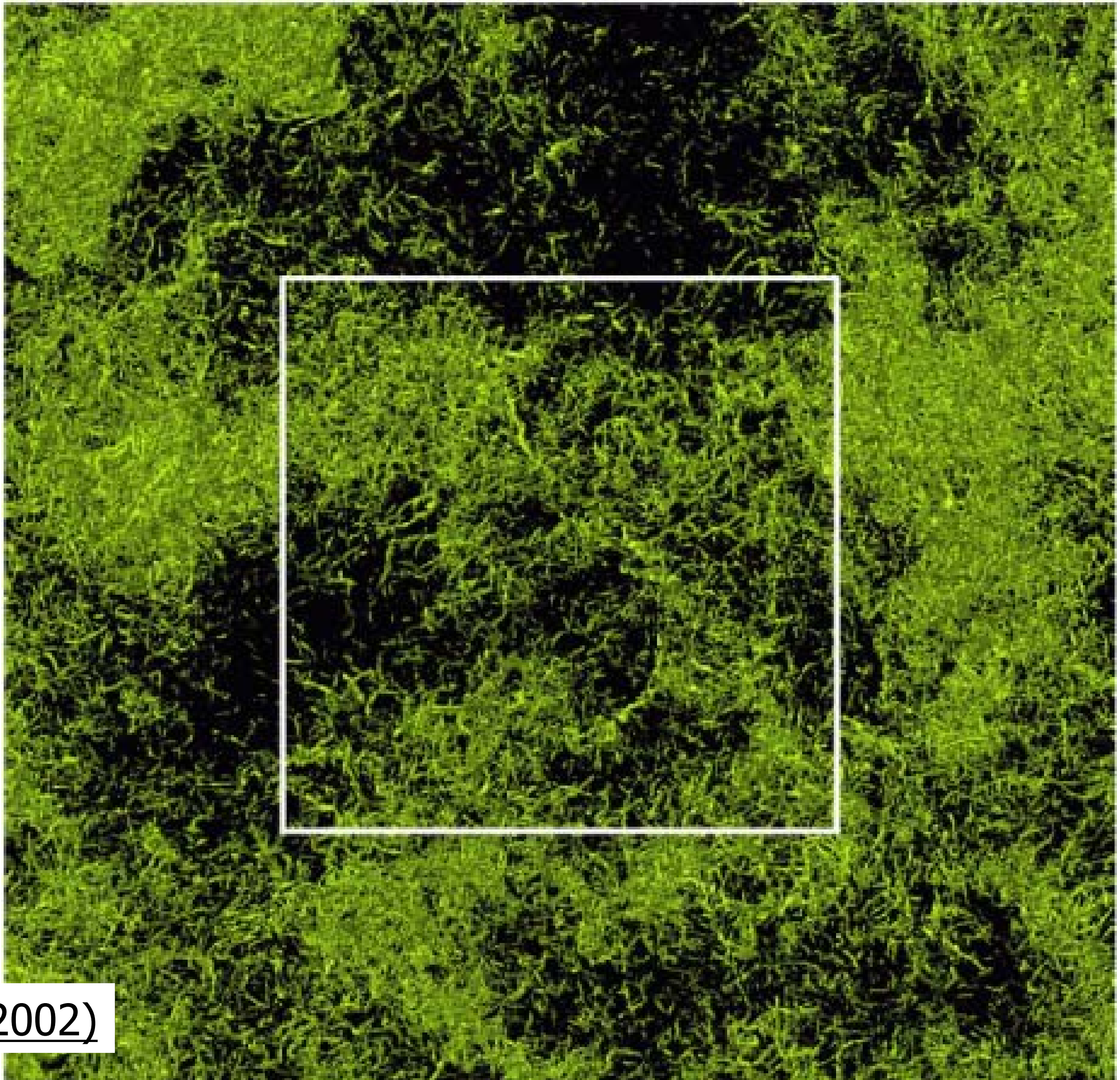
from YIUIK(SC2002)

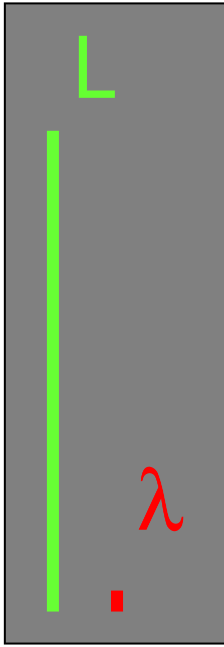
Image of Flow Field (Vorticity) by DNS with N^3=2048^3



from YIUIK(SC2002)

