ON IMPLICIT LES FOR TURBULENT FLOWS

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What is ILES (MILES) ?

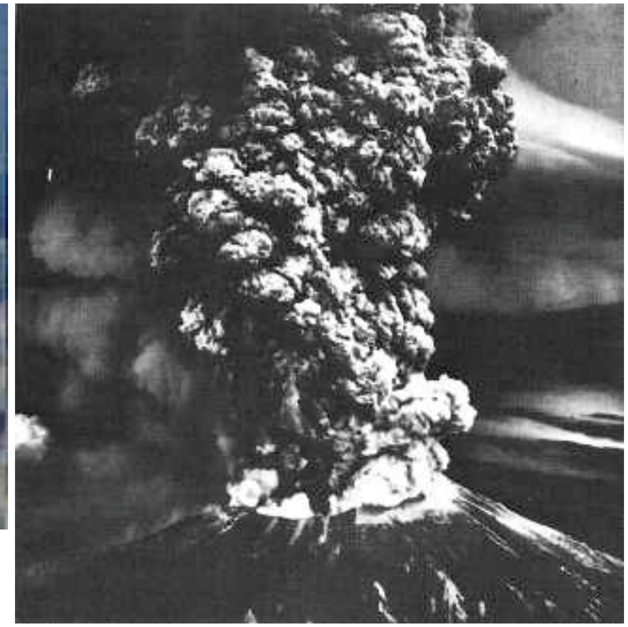
Historical Perspective & Motivation

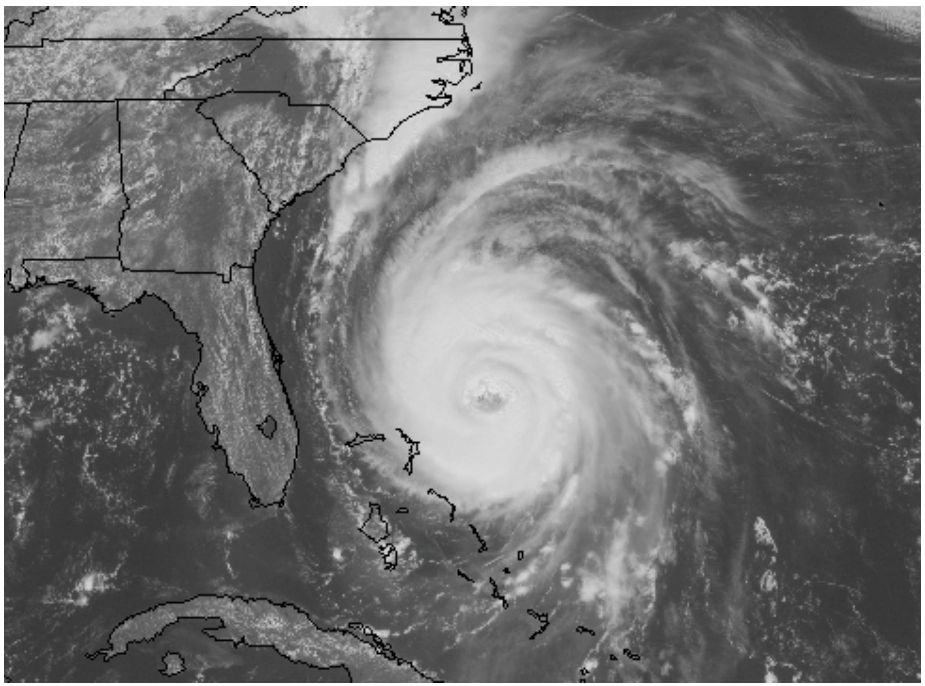
Capturing Physics with Numerics

Applications

canonical --> complex flow cases

Outlook



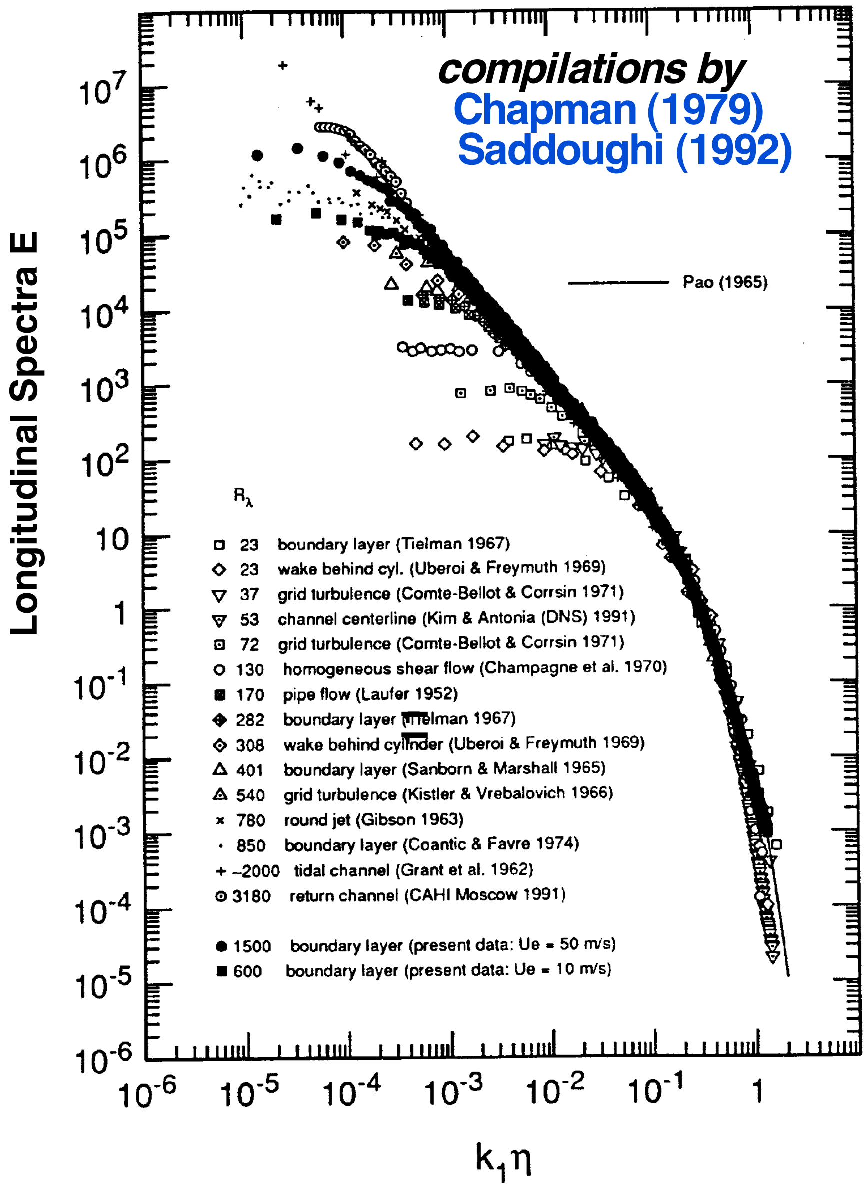


Numerical Simulation of Turbulent Flows is based on the N-S eqs.

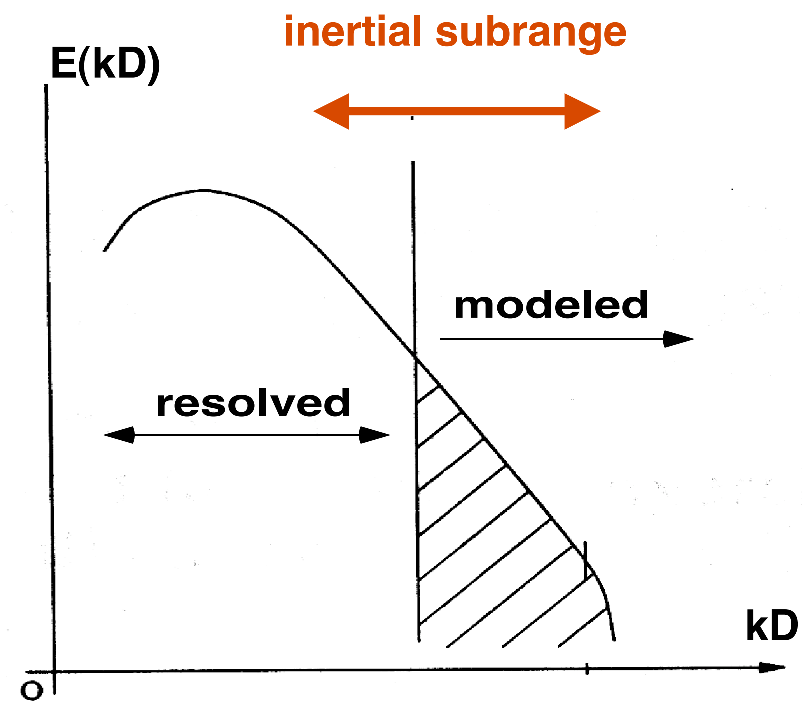
- **DNS, LES, RANS, ….**

DNS – ***solution for all scales without further assumptions*** **is prohibitive for most practical flows of interest !**

