Workshop on Petascale Computing:
Its Impact on Geophysical Modeling and Simulation
5-7 May 2008, NCAR Mesa Laboratory

DNS of Turbulence under Simple Geometrical Conditions

– Universality in Small Scale Statistics –

Y. Kaneda

Nagoya University

Collaboration:

Yokokawa M. (Earth Simulator Center → Riken)
Itakura K. (Earth Simulator Center)
Uno A. (Earth Simulator Center → Riken)

Ishihara T.
Moroshita K.
Ishida T.
(Nagoya Univ.)

Computation on: VPP500, VPP5000 at Nagoya Univ. C.C.
& Earth Simulator

21st Century COE Program
`Frontiers of Computational Science’

Outline of Talk

I) Background Idea of our DNS

II) Isotropic Turbulence

III) Anisotropic Turbulence
Mean Shear, Stratification, Uniform Magnetic field

IV) What can be done by petascale computing ?

Objective

= To Understand/Explore

the Physics/Universality of Turbulence

by Direct Numerical Simulation (DNS)

of Canonical Turbulence

universality
= statistical property insensitive to the detail of external large scale conditions,
such as the boundary conditions, forcing, initial conditions, etc.

→May Provide sound basis for turbulence modeling for more complicated flow fields

Kolmogorov's Idea

Universality

at sufficiently large Re

at sufficiently small scale (away from boundaries)

→ justifies the use of simple BC and forcing,
for the exploring the universality at small scales,
and to achieve high Re.

Outline of Talk

I) Background Idea

II) Isotropic Turbulence: some lessons

III) Anisotropic turbulence
Mean Shear, Stratification, Uniform Magnetic Field

IV) What can be done by peta scale computing ?

Basic Equation

Equation (Navier-Stokes)

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu\Delta\mathbf{u} + \mathbf{f}$$

$$\nabla\cdot\mathbf{u} = 0$$

B.C. 2π–periodic in x,y,z

$$\mathbf{u}(\mathbf{x}) = \sum_{|\mathbf{k}|<k_{\max}} \hat{\mathbf{u}}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}$$

Forcing

$$\mathbf{f}(\mathbf{x}) = \sum_{\mathbf{k}} \hat{\mathbf{f}}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \hat{\mathbf{f}}(\mathbf{k}) = c(k)\hat{\mathbf{u}}(\mathbf{k})$$

$$c(k) = \begin{cases} c & (k < 2.5) \\ 0 & \text{otherwise} \end{cases}$$

cf.Jimenez et al.

I.C. Random phase

$$E(k) = ak^4 \exp(-bk^2)$$

Use of Spectral method with phase shift method to remove alias error

See Yokokawa et al. (2002), Kaneda & Yokokawa (2005)

Two Series of DNS

Possible on
the Earth Simulator

VPP

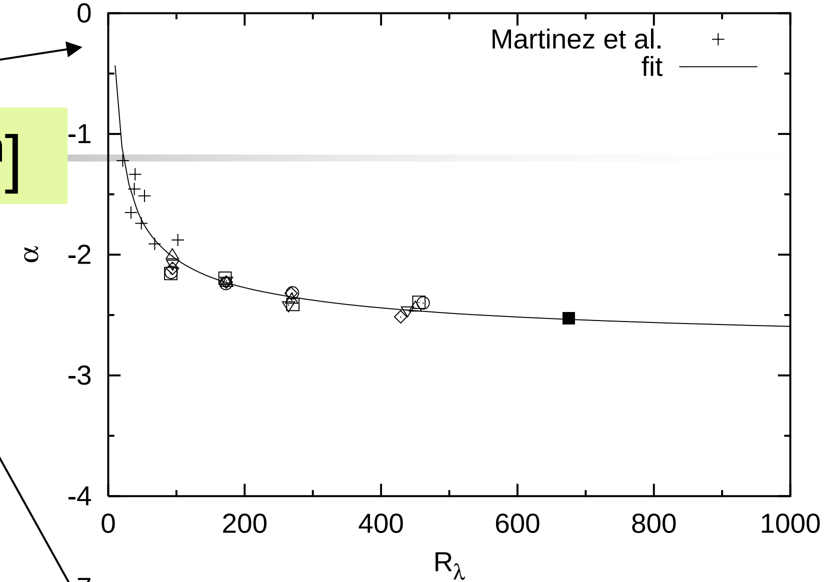
- Series 1 $(k_{max}\eta = 1)$
- Series 2 $(k_{max}\eta = 2)$