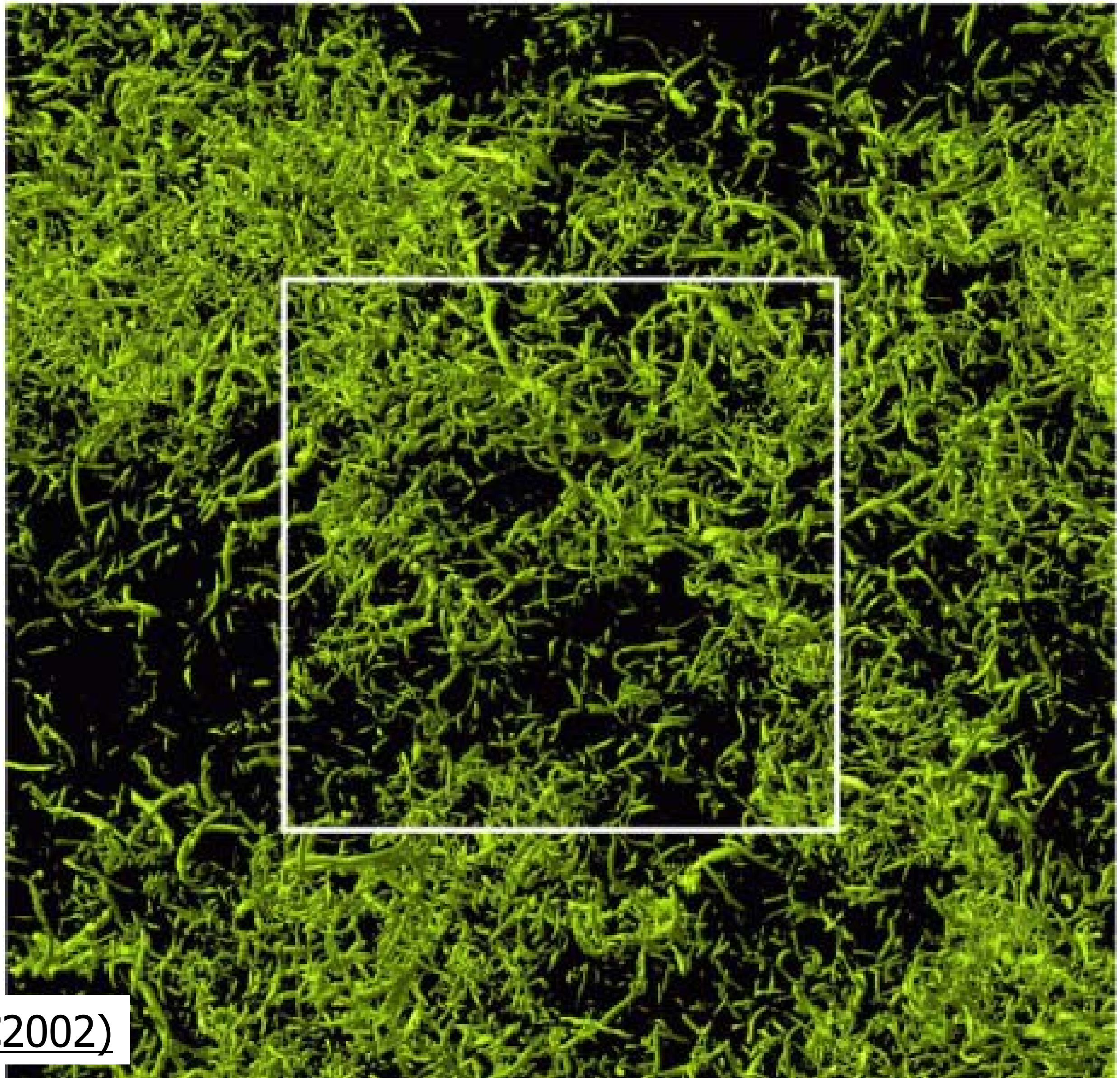
Close up view-1

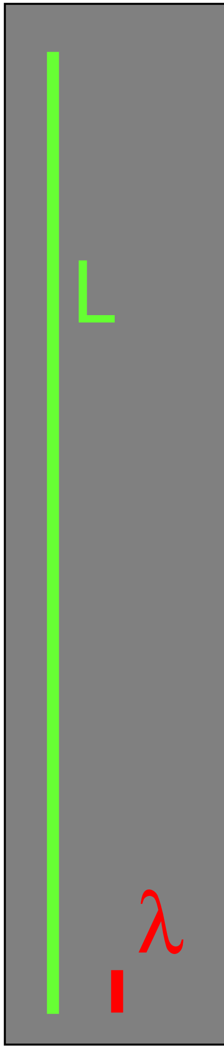




from YIUIK(SC2002)