Turbulent Flow Energy Spectra



Large Eddy Simulation (LES) Approach



LES Assumptions & Issues:

- based on unsteady N-S equations
- large scales resolved
- smaller scale features modeled
- desirable modeling choices
  - ➢ cutoff within inertial subrange
  - ➢ smooth transition at cutoff

The Modified Equation (ME)
A framework for LES analysis

- **The Modified Equation provides the effective differential equation satisfied by the numerical solution by the given method**

  reproduces the original PDE, and includes the implicit SGS models associated with "error" terms as effective source terms

$$U_t + \nabla \cdot F(U) = \nabla \cdot \tau(U)$$

"error" in divergence form (FV formulation …)

- **Derived via Taylor series expansion**
- **Compliments standard numerical analysis**

  provides <u>nonlinear</u> "error" contributions as well …

ME analysis of LES

$$\bar{f}(\mathbf{x}_P) = \frac{1}{\delta V_P} \int_{\Omega_P} f(\mathbf{x}')G(\mathbf{x}' - \mathbf{x}_P, \Delta)\,dV'$$

LES ingredients

- low-pass filter the Navier-Stokes equations
- finite volume, element or difference discretization

$$\mathbf{v} \longrightarrow \bar{\mathbf{v}}_N$$

Modified LES Equations

(satisfied by numerical solutions)

$$\mathbf{B} = \overline{\mathbf{v} \otimes \mathbf{v}} - \bar{\mathbf{v}} \otimes \bar{\mathbf{v}}$$

$$\partial(\bar{\mathbf{v}}) + \nabla \cdot (\bar{\mathbf{v}} \otimes \bar{\mathbf{v}}) = -\nabla \bar{p} + \nabla \cdot \bar{\mathbf{S}} - \nabla \cdot \mathbf{B} + \boldsymbol{\tau} + \mathbf{m}$$

- $\nabla \cdot \mathbf{B}$: explicit SGS stress model
- $\mathbf{m}$: commutation error term
- $\boldsymbol{\tau}$: discretization "error" term

"well-resolved" LES requires: $\boldsymbol{\tau} \ll \nabla \cdot \mathbf{B} + \mathbf{m}$

NOTE: In the absence of an accepted turbulence theory,
SGS modeling must be based on
➔ rational use of empirical info ➔ *pragmatic practice …*

$$\mathbf{B} = \overline{\bar{\mathbf{v}} \otimes \bar{\mathbf{v}}} - \bar{\bar{\mathbf{v}}} \otimes \bar{\bar{\mathbf{v}}}$$

$$\partial(\bar{\mathbf{v}}) + \nabla \cdot (\bar{\mathbf{v}} \otimes \bar{\mathbf{v}}) = -\nabla \bar{p} + \nabla \cdot \bar{\mathbf{S}} - \nabla \cdot \mathbf{B} + \cdots$$

conventional (explicit) SGS stress models

Functional models: most popular, e.g., Smagorinsky eddy-viscosity (*involving isotropic SGS's*):

$$\mathbf{B} = -2\nu_k \bar{\mathbf{D}}_\mathrm{N} \qquad \nu_k = c_D \Delta^2 \,\|\, \bar{\mathbf{D}}_\mathrm{N} \,\| \qquad \bar{\mathbf{D}}_\mathrm{N} = \tfrac{1}{2}(\nabla \cdot \bar{\mathbf{v}}_\mathrm{N} + \nabla \cdot \bar{\mathbf{v}}_\mathrm{N}{}^\mathrm{T})$$

basic limitation: (B) and strain rate (D) are largely uncorrelated & topologically different ➔ assumption (B ∝ D) is inappropriate !

Structural models: better, e.g., scale-similarity & approx. deconvolution (*involving anisotropic SGS's*):

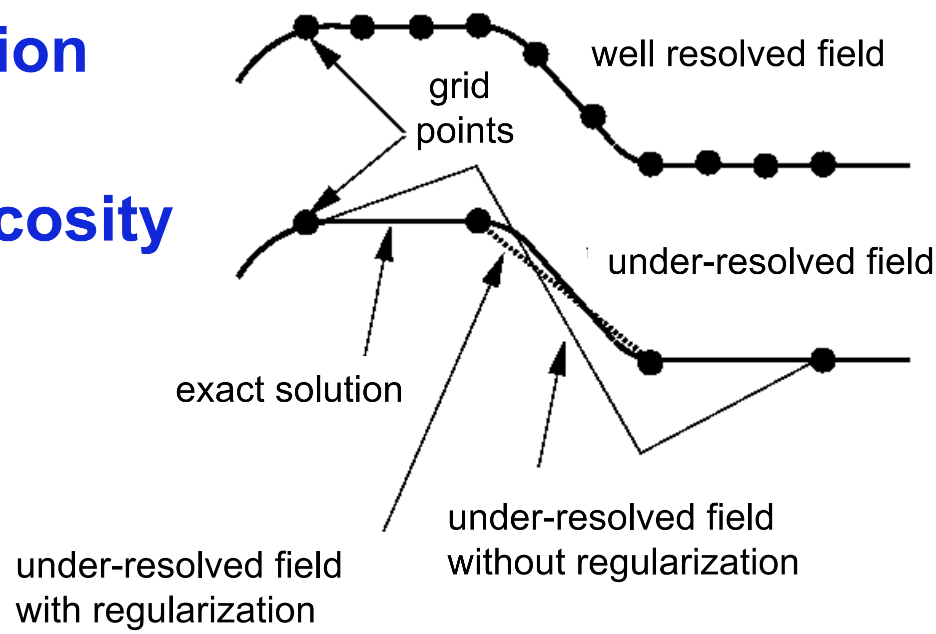
$$\mathbf{B}_2 = \overline{\bar{\mathbf{v}} \otimes \bar{\mathbf{v}}} - \bar{\bar{\mathbf{v}}}_N \otimes \bar{\bar{\mathbf{v}}}_N$$

- significantly more complex computationally
- typically, not dissipative enough by itself
- used with scalar eddy-viscosity type term in 'mixed' models, B= B_1 + B_2
  e.g., with $\mathbf{B}_1 = -2\nu_k \bar{\mathbf{D}}_\mathrm{N}$ ➔ which may defeat the potential gains …

--> non-conventional SGS modeling approaches need to be explored !

“Alternative” LES

- **hyperviscosity**
  Borue & Orszag
- **approximate deconvolution**
  Domaradzki, Adams
- ***ab-initio* scale separation**
  Temam, Hughes
- **spectral vanishing viscosity**
  Karniadakis
- **implicit SGS modeling**
  --> ILES, MILES



Implicit LES

- FV framework

  $$\text{"error" term} \rightarrow \nabla\cdot\boldsymbol{\tau}$$

- ME analysis

$$\partial(\overline{\mathbf{v}}) + \nabla\cdot(\overline{\mathbf{v}}\otimes\overline{\mathbf{v}}) =$$
$$-\nabla\overline{p} + \nabla\cdot\overline{\mathbf{S}} - \nabla\cdot\mathbf{B} + \nabla\cdot\boldsymbol{\tau} + \mathbf{m}$$

$$\mathbf{B} = \overline{\mathbf{v}\otimes\mathbf{v}} - \overline{\mathbf{v}}_N\otimes\overline{\mathbf{v}}_N$$

- ***No explicit filtering:*** **no commutation error term (m≡0);**

  discretization provides top-hat-shaped-kernel

  filtered values through $\bar{f}_P \equiv 1/\delta V_P \int_{\Omega_P} f dV$

- **B≡0:** ***minimal*** **SGS model, decoupled GS's & SGS's**

When based on stable (consistent) numerics, ***ILES converges*** **to DNS** ***to the same extent expected from any LES***

(***cutoff length*** *determined by explicit* ***or*** *implicit* filter --> 0)

When based on NFV numerics, **ILES is competitive with classical LES in the** ***LES realm proper*** (convectively dominated flows driven by large scale features)

ILES = Free Lunch ?

Not all implicit SGS modeling will work !

The numerical scheme has to be constructed such that lead truncation “errors“ satisfy required SGS-model properties i.e., **SGS physics must be built into the numerics !**

→ **nonlinear discretization is required**

Analogy:

Shock-capturing schemes designed under the requirements:

- Convergence to weak solution
- Entropy condition satisfied

Likewise: sharp-gradient capturing FV schemes can be viewed as relevant for ILES -- if we focus on the small scale characteristic features of turbulence ….