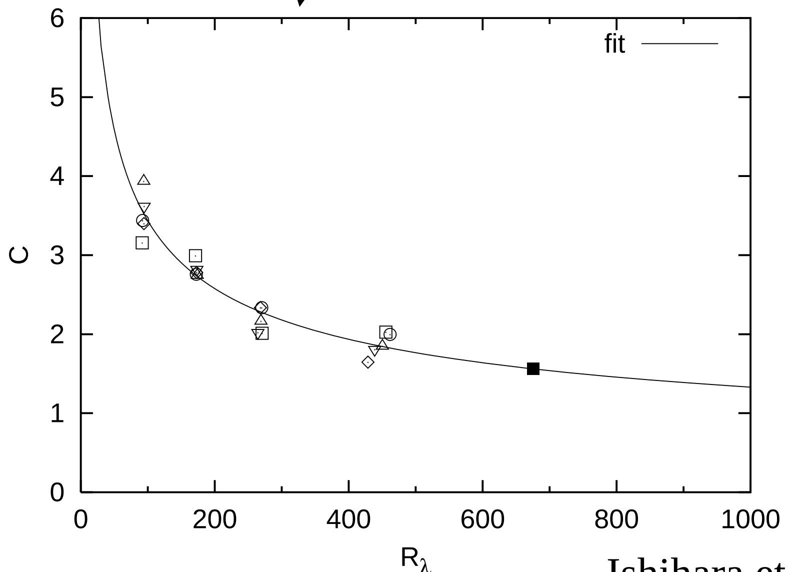
N	256^3	512^3	1024^3	2048^3	4096^3
R_λ	167	257	471	732	1131
R_λ	94	173	268	429	675

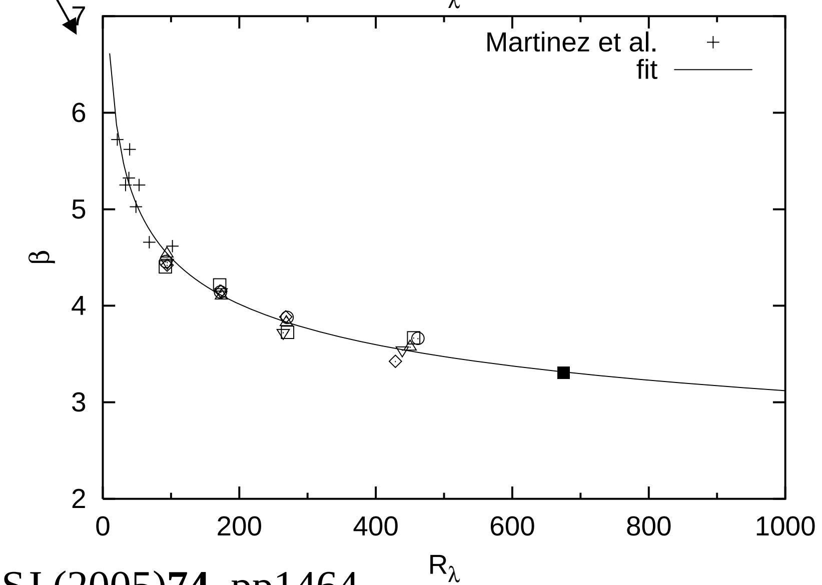
6.Energy spectrum in the near dissipation range