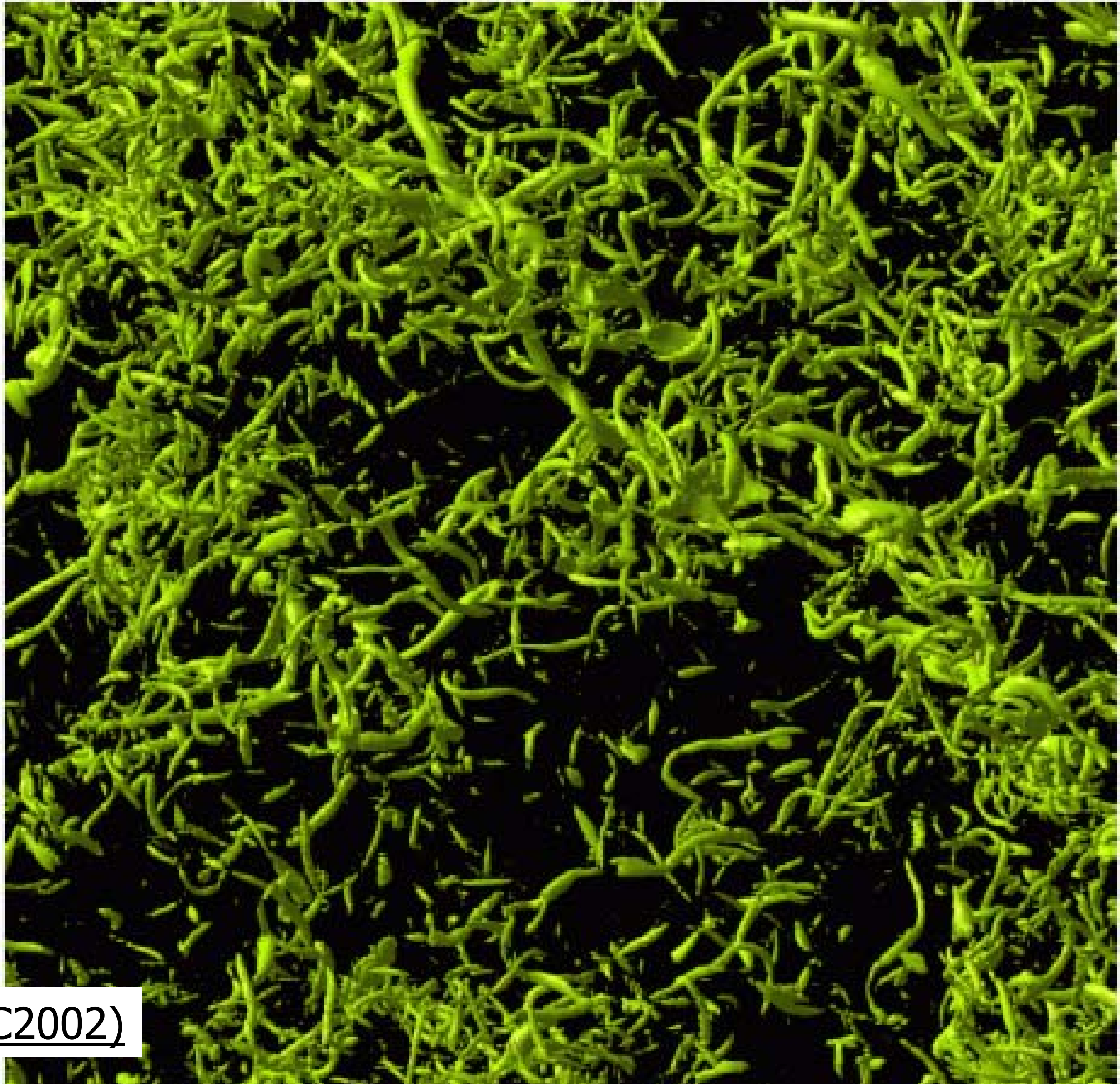
Close up view-2

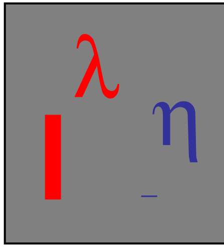




from YIUIK(SC2002)

Close up view-3





from YIUIK(SC2002)

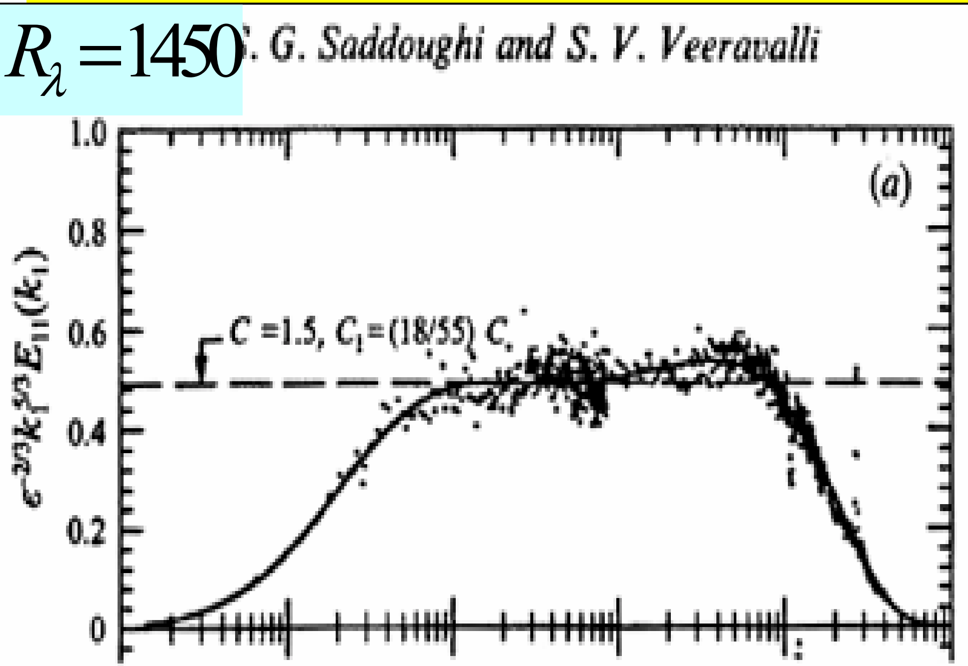
II) Some DNS Results

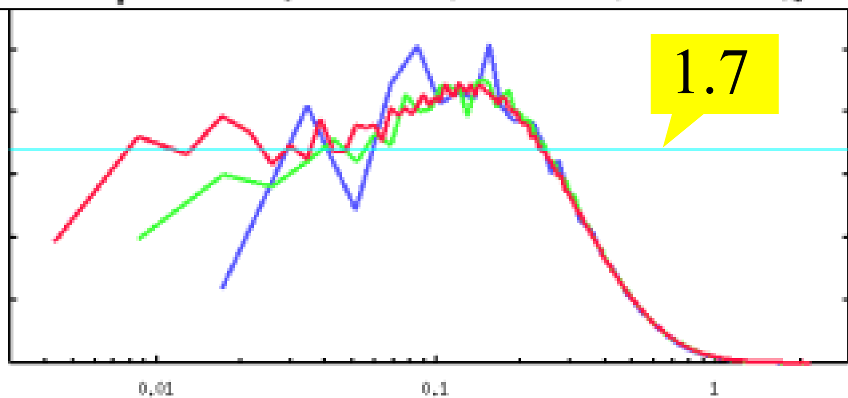
ower resolution: -1

m & energy transfer

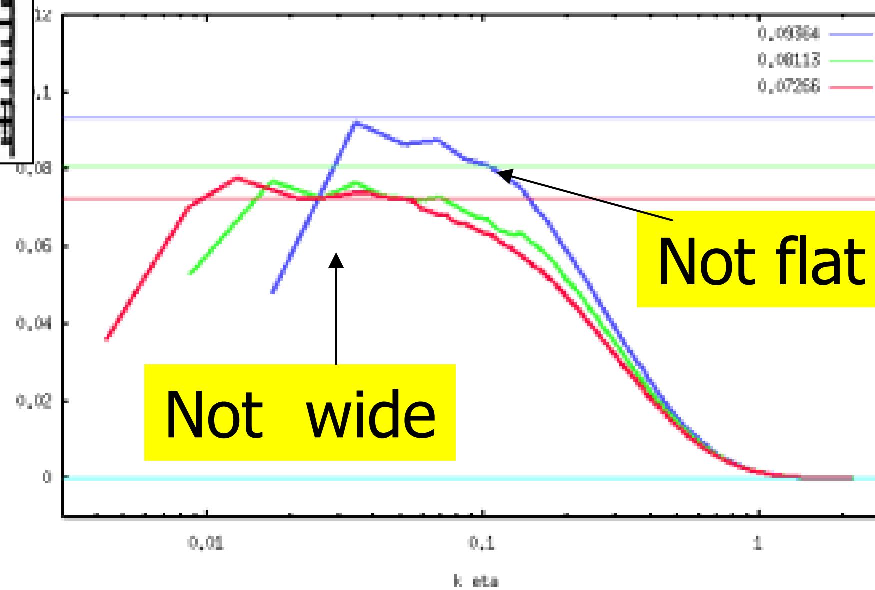
(at statistically steady state)

$$\Pi(k) = \int_k^\infty T(k)dk$$





$k\eta$



$k\eta$

cf. I&K,Statistical Theories and Computational Approaches to Turbulence, Springer(2002), ed. YK & Gotoh, pp.177