Implicit LES: Historical Precedents (courtesy, Bill Rider, LANL)

Smagorinsky's EV based on von Neumann-Richtmyer viscosity in 3D

$$C_{\mathrm{AV}} h^2 |u_x| u_x \Rightarrow C_{\mathrm{Smag}} h^2 \|\nabla u\| \nabla u$$

- J. Smagorinsky, *Advances in Geophysics*, Vol. 25, 1983, gives a history of the first weather calculations (Phillips) and a meeting where they were discussed. S's work followed from using vN's viscosity to cure ringing.

➔ first shock capturing and first LES have same basis !

Artificial viscosities (Q's) have become adaptive to the flow physics

- In 1955 Rosenbluth suggested Q's be turned off in expansions.
- Q's have been connected to the properties of the materials (Kurapatenko) and Riemann solvers (Dukowicz)
- Q's are now dynamic. Using methods from the high-resolution world (i.e., limiters) the Q's turn off in smooth resolved flow

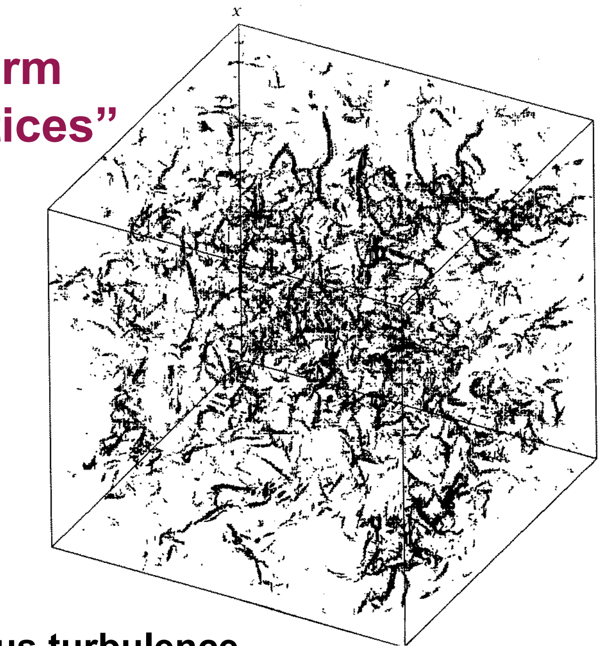
  ➔ *philosophically suggestive of the dynamic Smagorinsky model …*

➔ shock capturing methods and LES have evolved similarly !

Physical Requirements for nonlinear Implicit SGS Models

Inherent small-scale anisotropy of high-Re turbulent flows

- ➔ adaptiveness to local flow physics
- ➔ sharp velocity-gradient capturing



homogeneous turbulence
DNS, Vincent & Meneguzzi 1991

Inherently discrete nature of laboratory observables:

- ➔ conservative FV schemes

Other desirable requirements

- ➔ dissipative relevant solutions
- ➔ nonlinear stability
- ➔ positivity (where needed)

- ➔ Nonoscillatory FV (NFV)
- → FCT, PPM, MPDATA
- → Other NFV: e.g., Hybrid

Implicitly-Implemented SGS Modeling --> ILES

eng	**Local monotonicity preservation (MILES)** FCT [Boris '89, Boris, FFG, et al. '92, Fureby & FFG '99-'04]
astro	PPM [Porter, Woodward, et al., '94, '98, '00, …]
eng	Godunov's Riemann solvers [Knight et al. '00, …]
	Upwinding
eng	Third-Order Upwind-Biased Scheme [Kuwahara, …,'89, …]
geo	MPDATA [Margolin, Smolarkiewicz, Rider '00, '02, …]
	Vorticity confinement [Steinhoff et al. '92, ...]
eng	**Hybrid methods** [Youngs,'91,… Garnier et al. '99, Drikakis '02,…]
	Other related: approx. deconvolution [Adams, Domaradzki, ….]

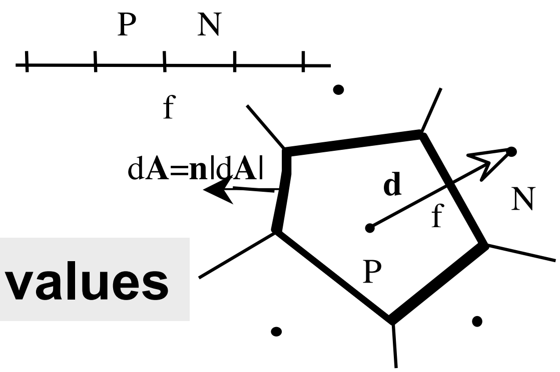
Modified LES Equation used as theoretical framework for ILES

➔ lead discretization "error" terms introduced by NFV schemes provide:

- ➔ implicit SGS models of ***mixed anisotropic*** type (Fureby & Grinstein 1999)
- ➔ regularized motion of ***discrete observables*** (Margolin & Rider 2002)

Finite Volume Discretization of the raw N-S eqs. for MILES (momentum equations exemplified)

Fureby & Grinstein, AIAAJ '99, JCP '02



Finite-volume (top-hat-shaped kernel filtered) values

$$f_P = \frac{1}{\delta V_P} \int_{\Omega_P} f dV$$

Use Gauss' theorem to obtain semi-discretized NSE; integrate over time with a multi-step method parametrized by *m*, {a_i, b_i},

$$\sum_{i=0}^{m} (\alpha_i (\mathbf{v})_P^{n+i} + \frac{\beta_i \Delta t}{\delta V_P} \sum_f [\mathbf{F}_f^{C,v} + \mathbf{F}_f^{D,v}]^{n+i})$$

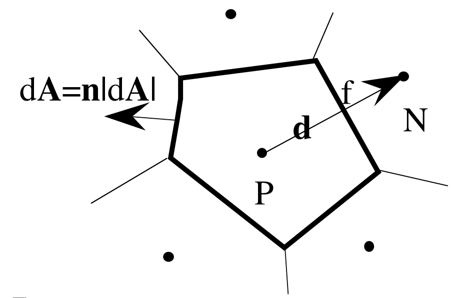
$$= -\sum_{i=0}^{m} \beta_i (\nabla p)_P^{n+i} \Delta t,$$

where, the {F's} are convective, diffusive, and auxiliary fluxes

Functional reconstruction based on Flux-Limiting

Example: momentum equation, 2nd. order fluxes

Blend High- & Low-order convective fluxes using flux limiter Γ



$$\mathbf{v}_f^C = \Gamma \mathbf{v}_f^{C,H} + (1-\Gamma)\mathbf{v}_f^{C,L}, \quad \Gamma = \Gamma(\mathbf{v}, \mathbf{x}, t)$$

$$\begin{cases} \mathbf{F}_f^{C,v,H} = F_f^{C,\rho}[l\mathbf{v}_P + (1-l)\mathbf{v}_N - \tfrac{1}{8}(\mathbf{d}\otimes\mathbf{d})\nabla^2\mathbf{v} + \ldots], \\ \mathbf{F}_f^{C,v,L} = F_f^{C,\rho}[\beta^+\mathbf{v}_P + \beta^-\mathbf{v}_N + (\beta^+ - \beta^-)(\nabla\mathbf{v})\mathbf{d} + \ldots]; \\ \qquad \beta^{\pm} = \tfrac{1}{2}(\mathbf{v}_f \cdot d\mathbf{A} \pm |\mathbf{v}_f \cdot d\mathbf{A}|)/|\mathbf{v}_f \cdot d\mathbf{A}|, \end{cases}$$

$$\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = -\nabla p + \nabla\cdot\mathbf{S} + \rho\mathbf{f}$$
$$+\nabla\cdot\{\rho(\mathbf{C}\mathbf{L}^T + \mathbf{L}\mathbf{C}^T + \chi^2\mathbf{L}\mathbf{d}\otimes\mathbf{L}\mathbf{d}) + \tfrac{1}{6}\mu(\mathbf{d}\otimes\mathbf{d})\nabla^3\mathbf{v} + \ldots\},$$

$$\mathbf{C} = \chi(\mathbf{v}\otimes\mathbf{d}) \qquad \mathbf{L} = \nabla\mathbf{v} \qquad \chi = \tfrac{1}{2}(1-\Gamma)(\beta^- - \beta^+)$$

MILES Modified Equation Analysis (CF & FFG, '99, '02,…)
Functional reconstruction based on Flux-Limiting
(e.g., momentum equation, 2nd. order fluxes)

