CLES.1 Computational Issues in Large Eddy Simulation

Mathematics-, mechanics-, LES-characterization of NS, reprise

$$\mathrm{D}M : \nabla \bullet \mathbf{U} = 0$$

$$\mathrm{D}\mathbf{P}: \ \mathrm{D}\mathbf{U}/\mathrm{D}t + \frac{1}{\rho_0}\nabla\rho - \upsilon\nabla^2\mathbf{U} + \rho/\rho_0\mathbf{g} = 0$$

Galilean invariance: $\mathrm{D}M$, $\mathrm{D}\mathbf{P}$ forms invariant under frame rectilinear $\mathbf{V}(t)$

NS *not* material frame indifferent for frame arbitrary $\mathbf{V}(t)$

random scalars: NS velocity component is a random variable

PDF: $f(V) \equiv \partial F/\partial V$, $V =$ sample space

CDF: $F(V)$ = probability of an event

mean: $\langle U \rangle \equiv \int_{-\infty}^{\infty} V f(V)\,\mathrm{d}V$

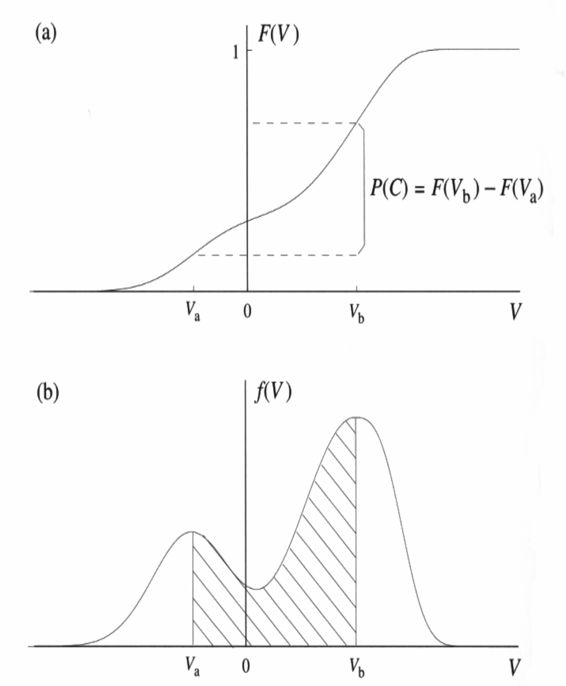
$\equiv$ definition of $f(V)$ for NS

fluctuation: $u = U - \langle U \rangle$

variance: $\mathrm{var}\langle U \rangle \equiv \langle u^2 \rangle = \int_{-\infty}^{\infty} (V - \langle U \rangle)^2 f(V)\,\mathrm{d}V$

std. deviation: $\mathrm{sdev}(U) = \langle u^2 \rangle^{1/2}$

n^{th} central moment: $\mu_0 \equiv \langle u^n \rangle$



CLES.2 Computational Issues in Large Eddy Simulation

NS velocity vector U(x,*t*) as multi-time, -point random vector field

one-point statics : $F(\mathbf{V},\mathbf{x},t) \equiv P\{U_i(\mathbf{x},t) < V_i, \quad i = 1,2,3\}$

$$f(\mathbf{V};\mathbf{x},t) = \partial^3 F(\mathbf{V},\mathbf{x},t)/\partial V_1 \partial V_2 \partial V_3$$

$$\left\langle \mathbf{U}(\mathbf{x},t) \right\rangle = \int_{-\infty}^{\infty} \mathrm{V} f(\mathbf{V};\mathbf{x},t)\,\mathrm{d}\mathbf{V}$$

$$\mathbf{u}(\mathbf{x},t) = \mathbf{U}(\mathbf{x},t) - \left\langle \mathbf{U}(\mathbf{x},t) \right\rangle$$