$C_K = 1.62 \pm 0.17$ Experimental values (from Sreenivasan 1995)

$C_K = 1.77$ ALHDIA (Kraichnan 1966) $C_K = 1.72$ LRA (Kaneda 1986)

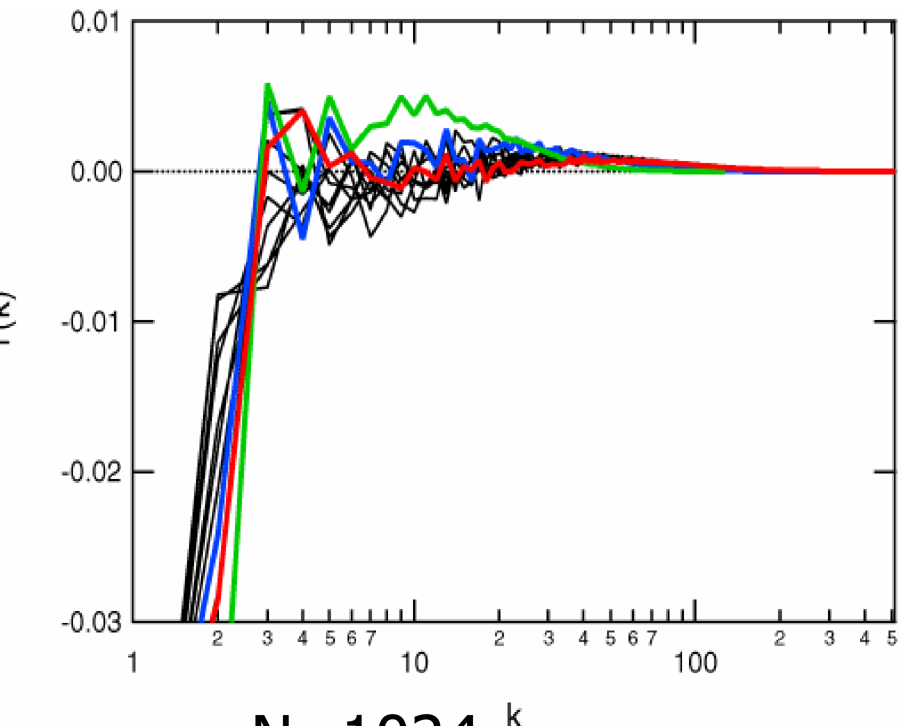
Some difference: -2

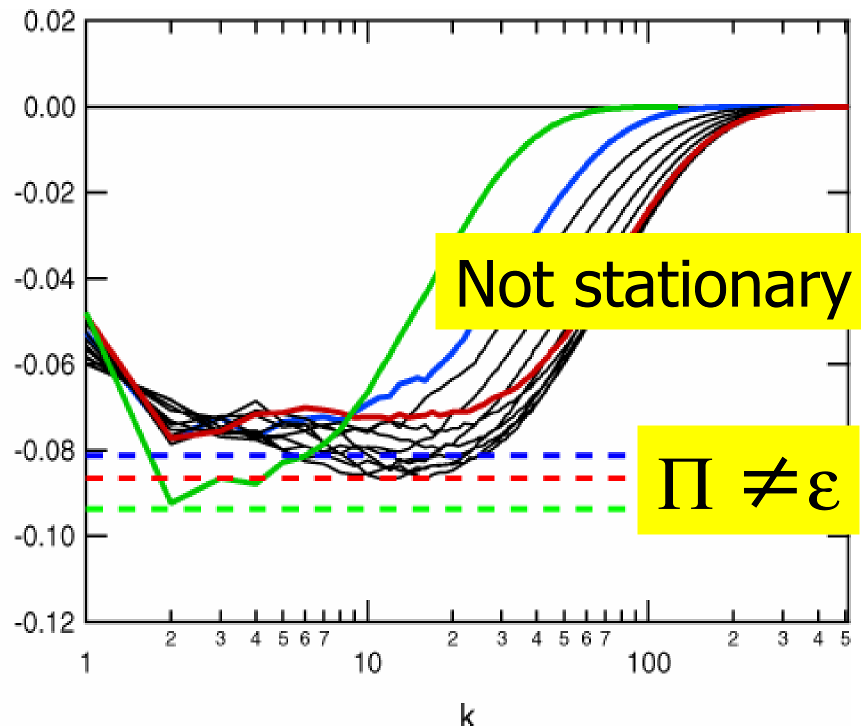
$$\left(\frac{\partial}{\partial t}+2\nu k^2\right)E(k)=T(k)$$

Energy Transfer

$T(k)$

$-\Pi(k)$





N=1024

cf. I&K,Statistical Theories and Computational Approaches to Turbulence, Springer(2002), ed. YK & Gotoh, pp.177

Analysis of the DNS data by ES

underway

- DNS's up to R_λ=1200 suggest

  Normalized dissipation ε **→ const, as R → ∞**
- **Energy Spectrum**
- **Scaling & Statistics of 4th order velocity moments**