$E(k)/(\varepsilon\nu^5)^{1/4} = C\,(k\eta)^{\alpha} \exp[-\beta(k\eta)^n]$

(n=1)







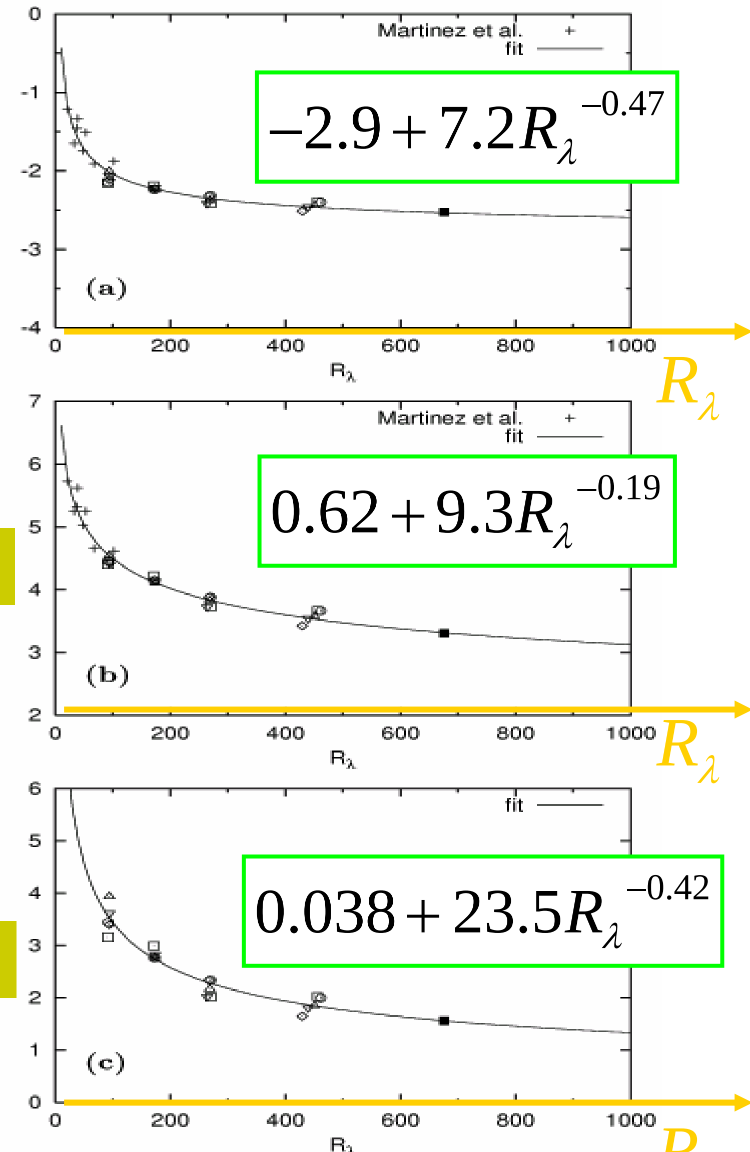
Ishihara et al. JPSJ (2005)**74**, pp1464

Dependence on R_λ

α, β and C approach to constants as $R_\lambda \rightarrow \infty$, but **the approach is slow**

e.g., $\beta(R_\lambda)-\beta_\infty / \beta_\infty \sim 2.61$, even at R_λ =10,000

+ : from Martinez, et al.(1997)



α: $-2.9 + 7.2 R_\lambda^{-0.47}$

β: $0.62 + 9.3 R_\lambda^{-0.19}$

C: $0.038 + 23.5 R_\lambda^{-0.42}$

Ishihara et al. JPSJ (2005)**74**, pp1464

II: Summary

1. DNS has reached at a stage where
   inertial subrange with $L/\eta \sim 1000$,

2. Some light on Asymptotic Small –Scale Statistics
   1. Normalized Energy Dissipation D (→ const)

   2. Dissipation range spectrum (→ converge to some form, but very slow)

   3. Statistics of velocity derivatives.
      Skewness, Flatness, 4^{th} order moments
      depend on Re (→ some kind of power laws, different at high R)