one - point, one-time : $\mathrm{cov}(U_i,U_j) = \left\langle u_i(\mathbf{x},t)\, u_j(\mathbf{x},t) \right\rangle \Rightarrow \tau_{ij}(\mathbf{x},t)$

two-point, one-time : $\mathrm{autocov}(U_i,U_j) \equiv R_{ij}(r) = \left\langle u_i(\mathbf{x},t)\, u_j(\mathbf{x}+\mathbf{r},t) \right\rangle$

energy spectrum : $R_{11}(\mathbf{0},t) = \left\langle u_1 u_1 \right\rangle = 2\int_0^{\infty} E_{11}(\kappa,t)\,\mathrm{d}\kappa$

an integral length scale : $L_{11}(\mathbf{x},t) \equiv \dfrac{1}{R_{11}(\mathbf{0},\mathbf{x},t)} \int_0^{\infty} R_{11}(r\hat{\mathrm{e}}_1,\mathbf{x},t)\,\mathrm{d}r$

homogeneous turbulence : $R_{ij}(\mathbf{r},\mathbf{x},t) \Rightarrow R_{ij}(\mathbf{r},t)$

homogeneous isotropic : $R_{ij}(\mathbf{r},\mathbf{x},t) \Rightarrow R_{ij}(\mathbf{r}^{\alpha},t^{\alpha})\ \forall\alpha$

one-point, two-time : $\mathrm{autocov}(U_i,U_j) \equiv R_{ij}(s) = \left\langle u_i(\mathbf{x},t)\, u_j(\mathbf{x},t+s) \right\rangle$

$$\mathrm{autocorr}\ \rho(s) = R_{ij}(s)/R_{ij}(0)$$

integral time scale : $\overline{\tau} \equiv \int_0^{\infty} \rho(s)\,\mathrm{d}s < \infty$

CLES.3 Computational Issues in Large Eddy Simulation

Spatially filtered NS velocity vector field, spectral forms

$$\text{mean}: \bar{U}_j(\mathbf{x},t) \equiv \int_\Delta G(\mathbf{x}-\mathbf{r};\Delta)\, U_i(\mathbf{r},t)\mathrm{d}\mathbf{r}$$

$$\text{fluctuation}: u_i' \equiv U_i - \bar{U}_i$$

$$\text{stress resolution}: \overline{U_i U_j} \equiv \bar{U}_i \bar{U}_j + L_{ij} + C_{ij} + R_{ij}$$

$$L_{ij} \equiv \overline{\bar{U}_i \bar{U}_j} - \bar{U}_i \bar{U}_j, \qquad L_{ij}^0 \equiv \overline{\bar{U}_i \bar{U}_j} - \bar{\bar{U}}_i \bar{\bar{U}}_j$$

$$C_{ij} \equiv \overline{\bar{U}_i u_j'} - \overline{\bar{U}_j u_i'}, \qquad C_{ij}^0 \equiv \overline{\bar{U}_i u_j'} + \overline{u_i' \bar{U}_j} - \bar{\bar{U}}_i \overline{u_j'} - \overline{u_i'} \bar{\bar{U}}_j$$

$$R_{ij} \equiv \overline{u_i' u_j'}, \qquad R_{ij}^0 \equiv \overline{u_i' u_j'} - \overline{u_i'}\,\overline{u_j'}$$

$$\text{spectral form}: \hat{U}(\kappa) \equiv \mathsf{F}\{U(x)\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(x)\mathrm{e}^{-\mathrm{i}\kappa x}\mathrm{d}x$$

$$\hat{\bar{U}}(\kappa) \equiv \mathsf{F}\{\bar{U}(x)\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} G(y)\mathrm{e}^{-\mathrm{i}\kappa y} U(x-y)\mathrm{e}^{-\mathrm{i}\kappa x}\mathrm{d}x\mathrm{d}y$$