  mean squares of $\nabla^2 p$, $\omega \cdot \omega$, $SS = \varepsilon/(2\nu)$

- **High order structure functions,**

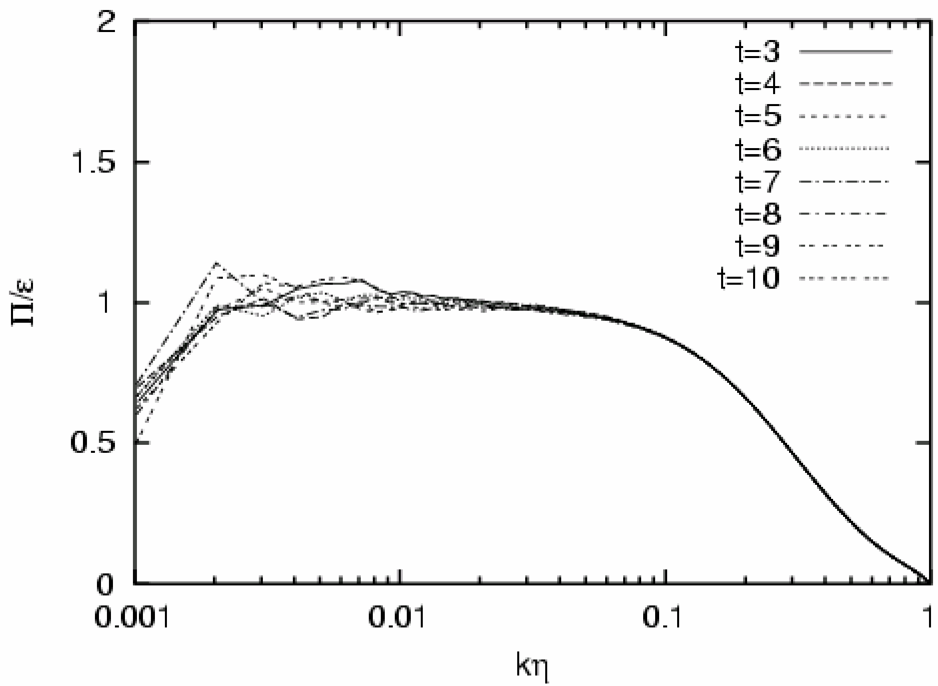
  pdf, joint-pdf, intermittency
- **Anisotropic scaling, effects of anisotropy,**
- **Inertial range structure,**
- **Dissipation range spectrum, ...**

- **Direct & Qualitative Examination of Theories**

Some difference from DNS with lower resolution: -2

$$\Pi \underset{?}{=} \varepsilon$$ (width, flat, stationarity)

$$\Pi(k) = \int_k^\infty T(k)dk$$

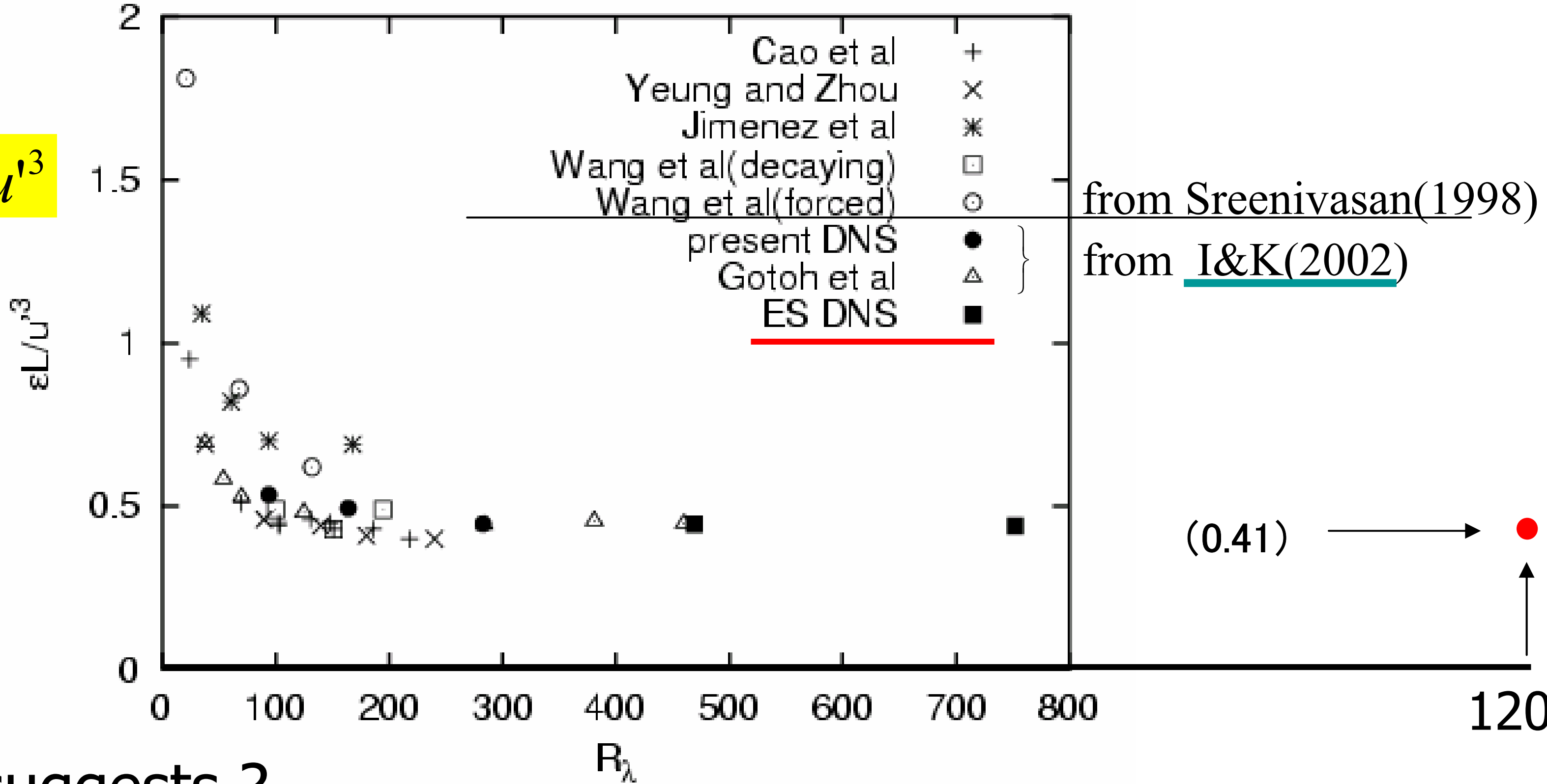


N=2048, $k_{max}\eta \sim 1$ R_λ~732

(from Phys Fluids 12(2003),L21-L24)

Normalized energy dissipation $\alpha \to$?
as $\nu \to 0$, or Re $\to \infty$

$\alpha = \varepsilon L / u'^3$



suggests ?