Blend High- & Low-order
convective fluxes
using flux limiter Γ

$$\mathbf{v}_f^C = \Gamma \mathbf{v}_f^{C,H} + (1-\Gamma)\mathbf{v}_f^{C,L}, \quad \Gamma = \Gamma(\mathbf{v},\mathbf{x},t)$$

$$\mathbf{C} = \chi(\mathbf{v} \otimes \mathbf{d}) \qquad \mathbf{L} = \nabla \mathbf{v} \qquad \chi = \tfrac{1}{2}(1-\Gamma)(\beta^- - \beta^+)$$

$$\partial_t(\rho\mathbf{v}) + \nabla \cdot (\rho\mathbf{v} \otimes \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{S} + \rho\mathbf{f}$$
$$+ \nabla \cdot \{\rho(\mathbf{C}\mathbf{L}^T + \mathbf{L}\mathbf{C}^T + \chi^2 \mathbf{L}\mathbf{d} \otimes \mathbf{L}\mathbf{d}) + \tfrac{1}{6}\mu(\mathbf{d} \otimes \mathbf{d})\nabla^3\mathbf{v} + \ldots\},$$

generalized eddy-viscosity *anisotropic scale-similarity* ***MILES***

lead-order convective truncation

lead-order viscous truncation

$$\partial_t(\bar{\rho}\tilde{\mathbf{v}}) + \nabla \cdot (\bar{\rho}\tilde{\mathbf{v}} \otimes \tilde{\mathbf{v}}) = -\nabla \bar{p} + \nabla \cdot (\bar{\mathbf{S}}) + \bar{\rho}\tilde{\mathbf{f}}$$
$$- \nabla \cdot (\mathbf{B}) - \tfrac{1}{8}\nabla \cdot \{(\mathbf{d} \otimes \mathbf{d})\nabla^2\tilde{\mathbf{v}} + \tfrac{1}{6}\mu\nabla \cdot (\mathbf{d} \otimes \mathbf{d})\nabla^3\tilde{\mathbf{v}} + \ldots$$