$$= \hat{G}(\kappa)\hat{U}(\kappa)$$

$$\text{energy spectrum}: \bar{E}_{11}(\kappa) \equiv \frac{1}{\pi}\int_{-\infty}^{\infty} \bar{R}(r)\mathrm{e}^{-\mathrm{i}\kappa x}\mathrm{d}r = \frac{1}{\pi}\int_{-\infty}^{\infty} \left\langle \bar{u}(x-r)\bar{u}(x)\right\rangle \mathrm{e}^{-\mathrm{i}\kappa r}\mathrm{d}x\mathrm{d}r$$

$$= \left|\hat{G}(\kappa)\right|^2 E_{11}(\kappa)$$

CLES.4 Computational Issues in Large Eddy Simulation

Gaussian filter, spectral resolution, statistically homogeneous $U(x)$

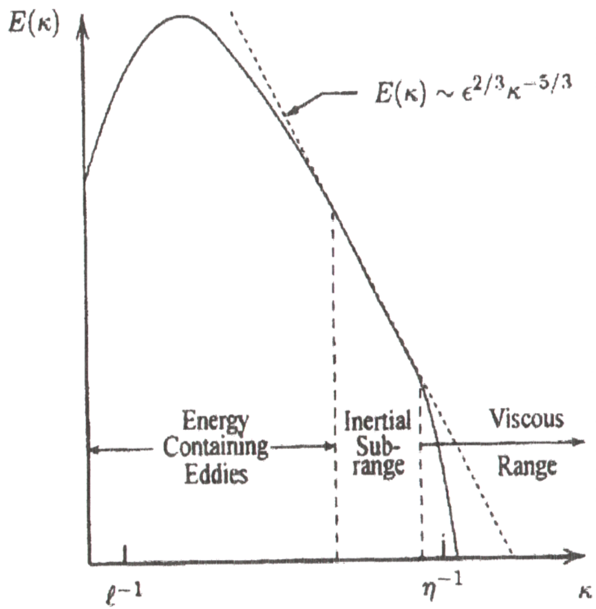
filter width : $\Delta \sim L_{11}/6$ resolves energetic eddies

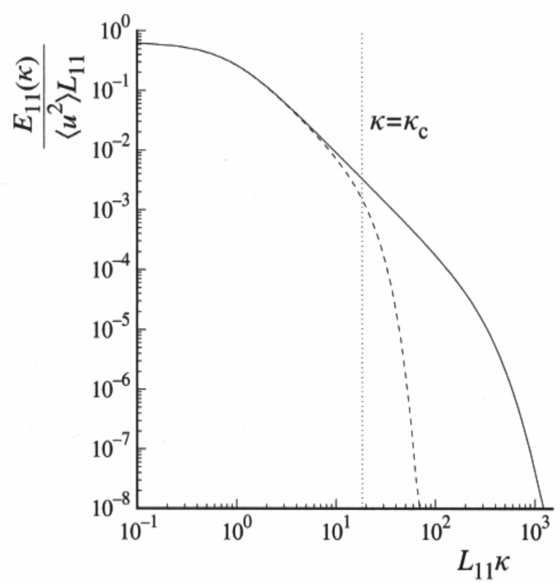
$$L_{11} \equiv \frac{1}{\langle uu \rangle} \int U(x+r)u(x)\mathrm{d}r$$

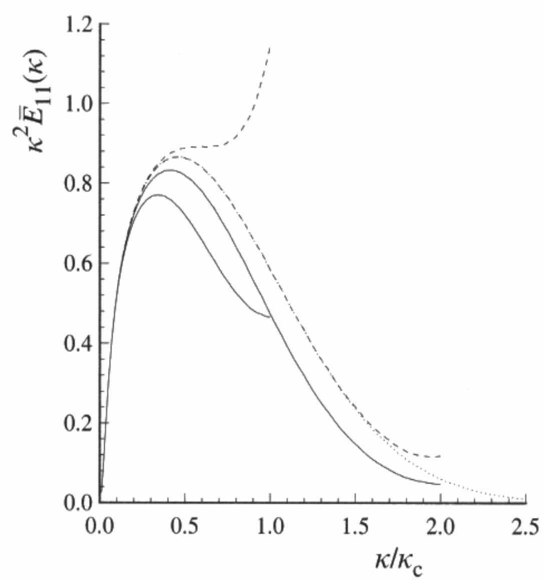
mesh resolution : $\kappa_r = \pi/h$, resolved mode limit