Approaches to a constant as Re → ∞

(from Phys Fluids 12(2003), L21-L24)

Energy Spectrum

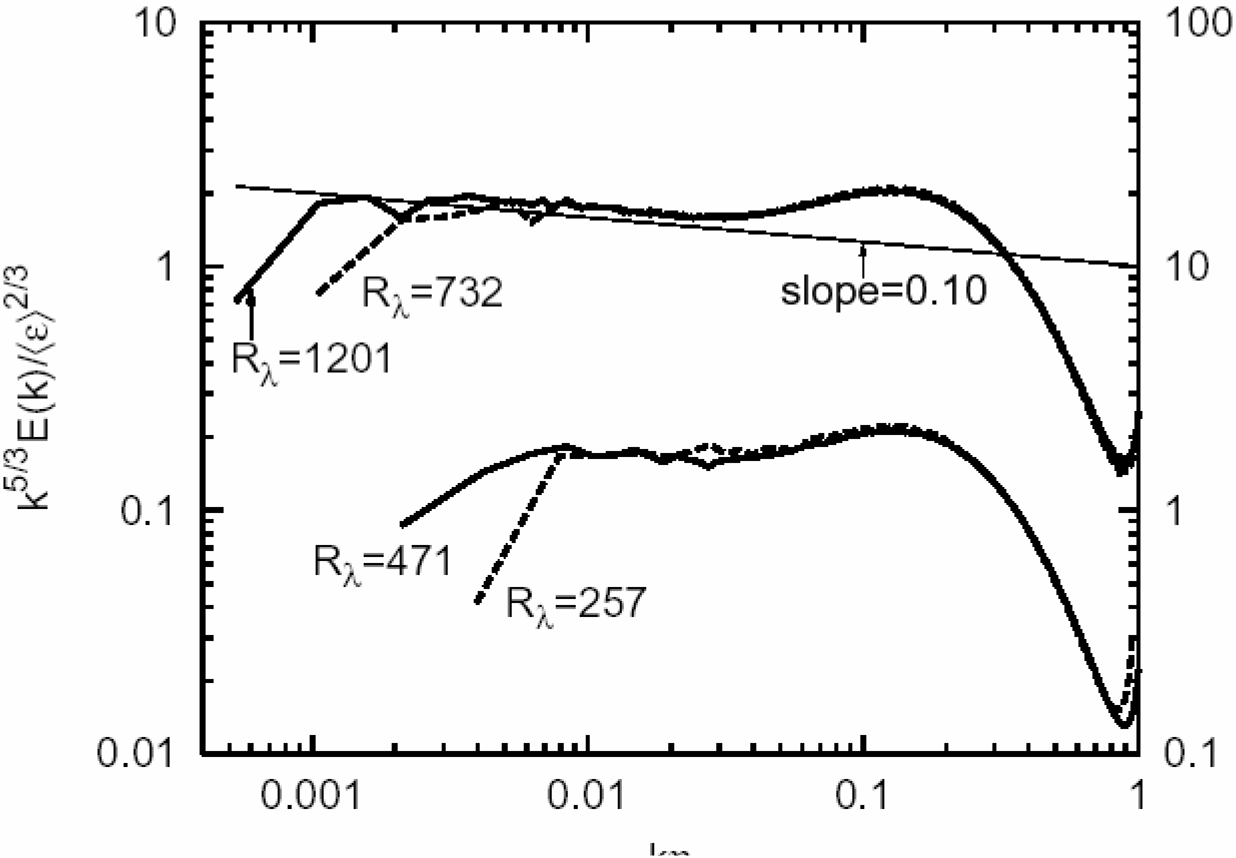


FIG. 5: Compensated energy spectra from DNSs with (A) 512^3, 1024^3, and (B) 2048^3, 4096^3 grid points. Scales on the right and left are for (A) and (B), respectively.

(from Phys Fluids 12(2003), L21-L24)

Exponent of 2nd order velocity structure func.