   4. PDF of Eulerian and Lagrangian accelerations
      Wider for Lagrangian than Eulerian
      Wider for higher time derivatives

Outline of Talk

I) Background Idea & Overview of our DNS

II) Isotropic Turbulence

III) Anisotropic turbulence
Mean Shear, Stratification, Uniform Magnetic field

IV) What can be done by petascale computing ?

Turbulence
= a system of huge degree of freedom

A paradigm of
Studies of systems of huge degree of freedom

→

Thermodynamics and Statistical Mechanics
for thermal equilibrium state

Analogy with
Statistical Mechanics for Near Equilibrium System

I. **Two kinds of universality**

characterizing the macroscopic state of the equilibrium system

not only

a) Equilibrium state itself,   like Boyle-Charles' law

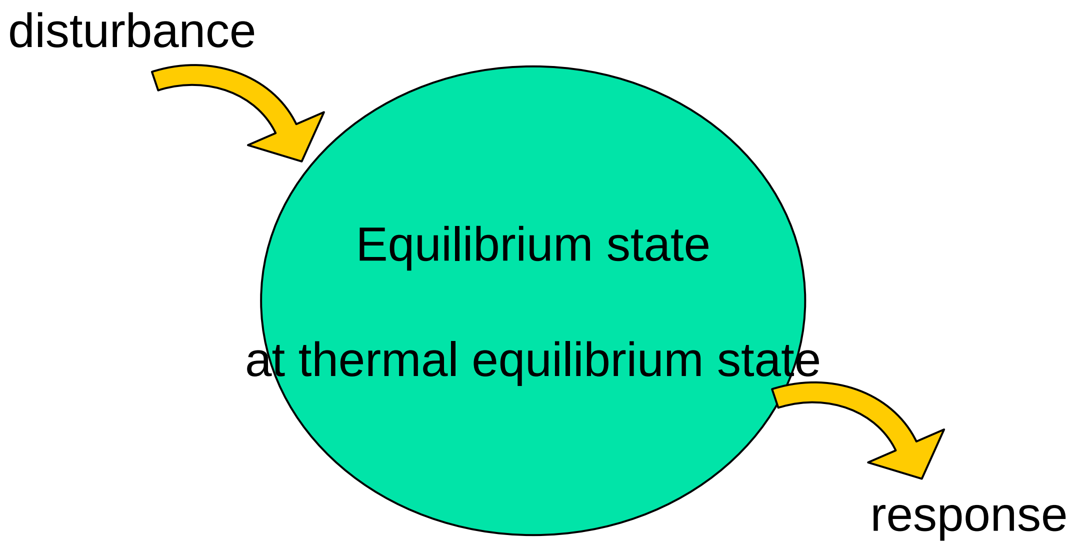
but also

b) **Response** to disturbance ⟷ **Universality of the 2nd Kind**

II. Thermal equilibrium state ←→ Universal equilibrium state at small scale

influence of external force, mean flow, etc. at small scale may be regarded as disturbance.

How dose the equilibrium state respond to the disturbance ?