$\kappa_c = \pi/\Delta$, filter cut off

$h/\Delta \sim \kappa_c/\kappa_r \leq 1/2$ for 80% energy in 3-D







CLES.5 Computational Issues in Large Eddy Simulation

NS equations, statistical Reynolds form : $\langle \mathbf{U} \rangle \equiv \int_{-\infty}^{\infty} \mathbf{V} f(\mathbf{V})\, d\mathbf{V}$

$$\langle DM \rangle : \nabla \bullet \langle \mathbf{U} \rangle = 0 = \nabla \bullet \langle \mathbf{u} \rangle$$

$$\langle D\mathbf{P} \rangle : D\langle \mathbf{U} \rangle / Dt + \frac{1}{\rho_0}\nabla \langle p \rangle - \upsilon \nabla^2 \langle \mathbf{U} \rangle + \left\langle \frac{\rho}{\rho_0} \right\rangle \mathbf{g} + \nabla \langle u_i u_j \rangle = 0$$

$$\langle \nabla \bullet D\mathbf{P} \rangle : -\frac{1}{\rho_0}\nabla^2 \langle p \rangle - \partial^2 \left[\langle U_i \rangle \langle U_j \rangle + \langle u_i u_j \rangle \right] / \partial x_i \partial x_j = 0$$

Reynolds stress : $\langle u_i u_j \rangle = (2/3)\, k \delta_{ij} + \tau_{ij}^r, \qquad \tau_{ij}^r \cong -\upsilon\, 2 \langle S_{ij} \rangle$

NS equations, spatially filtered form : $\bar{\mathbf{U}} \equiv \int_{\Delta} G(\mathbf{x}, \mathbf{r}; \Delta)\, \mathbf{U}(\mathbf{r}, t)\, d\mathbf{r}$

$$\overline{DM} : \nabla \bullet \bar{\mathbf{U}} = 0 = \nabla \bullet \bar{\mathbf{u}}'$$

$$\overline{D\mathbf{P}} : D\bar{\mathbf{U}} / Dt + \frac{1}{\rho_0}\nabla \bar{p} - \upsilon \nabla^2 \bar{\mathbf{U}} + \frac{\bar{\rho}}{\rho_0} \mathbf{g} + \nabla \tau_{ij}^R = 0$$

$$\overline{\nabla \bullet D\mathbf{P}} : -\frac{1}{\rho_0}\nabla^2 \bar{p} - \partial^2 \left[U_i U_j + \tau_{ij}^R \right] / \partial x_i \partial x_j = 0$$

Reynolds stress : $\tau_{ij}^R = (2/3)\, k_r \delta_{ij} + \tau_{ij}^r \equiv L_{ij} + C_{ij} + R_{ij}$

SGS Reynolds : $R_{ij}^o \equiv \overline{u_i' u_j'} - \bar{u}_i' \bar{u}_j' = -\upsilon_r 2 \bar{S}_{ij}$

Smagorinsky : $\upsilon_r \equiv \ell_s^2\, \bar{S}, \ell_s \equiv C_s \Delta\ , \bar{S} \equiv (2 \bar{S}_{ij} \bar{S}_{ij})^{1/2}$

CLES.6 Computational Issues in Large Eddy Simulation

Comparison of features/ limitations of processed NS systems

statististical form : precisely describes velocity vector field random character
clearly defines moments, covariance, length & time scales
energy spectrum Fourier transform related
mean velocity defines the PDF
how to determine in absence of experiments ?