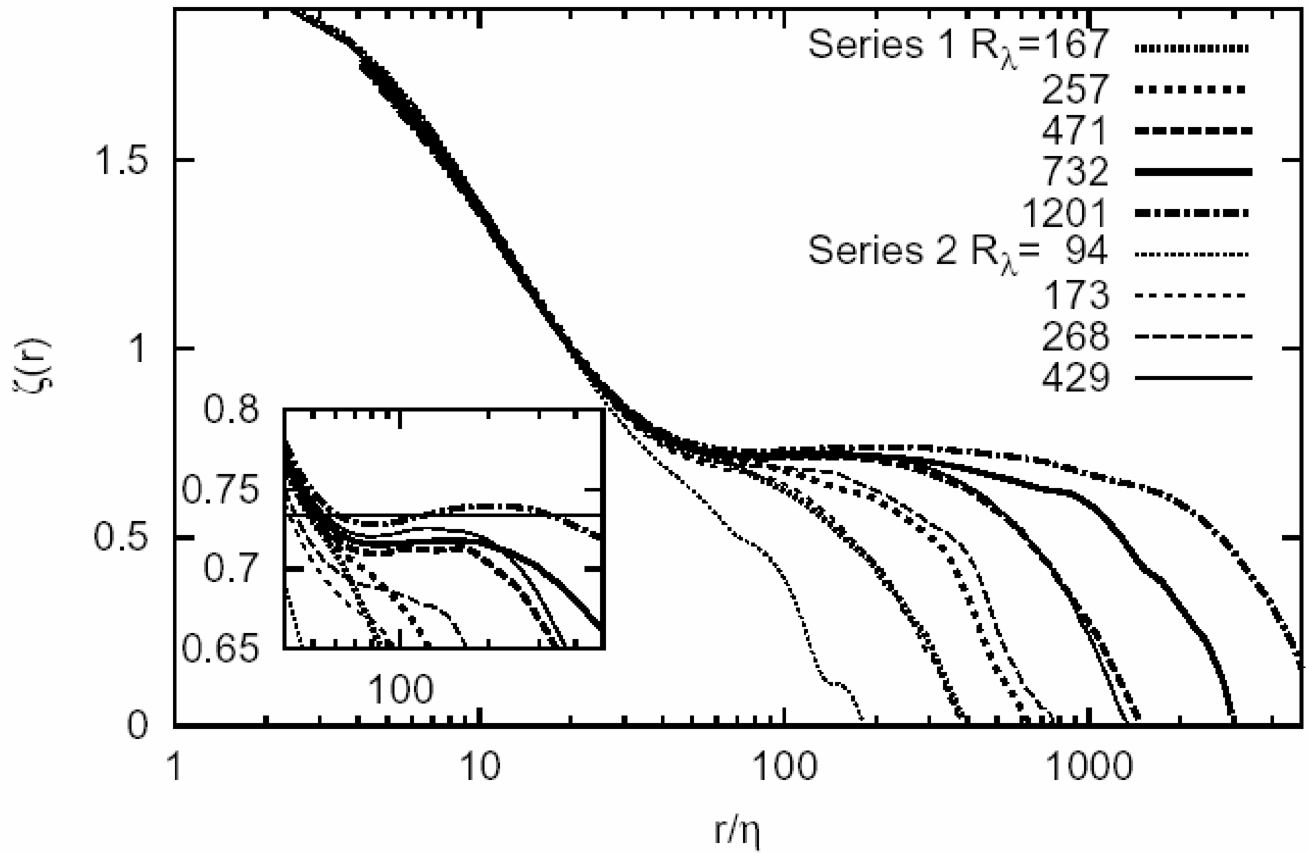
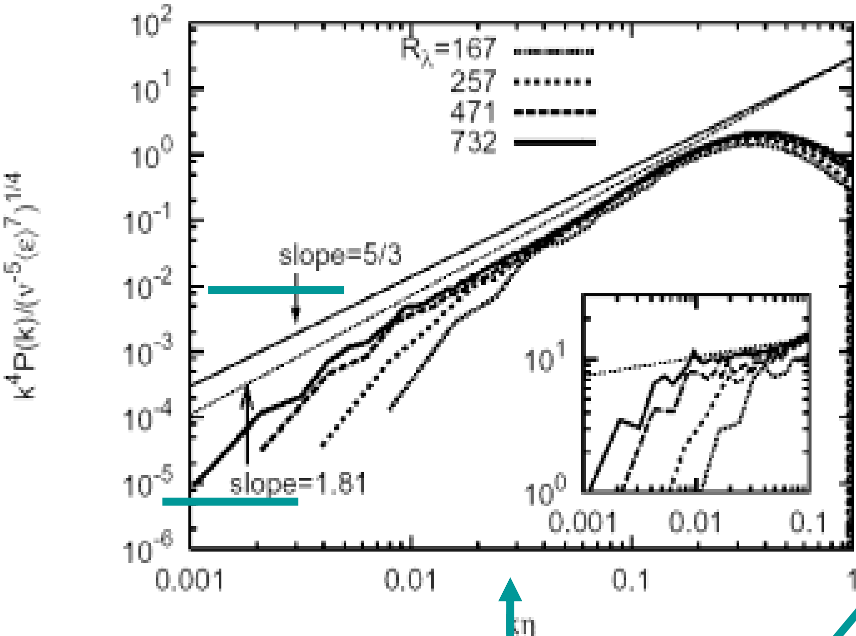


FIG. 6: Local slope $\zeta(r)$ of $f_0(r)$ versus r/η. The inset is an enlargement of the range $40 < r/\eta < 500$. The straight line shows $\zeta(r) = 0.734$.

>2/3

(from Phys Fluids 15(2003), L21-L24)

Normalized Spectra of $<(\nabla^2 p)^2>$, Ω and D



Spectra of

$<(\nabla^2 p)^2>$

Ω: Square of $\omega\omega$

D: Square of SS=$\varepsilon/(2\nu)$

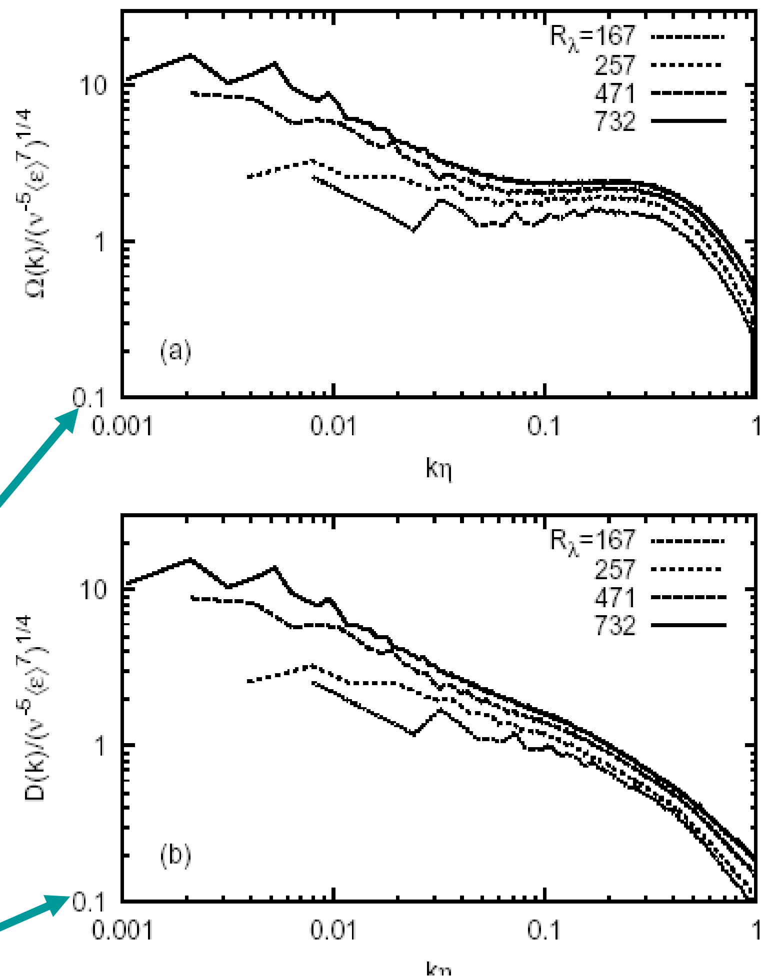


Fig. 3. Normalized spectra (a) $\Omega(k)/(\nu^{-5}\langle\epsilon\rangle^7)^{1/4}$ and (b) $D(k)/(\nu^{-5}\langle\epsilon\rangle^7)^{1/4}$ versus $k\eta$ in Runs 256, 512, 1024 and 2048.