disturbance
Equilibrium state
at thermal equilibrium state
response

Thermal Equilibrium system

Disturbance

X
grad ϕ
grad T
grad c

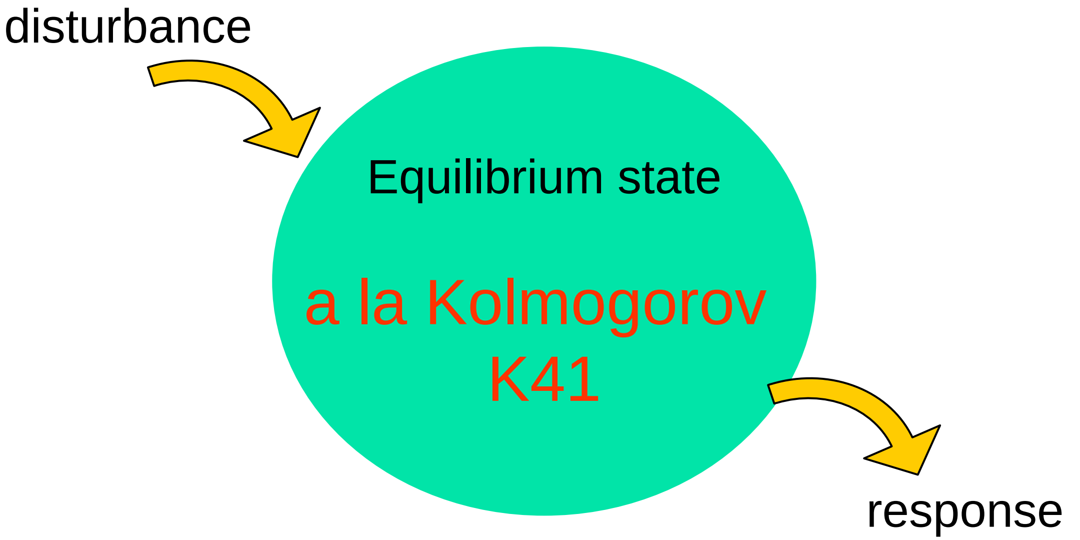
Equilibrium state

Linear response

$F = CX$	(Hooke's law)
$J = C'\ \mathrm{grad}\ \phi = \sigma E$	(Ohm's law)
$J = C''\ \mathrm{grad}\ T$	(Fourier's law)
$J = C'''\ \mathrm{grad}\ c$	(Fick's law)

Equilibrium State of Turbulence

How about turbulence ?


disturbance
Equilibrium state
a la Kolmogorov
K41
response

Disturbance

1. Mean Shear
2. Buoyancy by Stratification
3. Magneto-Hydrodynamic Force

Turbulent Shear Flow

NS-equation Local co-ordinate $\boldsymbol{v} = <\boldsymbol{v}> + \tilde{\boldsymbol{v}}$

$$\frac{\partial}{\partial t}\tilde{\boldsymbol{v}}(\boldsymbol{r},t) = -(\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} - \nabla q + \nu\nabla^2\tilde{\boldsymbol{v}} + \boxed{\boldsymbol{M},}$$

$$\underline{M_i} = S_{mn} r_n \frac{\partial \tilde{v}_j}{\partial r_m} + S_{ij}\tilde{v}_j$$

<u>Effect of mean shear</u>

Local strain rate of mean flow

$$\text{for } r \ll L, \; <\boldsymbol{v}> \sim S\boldsymbol{r}$$

$$(\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} \sim v_\ell^2/\ell, \qquad \nu\nabla^2\tilde{\boldsymbol{v}} \sim \nu v_\ell/\ell^2, \qquad \boldsymbol{M} \sim S v_\ell,$$

$$\tau_N \sim \ell/v_\ell, \qquad \tau_\nu \sim \ell^2/\nu, \qquad \tau_E \sim 1/S,$$

$$\boxed{\frac{\boldsymbol{M}}{(\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}}} \sim \frac{S v_\ell}{v_\ell^2/\ell} = \frac{S\ell}{v_\ell}} \propto S\ell^{2/3}/\epsilon^{1/3} \ll 1$$

$$\text{for } \ell \ll \ell_E = (\epsilon^{1/3}/S)^{3/2}.$$

Ishihara et al. PRL(2002) **88**, 15-#154501

Boussinesq approximation

$$\frac{\partial}{\partial t}\mathbf{u} = -(\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla p + \nu\nabla^2\mathbf{u} \boxed{-N\rho\mathbf{e}_3},$$