filtered form : NS system is identical appearing !
filter function does not (yet) appear explicitly
resolution clearly defined by κ_c, κ_r, Δ and h
closure for R_{ij} not included in theory
boundary condition form not precise

comparative limitations : both detailed only for homogeneous, isotropic turbulence
Boussinesq- type closure model
ℓ_s requires van Driest damping
conversion to CFD form faces additional problems
convolution and differentiation do not commute
boundary conditions
accuracy/convergence/well-posedness/closure

CLES.7 Computational Issues in Large Eddy Simulation

Fundamental issues, CFD implementation of LES NS form (John, 2004)

error generated assuming filtering, differentiation operations commute
on bounded domains, identify, correct
error due to approximation of Gaussian filter
low order TS $\Rightarrow$ *Taylor* LES
higher order (Pade′) TS $\Rightarrow$ *rational* LES
order of Smagorinsky closure incompatible
fourth order rational leads to R_{ij} model, but theory difficulties

CFD solution boundedness in kinetic energy
weak form yields consistency

CFD algorithm stability, accuracy
numerical dissipation boundedness, control
boundary conditions

mathematical rigor implementation analysis
existence, uniqueness(by data), convergence estimates
mathematical vs. physical arguments

CLES.8 Computational Issues in Large Eddy Simulation

Summary CFD LES NS implementation, notation!!

$$\overline{\mathrm{D}M} : \nabla \bullet \bar{\mathbf{U}} = 0 = \nabla \bullet \bar{\mathbf{u}}' = \nabla \bullet \mathbf{w}$$

$$\overline{\mathrm{D}\mathbf{P}} : \; \mathsf{L}(\bar{\mathbf{U}}) = \partial \bar{\mathbf{U}}/\partial t + \bar{\mathbf{U}} \bullet \nabla \bar{\mathbf{U}} + \frac{1}{\rho_0} \nabla \bar{\rho} - \upsilon \nabla^2 \bar{\mathbf{U}} + \nabla(\overline{u_i' u_j'}) = 0$$

$$\mathsf{L}(\mathbf{w}) = \mathbf{w}_t + \mathbf{w} \bullet \nabla \mathbf{w} + \nabla r - \nabla \bullet \big((2\upsilon + \upsilon_{\mathrm{T}})\mathsf{D}(\mathbf{w})\big)$$

$$+ \nabla \bullet \frac{\delta^2}{2\gamma}\left[\mathrm{A}(\nabla \mathbf{w} \nabla \mathbf{w}^T) \right] - \mathbf{f} = 0$$

Term definitions as function of auxiliary problem or convolution

laminar NS : $\upsilon_T = 0, \; A = 0$

Smagorinsky : $\upsilon_T = c_s \delta^2 \; \|\mathsf{D}(\mathbf{w})\|_F , \; A = 0$

Taylor LES : $\upsilon_T = c_s \delta^2 \; \|\mathsf{D}(\mathbf{w})\|_F , \; A = \boxed{\mathrm{I}}$

rational LES with auxiliary problem (homogeneous Neumann BCs)

Smagorinsky : $\upsilon_T = c_s \delta^2 \; \|\mathsf{D}(\mathbf{w})\|_F , \; A = \left[\mathrm{I} - \frac{\delta^2}{4\gamma} \nabla^2 \right]^{-1}$

Iliescu-Layton : $\upsilon_T = c_s \delta^2 \; \|\mathbf{w} - A\mathbf{w}\|_2$

rational LES with convolution

Smagorinsky : $\upsilon_T = c_s \delta^2 \; \|\mathsf{D}(\mathbf{w})\|_F , \; A = G(\delta)^* \equiv g_\delta^*$

Iliescu-Layton : $\upsilon_T = c_s \delta^2 \; \|\mathbf{w} - A\mathbf{w}\|_2 , \; A = g_\delta^*$