conventional LES

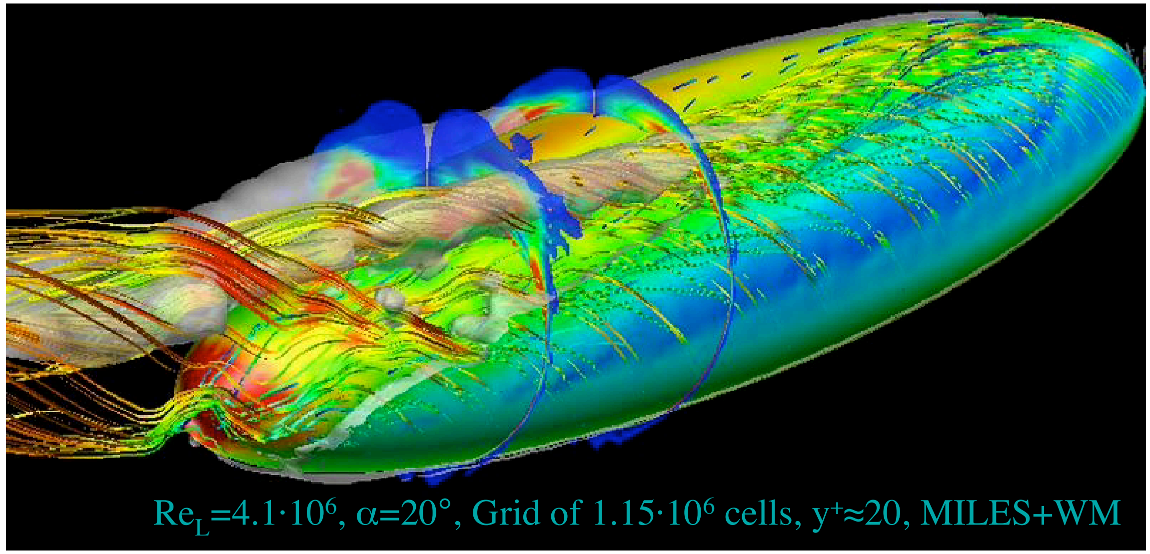
explicit SGS model

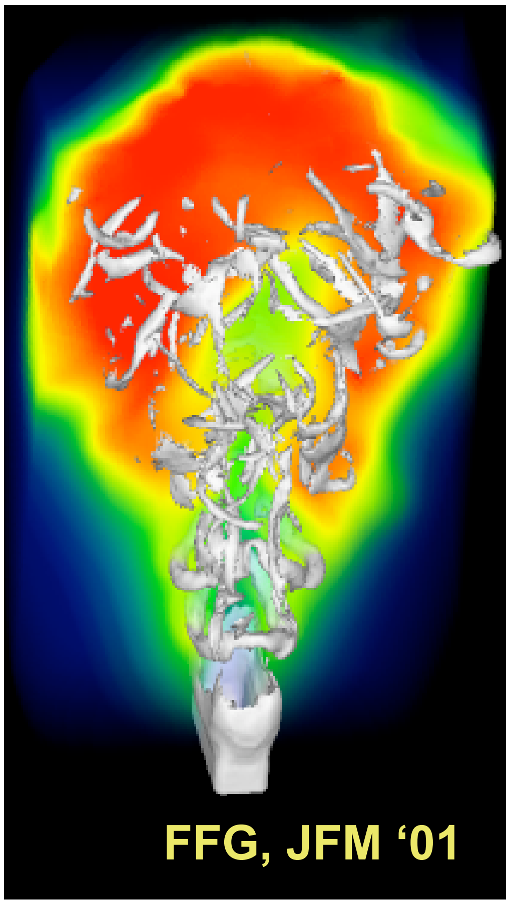
lead truncation terms

Extensive MILES applications …

- canonical --> complex
- free & wall bounded
- **competitive with LES !**

Fureby et al., AIAA J. ’04

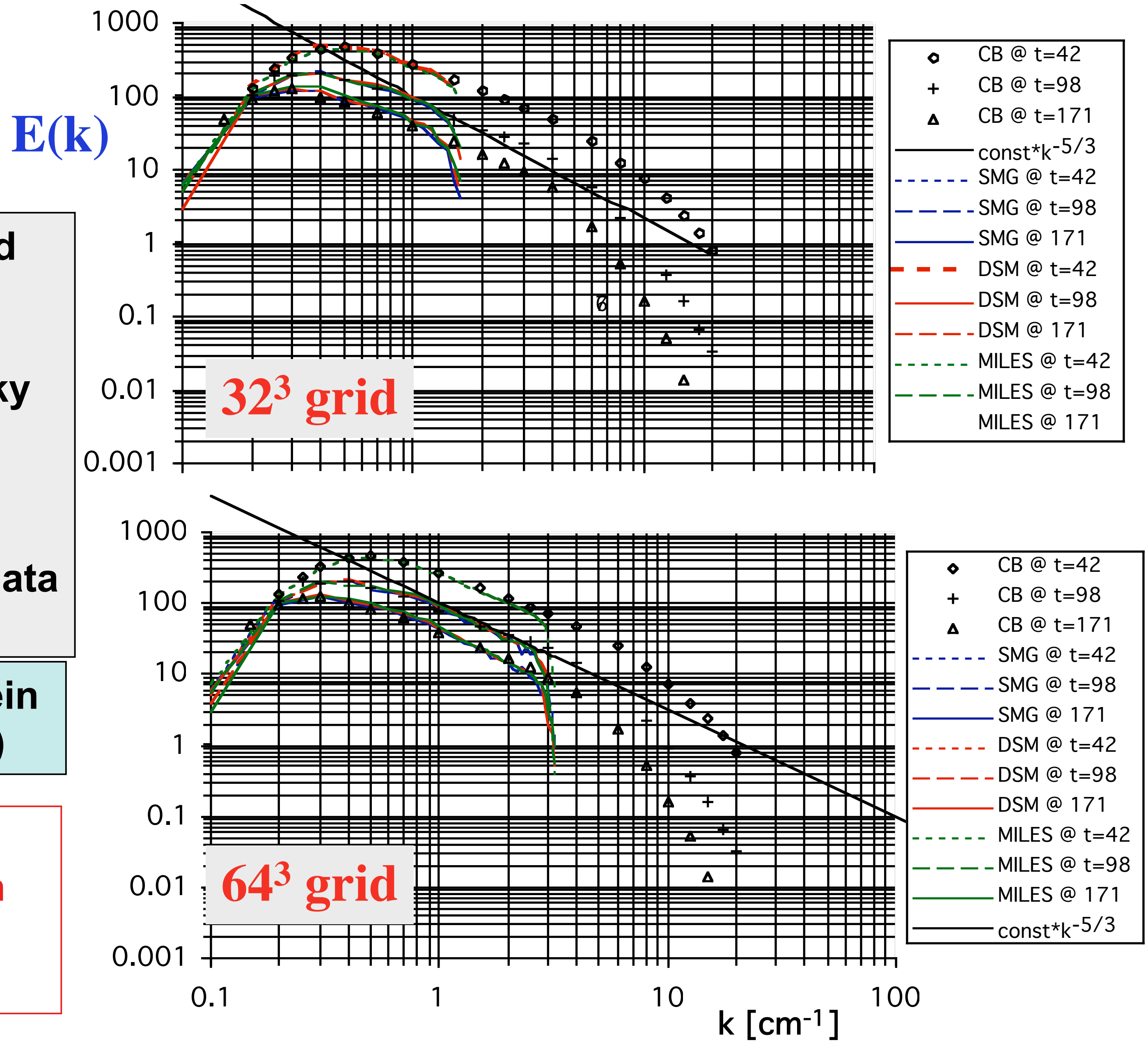




FFG, JFM ‘01

challenging new needs
Boris et al., 2003

TURBULENCE DECAY RATES CAPTURED WITH LES



MILES : FCT-based
DSM : Differential Stress Model
SMG : Smagorinsky Model

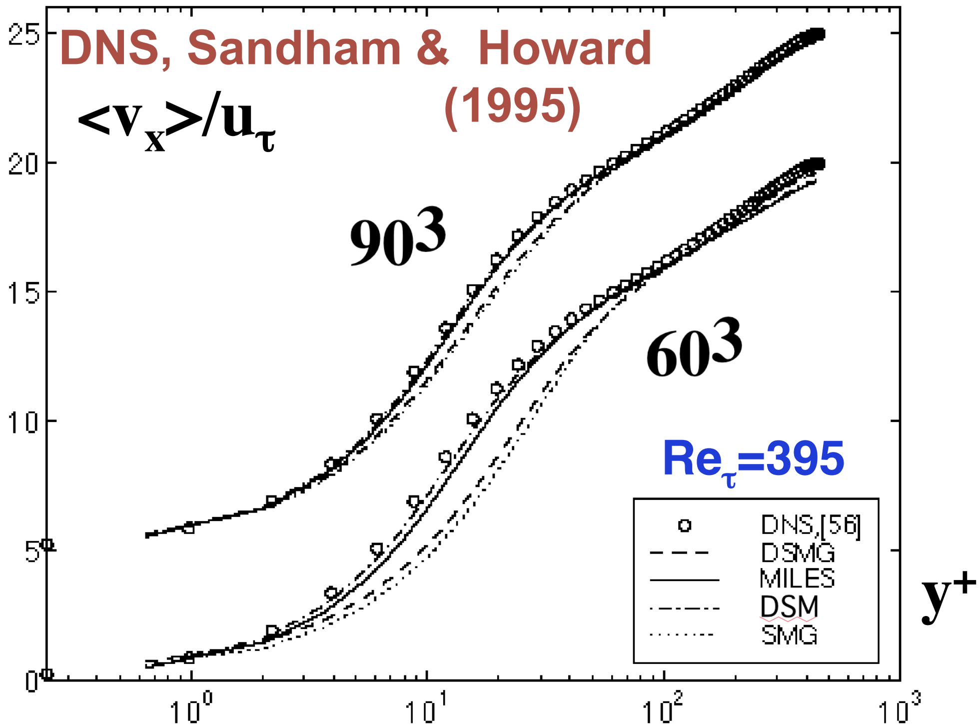
CB : Comte-Bellot Laboratory Data (JFM '71)

Fureby & Grinstein
JCP (Sept. '02)

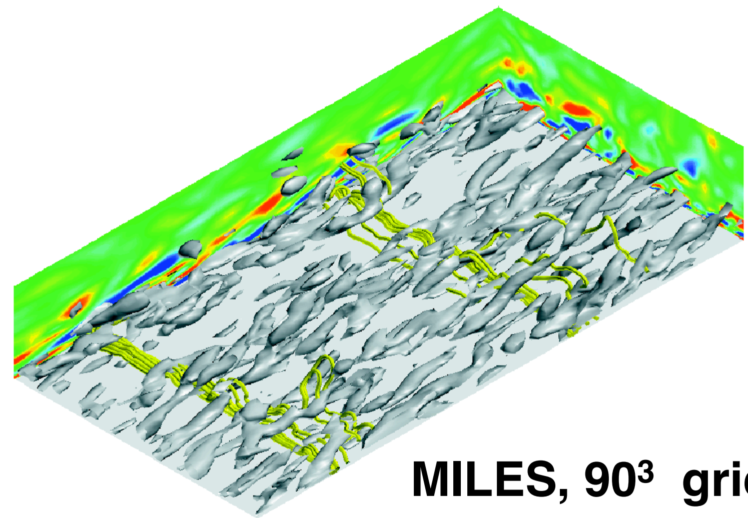
Excellent recent comparisons with JHU data
(B.Rider, X-7)

Turbulent Channel Flows

Fureby & Grinstein, JCP 2002



typical cost:
SMG=1, MILES=0.90, DSM=1.60



MILES, 90^3 grid

MILES : FCT-based
DSM : Differential Stress Model
SMG : Smagorinsky Model
DSMG : Dynamic Smagorinsky Model

MILES reproduces first & second order moments of the velocity field

- **almost as accurately as significantly more-complex SGS models**
- **better than isotropic eddy viscosity models**

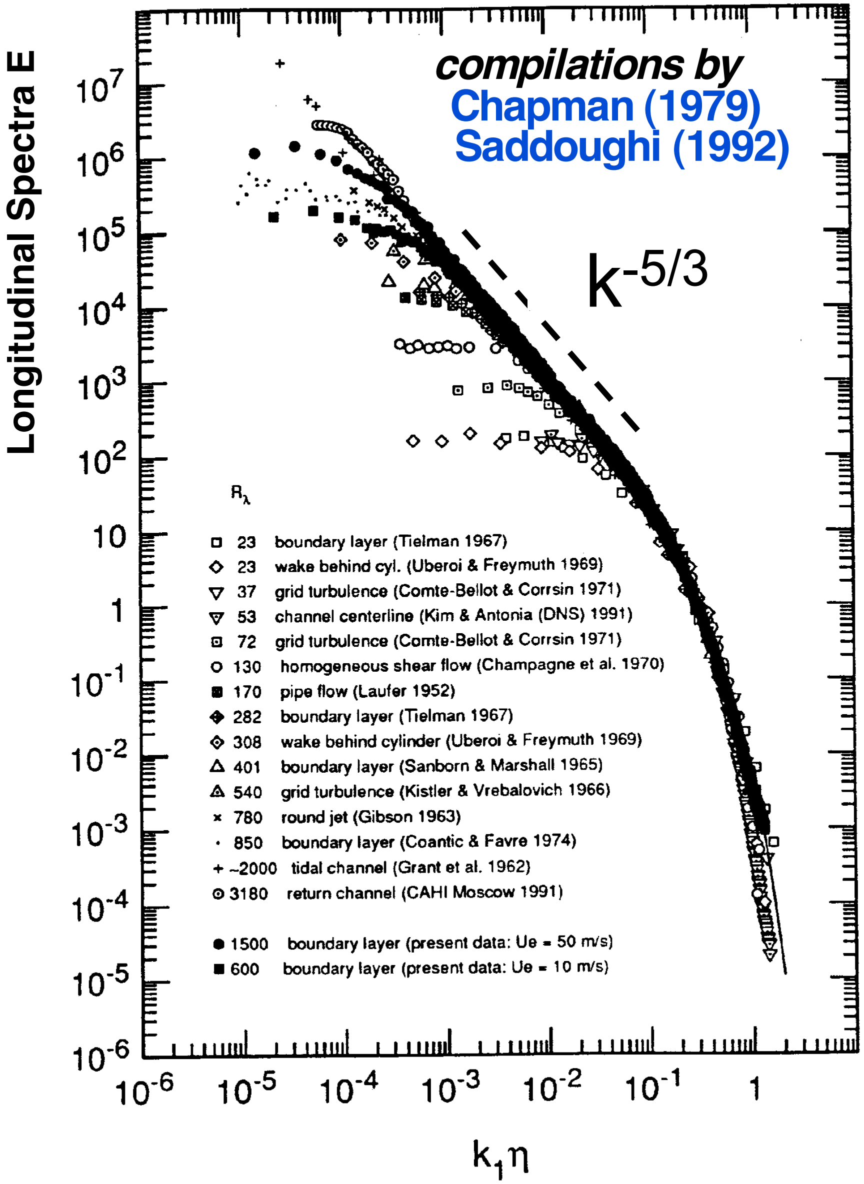
Recent Validation Studies:

Transition & turbulence decay in

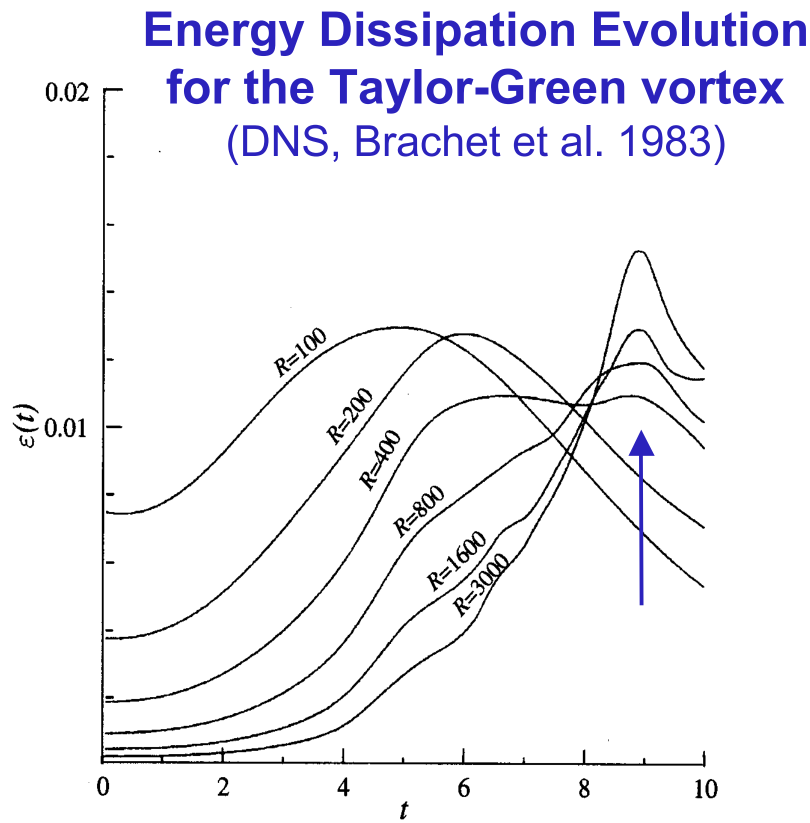
the Taylor-Green Vortex

Empirical Laws of High-Re Developed Turbulence

Inertial Subrange



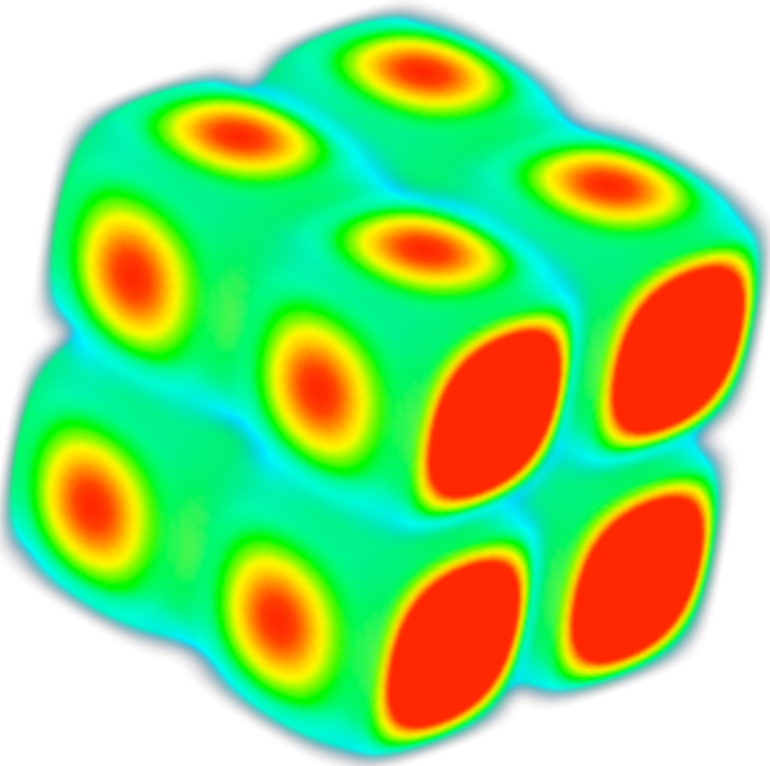
Finite Energy Dissipation



finite positive
(ν-independent)
limit for high-Re

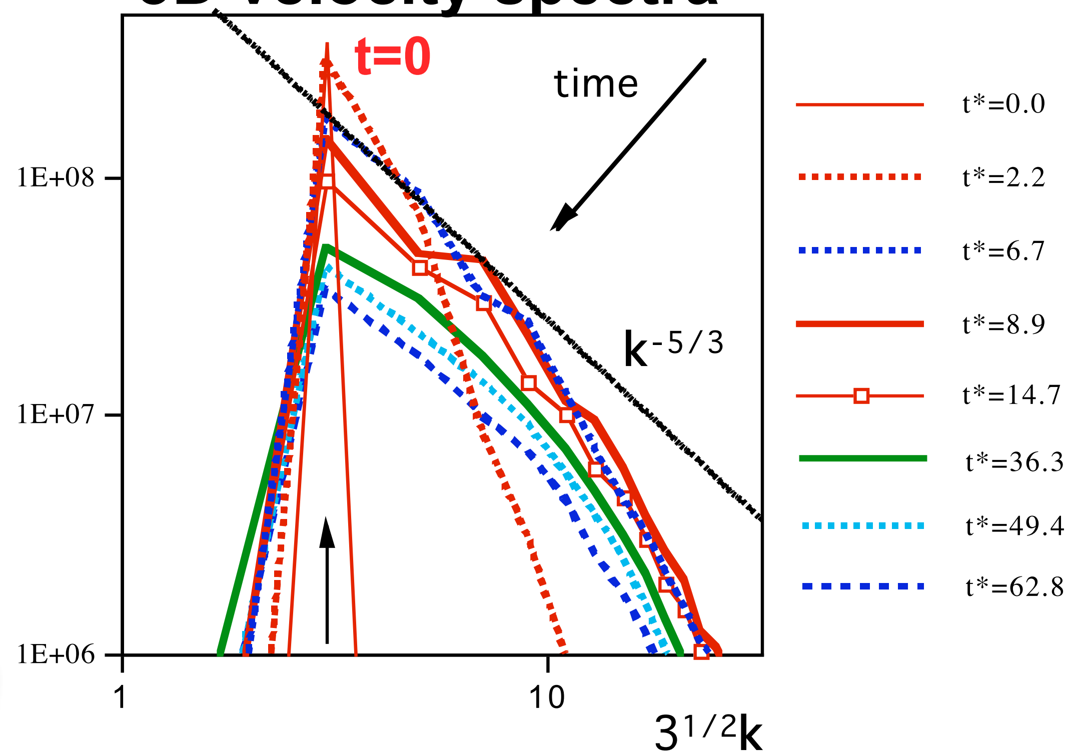
Evolution of the Taylor-Green Vortex

LES vs. MILES, various limiters (FCT, hybrid ...)



vorticity magnitude

3D velocity spectra



$u_o = U_o \sin(x)\ \cos(y)\ \cos(z),$

$v_o = -\ U_o \cos(x)\ \sin(y)\ \cos\ (z),$

$w_o = 0,$

$P_o = P_{oo} + [\rho(U_o)^2/16]$

$\times\ [\ 2 + \cos(2z)\ ] \cdot [\ \cos(2x) + \cos(2y)]$

Mach number ~ 0.3

FFG, Drikakis, Fureby, Youngs, DLES6, Poitiers, 2005

ILES of Turbulent Flows with NFV Schemes

- ***A "natural" extension of shock-capturing concepts for compressible turbulent flow …***

- ***The effects of the SGS physics on the GS's are incorporated in the functional reconstruction of the convective fluxes; focus on near cutoff emulation of***
  - *inherently discrete nature of observables*
  - *small-scale vorticity organization: worms*

- ***ILES has been successfully applied to broad range of free and wall-bounded flows in engineering, geophysics, and astrophysics;*** *canonical --> complex flows*