$$\nabla\cdot\mathbf{u} = 0,$$

Buoyancy by Stratification

$$\frac{\partial}{\partial t}\rho = -(\mathbf{u}\cdot\nabla)\rho + \kappa\nabla^2\rho \boxed{+Nu_3},$$

$$\tau_N \sim \ell/v_\ell, \qquad \tau_\nu \sim \ell^2/\nu, \qquad \tau_E \sim 1/N,$$

$$\tau_N/\tau_E \sim \delta(k) \equiv N/[kv(k)] \ll 1,$$

$$B_i(\mathbf{k},t) = -\frac{1}{(2\pi)^3}\int d^3\mathbf{r}\langle u_i(\mathbf{x}+\mathbf{r},t)\rho(\mathbf{x},t)\rangle e^{-i\mathbf{k}\cdot\mathbf{r}}.$$

$$P(\mathbf{k},t) = \frac{1}{(2\pi)^3}\int d^3\mathbf{r}\langle \rho(\mathbf{x}+\mathbf{r},t)\rho(\mathbf{x},t)\rangle e^{-i\mathbf{k}\cdot\mathbf{r}},$$

Kaneda & Yoshida, New J. Physics (2004) **6**-#34.

MHD approximation

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot \mathrm{grad})\,\boldsymbol{u} = -\frac{1}{\rho}\mathrm{grad}p + \nu\triangle\boldsymbol{u} + \boxed{\frac{1}{\rho}\boldsymbol{F}},$$

$$\mathrm{div}\boldsymbol{u} = 0,$$

Magnetic force

$$\frac{\partial \boldsymbol{B}}{\partial t} = (\boldsymbol{B}\cdot \mathrm{grad})\,\boldsymbol{u} - (\boldsymbol{u}\cdot \mathrm{grad})\,\boldsymbol{B} + \eta_{\mathrm{e}}\triangle\boldsymbol{B}$$

$$\mathrm{div}\boldsymbol{B} = 0$$

$$\boldsymbol{F} = \frac{1}{\mu_{\mathrm{e}}}(\boldsymbol{B}\cdot \mathrm{grad})\,\boldsymbol{B}$$

quasi-static approximation

$$\begin{aligned}\boldsymbol{F}' &= \frac{1}{\mu_{\mathrm{e}}}(\boldsymbol{B}\cdot \mathrm{grad})\,\boldsymbol{B}\\ &\simeq \frac{1}{\mu_{\mathrm{e}}}(\boldsymbol{B}_0\cdot \mathrm{grad})\,\boldsymbol{b} \quad + O(b^2)\\ &= -\frac{\sigma_{\mathrm{e}}}{\rho_{\mathrm{e}}}\triangle^{-1}(\boldsymbol{B}_0\cdot \mathrm{grad})^2\,\boldsymbol{u}\end{aligned}$$

Ishida & Kaneda, Phys. Fluids(2007) **19-**#075104

Two kind of measures
characterizing the universal equilibrium state

$\Delta\, \mathbf{Q_{ij}}$

$$<u_i(\mathbf{k})u_j(-\mathbf{k})> = \; Q_{ij}(\mathbf{k}) = \underline{Q_{ij}{}^{0}(\mathbf{k})} + \underline{C_{ij\alpha\beta}(\mathbf{k})}S_{\alpha\beta}$$

Not only

1) Equilibrium state itself

$$Q_{ij}^{(0)}(\mathbf{k}) = \frac{C_K}{4\pi}\varepsilon^{2/3}k^{-11/3}P_{ij}(\mathbf{k})$$

$$P_{ij}(\mathbf{k}) = \delta_{ij} - \hat{k}_i\hat{k}_j,\; \hat{k}_i = k_i/k$$

but also

2) Response to disturbance

Similar to stress vs. rate of strain relation:

$$\tau_{ij} = C_{ij\alpha\beta}\, S_{\alpha\beta}$$

(justified by the Linear response theory for non-equilibrium system)