(from J.Phys.Soc Jpn (2003), 983-986)

Compensated Spectra of Ω and D

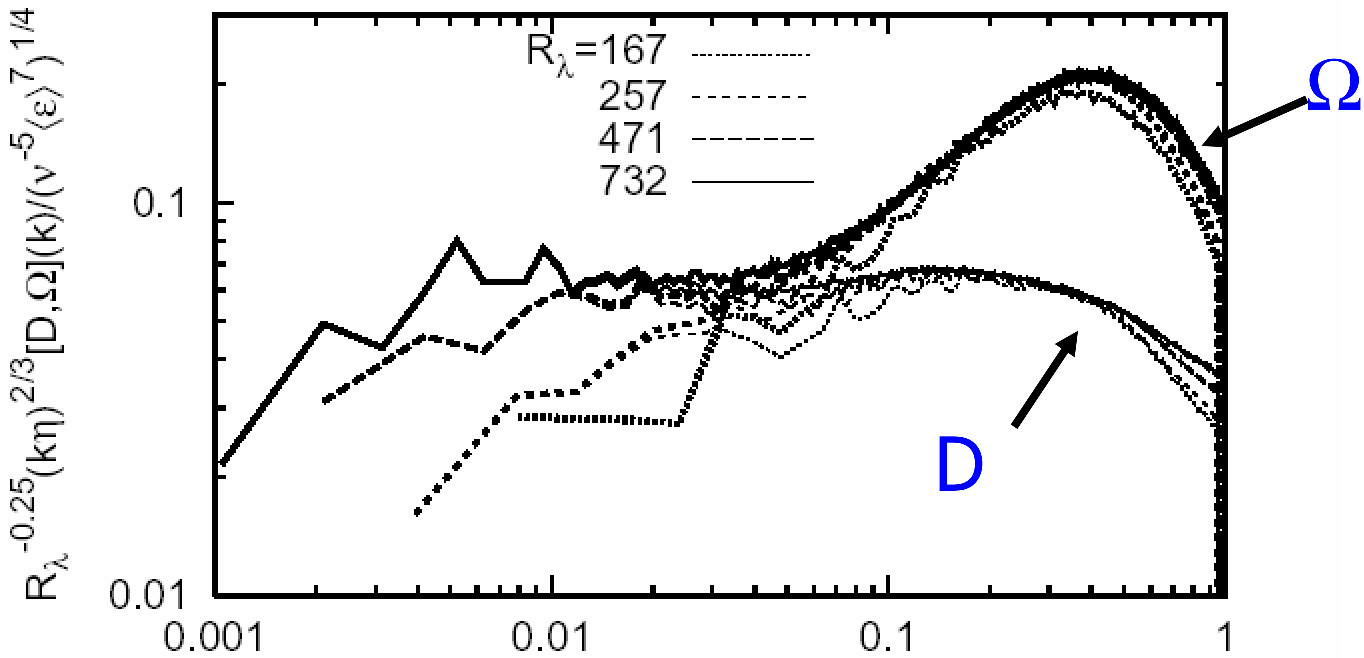


Fig. 5. $\Omega(k)$ (thick lines) and $D(k)$ (thin lines) spectra compensated by $R_\lambda^{-0.25}(k\eta)^{2/3}/(\nu^{-5}\langle\epsilon\rangle^7)^{1/4}$.

(from J.Phys.Soc Jpn (2003), 983-986)

according to DNS

- Scaling of $\nabla^2 p$, $\omega\cdot\omega$ & SS = $\varepsilon/(2\nu)$ → k^{ζ}
  - Anomalous scaling

  with $\zeta \sim 5/3$, m<0, n<0, (m, n≒0 ~ -2/3 ?)

A question: Why are they different ?

NOTE: $\nabla^2 \mathbf{p}$ **=** $(1/2)\omega\cdot\omega - \mathbf{SS}$ **,**

$\nabla^2 \mathbf{p}$ **,** $\omega\cdot\omega$ & **SS**

→ **dimensionally the same; (du/dx)(du/dx)**

(density ignored)

$$A(k)=\langle f(k)f(-k)\rangle=?$$
$$(\ f=-\nabla^2 p\ ,\ \omega\cdot\omega\ ,\ SS=\varepsilon/(2\nu)\ )$$

- $f(k)=-C_{abcd} \overset{\Delta}{\sum_{k=p+q}} p_a q_b u_c(p) u_d(q)$

for	(i)	$f=-\nabla^2 p$	→	$C_{abcd}=\delta_{ad}\,\delta_{bc}$
	(ii)	$f=\omega\cdot\omega$	→	$C_{abcd}=\varepsilon_{iac}\varepsilon_{ibd}=\delta_{ab}\,\delta_{cd}-\delta_{ad}\,\delta_{bc}$
	(iii)	$f=SS$	→	$C_{abcd}=(\delta_{ab}\,\delta_{cd}+\delta_{ad}\delta_{bc})/2$

$A=\langle f(k)f(-k)\rangle$

$$=\langle C_{abcd} \overset{\Delta}{\sum} p_a q_b\, u_c(p)u_d(q)\ f(k)\ \times C_{a'b'c'd'} \overset{\Delta}{\sum} p'_{a'} q'_{b'} u_{c'}(p')u_{d'}(q')\rangle$$

$$=C_{abcd}C_{a'b'c'd'} \overset{\Delta}{\sum}\overset{\Delta}{\sum} p_a q_b p'_{a'} q'_{b}\ \langle u_c(p)u_d(q)\ u_{c'}(p')u_{d'}(q')\rangle$$

Conclusion III

- A new stage of DNS may
  "catch the tail" of universality/scaling ?
  scaling range r : $L >> r >> \eta$ with $\Pi \sim \varepsilon$

  – R_λ=700 ~1200 > R_λ in Laboratory experiments

→ Direct & Quantitative Examination of Hypotheses/Theories such as K41, RSH, etc ?

The End

Thank you for your attention !