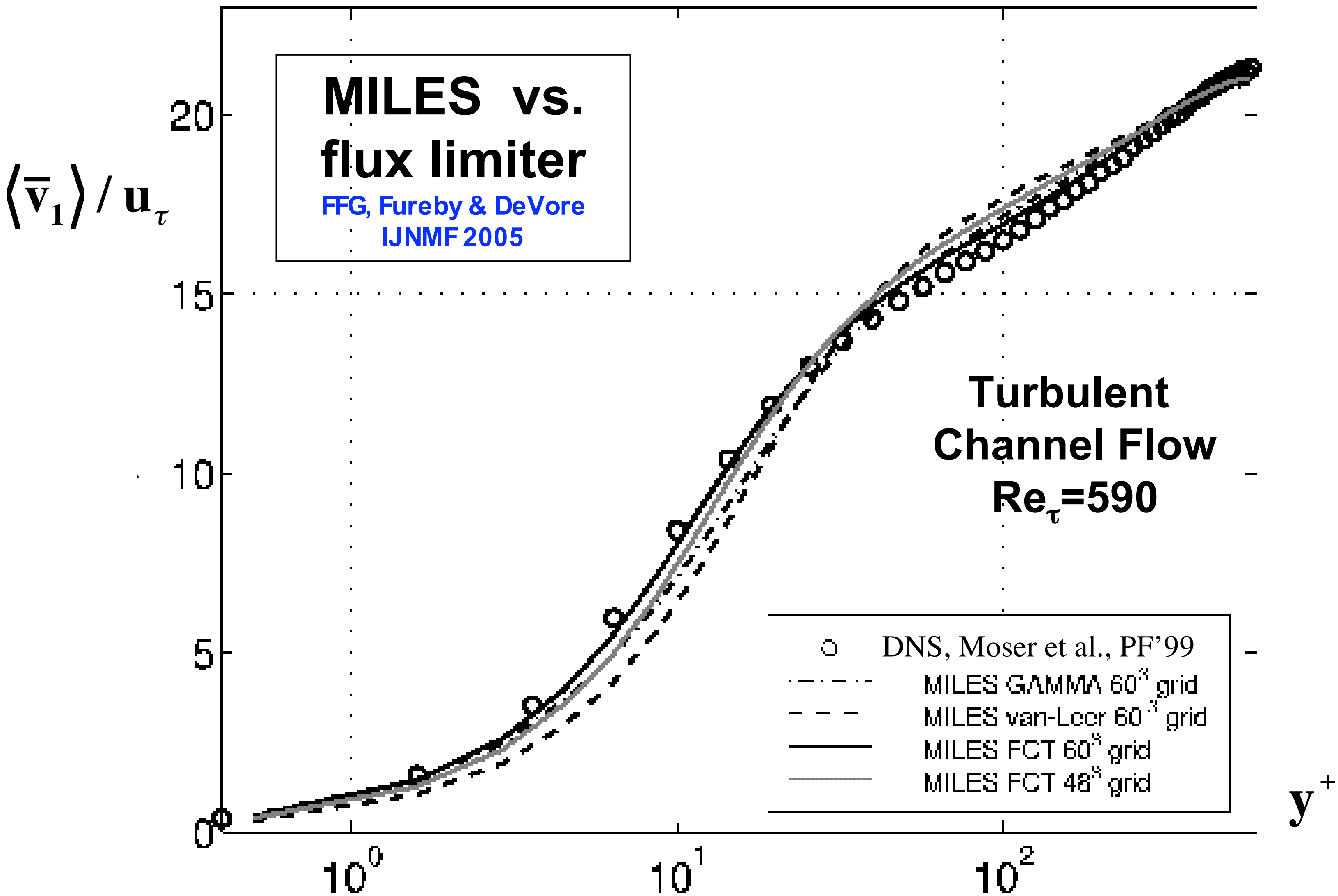
- **Modified LES Equation as theoretical framework for ILES**

  ➔ **lead discretization "error" terms provide:**

  ➔ **implicit SGS models of mixed anisotropic type**

  ➔ **regularized motion of discrete observables**

- ***implicit SGS model depends on scheme specifics, …***

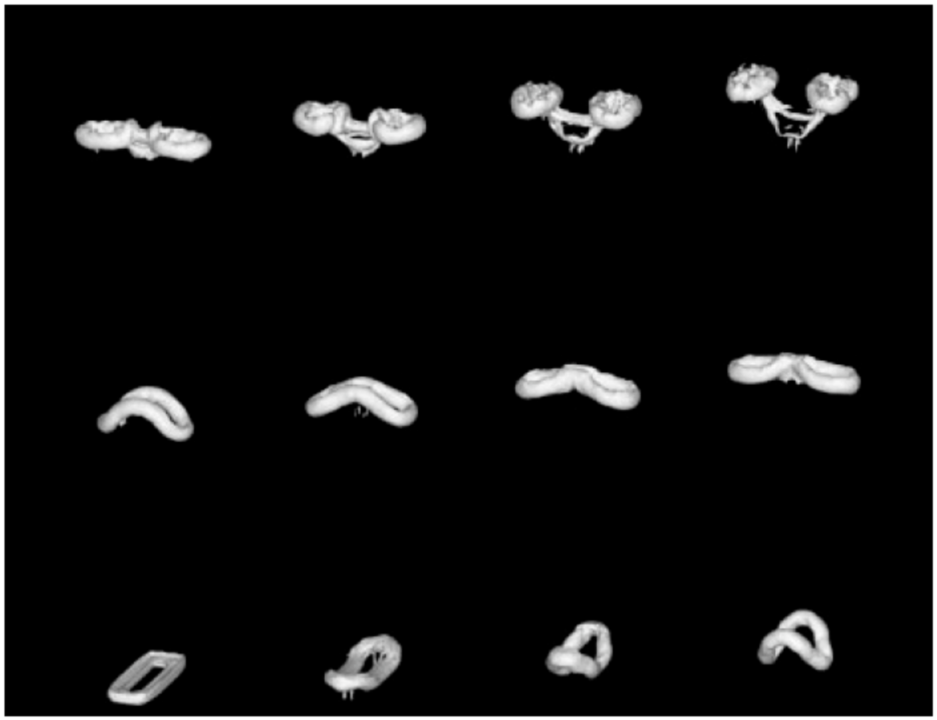


TVD is generally too diffusive … locally monotonic schemes, e.g., FCT, GAMMA, (and PPM) appear to work best for ILES ("better" worm emulation …)

FCT-based MILES of Rectangular Jets
with 2D⊗1D splitting (transverse ⊗ streamwise)