Summary –III

For turbulence,
We don't know the pdf nor Hamiltonian in contrast to thermal equilibrium state

But we may assume
1) the existence of equilibrium state at small scale
(Universal) Local equilibrium state *a la* K41,
disturbance can be treated as perturbation to the inherent equilibrium state determined by the NS-dynamics

and see

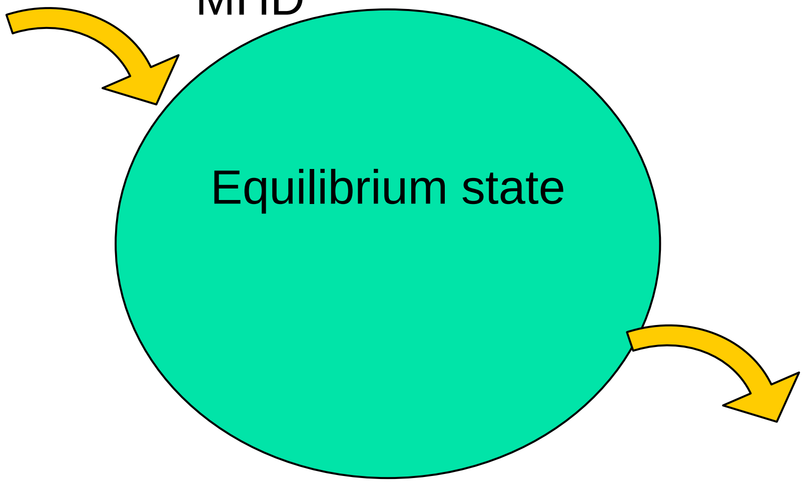
2) the response ← small disturbance
disturbances tested: Mean Shear, Stratification, MHD
(scalar field under mean scalar gradient, pressure spectrum in shear, jet . …)

But
3) The **anisotropy may remain large** even at small scales,
if Re is not high enough, so that the inertial subrange is not wide.

Summary –III

Mean shear
Stratification
MHD

Disturbance; X



Response: J

$$J_{ij} = \Delta Q_{ij} = C_{ijkm} X_{km}$$

Universal at high Re,
Independent of X

Outline of Talk

I) Background Idea & Overview of our DNS

II) Isotropic Turbulence

III) Anisotropic Turbulence
Mean Shear flow, Stratification, Uniform Magnetic Field

IV) What can be done by petascale computing ?

If $\epsilon/[U^3/L] \to const$, then

$$\frac{L}{\eta} \propto Re^{3/4}, \qquad \frac{T}{\tau_c} \propto Re^{3/4}, \quad \frac{T}{\tau_\nu} \propto Re^{1/2} \quad R_\lambda \propto Re^{1/2}$$

$$\frac{\tau_c U}{\Delta} \sim 1, \quad \frac{\nu \tau_\nu}{\Delta^2} \sim 1$$

$$N \propto \frac{L}{\eta} \quad \to \text{Computational Load} \;\; W \propto (N \log N)^3 \frac{T}{\tau_c}$$

$$\boxed{W \propto N^4 \propto Re^3 \propto R_\lambda^6}$$

- $N^3 = 4096^3$ DNS on ES:

  40TFlops, 10TB → 16.4 Tflops, 7.2 TB,

For N=12,000

3.2Pflops, 270 TB, 1Pflops, 200TB

Sustained performance ? Memory,

Isotropic Turbulence

(i) Low and high wave number range

Influence of Computation domain size, Resolution

(ii) Re dependence

(iii) High order statistics

A Constraint on DNS

~80?