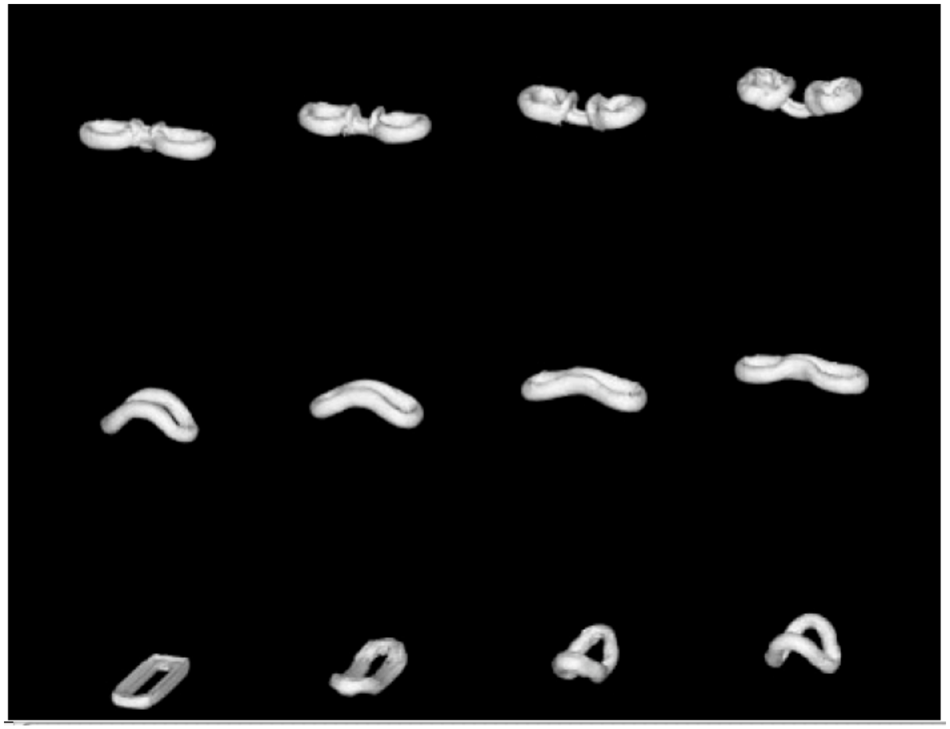
FFG, Fureby & DeVore, IJNMF 2005

positivity- but not monotonicity-preserving



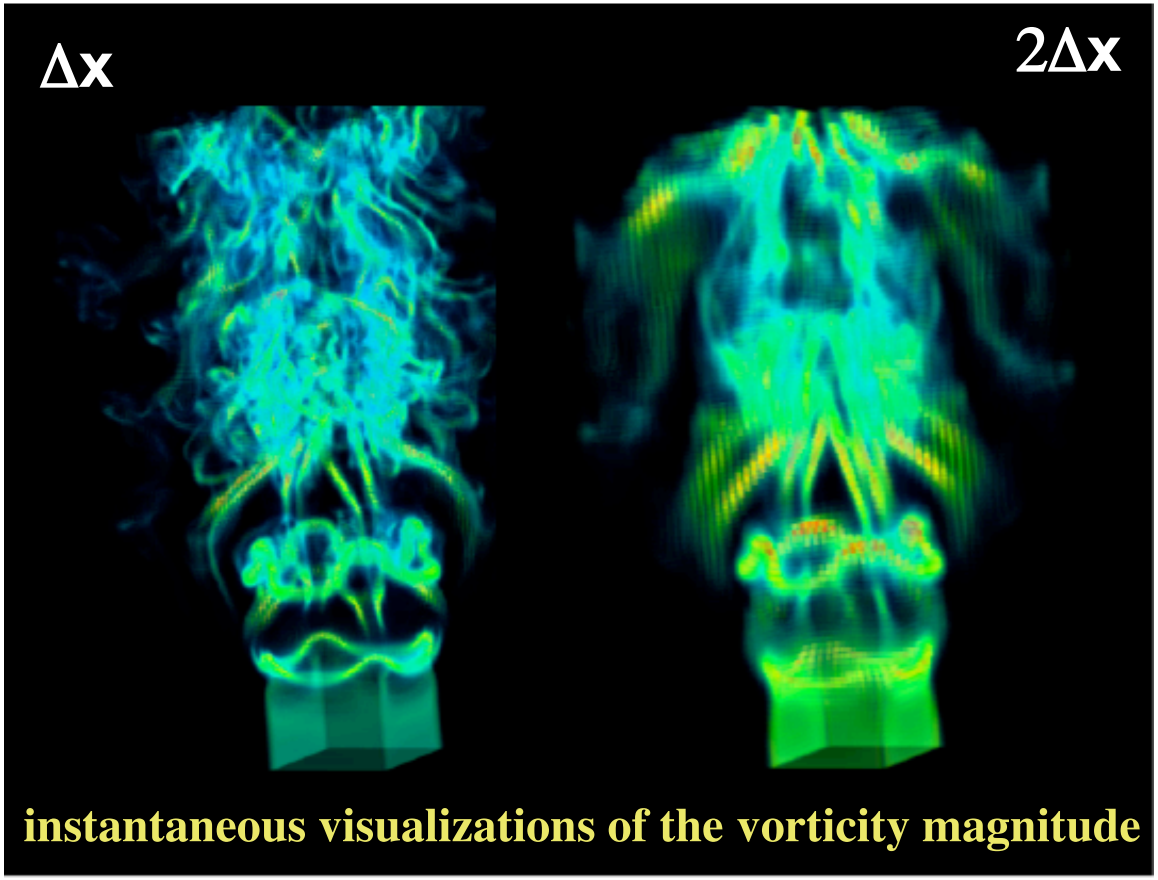
using Zalesak's 2D FCT limiter

with additional pre-limiting step enforcing local (FCT) monotonicity in each direction

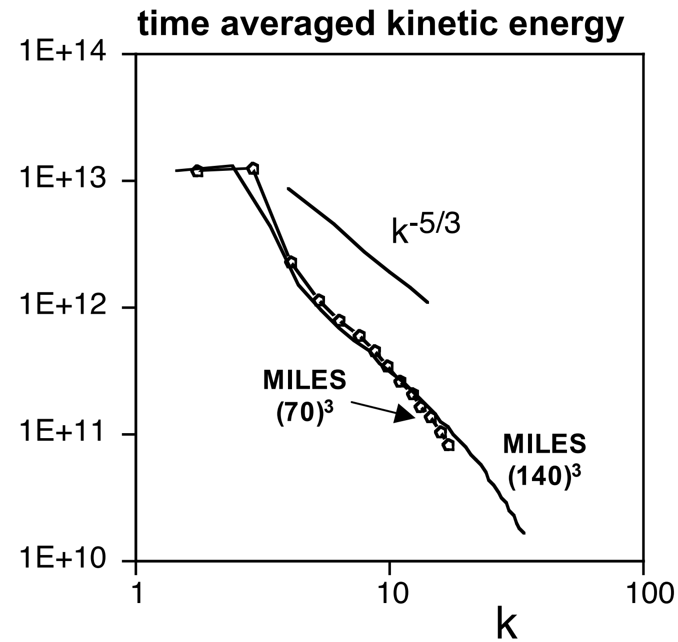


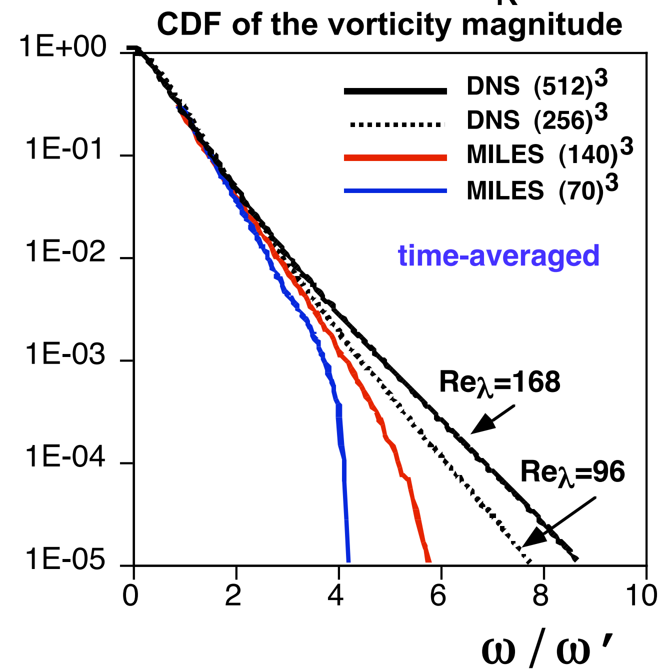
using DeVore's 2D FCT limiter

ILES (or LES) “convergence” ….



FFG & Devore PF ‘96, FFG JFM ‘01





- LES “observations” directly affected by (explicit or implicit) filter-length cutoff …

Some Open Issues of ILES based on NFV schemes

- *relevant differences / similarities*
  - *flux-limiting vs. upwinding*
  - *interplay between discrete & continuous equations*
  - *scale separation, filtering analogues*
- *building physics into scheme to improve on*
  - *global performance, dissipation & backscatter*
- *dependence on algorithm specifics (the ILES "knobs"), e.g.,*
  - *flux limiter, low & high order schemes, gridding*

Challenges and Directions for Future ILES Development

- *appropriate theoretical framework (ME, …)*
- *a priori vs. a posteriori tests: what's meaningful for ILES ?*
- *effective "mixed" explicit / implicit SGS modeling of small-scale driven mixing & combustion, stochastic backscatter (inherently difficult for all LES !)*

Implicit LES
Recent Background

Invited Special Sessions

"VLES", 2001 ECCOMAS, Swansea UK
--> **special section of 2002 IJNMF**

"Alternative LES", 2002 AIAA-ASM, Reno NV
--> **special section of 2002 ASME JFE**

"ILES"
2003 CSE-SIAM, San Diego CA
2003 AIAA-CFD, Orlando FL
2004 IGPP-CNLS LANL Workshops
--> Cambridge UP ILES Book, 2006

IMPLICIT LARGE EDDY SIMULATION: COMPUTING TURBULENT FLUID DYNAMICS (Cambridge University Press, 2005-2006)

Editors:
Fernando F. Grinstein, Len Margolin, and Bill Rider

INTRODUCTION

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1. Historical Introduction (Boris)
2. ILES for Turbulent Flows: A Rationale (Grinstein, Margolin, Rider)

SECTION B - CAPTURING PHYSICS WITH NUMERICS

3. Subgrid Scale Modeling: Issues and Approaches (Sagaut)
4. Numerics for ILES
    a. Limiting Algorithms (Drikakis,Grinstein, Fureby,Youngs)
    b. Piecewise Parabolic Method (Woodward, Porter)
    c. Lagrangean Remap Method (Youngs)
    d. MPDATA (Smolarkiewicz, Margolin)
    e. Vorticity Confinement (Steinhoff)
5. Numerical Regularization (Rider, Margolin,Fureby)
6. Approximate Deconvolution (Adams, Domaradzki)

SECTION C - VERIFICATION AND VALIDATION

7. Homogeneous Turbulence (Woodward, Porter)
8. Vortex Dynamics and Transition to Turbulence (Grinstein)
9. Instabilities and Symmetry Breaking (Drikakis)
10. Incompressible Wall Bounded Flows (Fureby)
11. Compressible Turbulent Shear Flows (Knight, Adams, Fureby)
12. Studies Based on Vorticity Confinement (Steinhoff)
13. Rayleigh-Taylor and Richtmyer Meshkov Mixing (Youngs)

SECTION D - FRONTIER FLOWS

14. Studies of Geophysics (Smolarkiewicz, Margolin)
15. Studies of Astrophysics (Porter, Woodward)
16. Complex Engineering Turbulent Flows (Fureby)
17. Large Scale Urban Simulations (Patnaik, Grinstein, Boris)

Bibliography

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