See eg., Ishida et al. JFM(2006), **564**,pp455

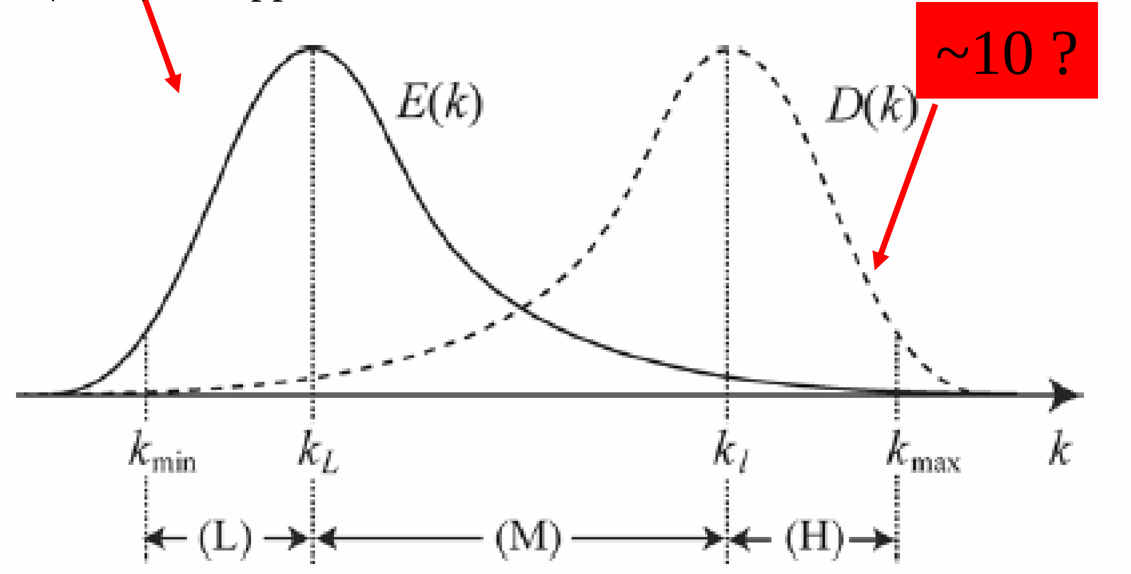
~2000

See eg. Schumaher et al.
New J. Phys (2007) **9**, pp89.

~10 ?

Wave-number range

$[k_{min}, k_{max}]$



Kaneda & Ishihara, JOT(2006) **7**-20,pp1

# of grid points in one direction

$$\frac{N}{2} \sim \frac{k_{max}}{k_{min}} = \frac{1/L}{k_{min}} \times \frac{1/\eta}{1/L} \times \frac{k_{max}}{1/\eta}$$

Anisotropic Turbulence

(i) Beyond scaling

→ Universal constants

(ii) Wall Bounded Turbulence

Universal Constants ?

When applied to Shear Flow Turbulence,

LRA gives not only the form

$$<u_i(\mathbf{k})u_j(-\mathbf{k})> = \quad Q_{ij}(\mathbf{k}) = Q_{ij}{}^{0}(\mathbf{k}) + C_{ij\alpha\beta}(\mathbf{k})S_{\alpha\beta}$$

$$a(k) = A\varepsilon^{1/3}k^{-13/3},\ b(k) = B\varepsilon^{1/3}k^{-13/3}$$

$$C_{ij\alpha\beta}(\mathbf{k}) = a(k)\left[P_{i\alpha}(\mathbf{k})P_{j\beta}(\mathbf{k}) + P_{i\beta}(\mathbf{k})P_{j\alpha}(\mathbf{k})\right] + b(k)P_{ij}(\mathbf{k})\hat{k}_\alpha\hat{k}_\beta$$

but also gives an estimate of the universal constants A and B.

LRA =Lagrangian Renormalized Approximation

Summary –IV

Want can be done by petascale computing?

1. Isotropic turbulence
   Larger domain, Higher resolution,
   Higher Re → Asymptotic statistics for Re →∞,
   Anomalous scaling/Intermittency

2. Anisotropic turbulence
   universality ?
   not only scaling, but also constants

3. Wall bounded turbulence with inertial subrange →?

The End