CLES.9 Computational Issues in Large Eddy Simulation

Notation synopsis for LES CFD theoretical constructions

Lebesgue space: $L^p(\Omega)$ is the space of all measurable functions $\upsilon(\mathbf{x})$

$$\|\upsilon\|_{L^p(\Omega)} := \left[\int_\Omega |\upsilon(\mathbf{x})|^p \,\mathrm{d}\mathbf{x}\right]^{1/p} < \infty, \quad p \in (1,\infty)$$

$$q = \text{conjugate exponent of } p \in (1,\infty), \text{ hence } p^{-1} + q^{-1} = 1$$

$$\text{then } \langle \upsilon, w \rangle \equiv \int_\Omega \upsilon(\mathbf{x})\, w(\mathbf{x})\,\mathrm{d}\mathbf{x}, \quad \upsilon \in L^p, \quad w \in L^q$$

Sobolev space : $W^{m,p}(\Omega)$ is the space of all functions for which

$$\|\upsilon\|_{W^{m,p}(\Omega)} := \left[\sum_{0\le|\alpha|\le m} \|\mathrm{D}^\alpha \upsilon\|^p_{L^p(\Omega)}\right]^{1/p} < \infty, \quad p \in (1,\infty)$$

$$\mathrm{D}^\alpha \upsilon(\mathbf{x}) := \partial^m \upsilon / \partial x^{\alpha_1} \partial y^{\alpha_2} \partial z^{\alpha_3}(\mathbf{x}), \quad x = (x,y,z) \in \mathbb{R}^3$$

$$|\alpha| = \sum_{i=1}^{d} \alpha_i = m$$

Hilbert space: is Sobolev space with $p = 2$, hence

$$H^m(\Omega) \equiv W^{m,2}(\Omega)$$

$$L^p(\Omega) \equiv W^{0,p}(\Omega)$$

Notation continued, convolution, Fourier transform

$$\text{convolution}: \left(f*g\right)(y) \equiv \int_{\mathbb{R}} f(y-x)\, g(x)\, \mathrm{d}x = \int_{\mathbb{R}} f(x)\, g(y-x)\, \mathrm{d}x = g*f$$

$$\text{Fourier transform}: \mathcal{F}(f)(y) = \int_{\mathbb{R}} f(x)\, \mathrm{e}^{-\mathrm{i}xy} \mathrm{d}x$$

$$\mathcal{F}^{-1}(F)(x) = \frac{1}{2\pi}\int_{\mathbb{R}} F(y)\, \mathrm{e}^{\mathrm{i}xy} \mathrm{d}x$$

$$\mathcal{F}(f*g) = \mathcal{F}(f)\,\mathcal{F}(g),\ \mathcal{F}(fg) = \mathcal{F}(f)*\mathcal{F}(g)$$

$$\text{differentiation}: \text{for } f \text{ differentiable and bounded, } f(x \Rightarrow \infty) = 0$$

$$y\mathrm{F}(f)(y) = -\mathrm{i}\mathcal{F}(f')(y)$$

$$\|y\|_2^2\ \mathrm{F}(\mathbf{f}) = -\mathcal{F}\left(\Delta\mathbf{f} \equiv \nabla^2\mathbf{f}\right)$$

$$\frac{1}{\|y\|_2^2}\mathrm{F}(\mathbf{f}) = -\mathcal{F}\left(\Delta^{-1}\mathbf{f}\right)$$

$$\frac{1}{1+c\|y\|_2^2}\mathrm{F}(\mathbf{f}) = \mathcal{F}\left(\left(\mathrm{I}-c\Delta\right)^{-1}\mathbf{f}\right)$$

$$\text{boundedness}: \text{for } f\in L^p,\ g\in L^q,\ p^{-1}+q^{-1}\geq 1,\ r^{-1} = p^{-1}+q^{-1}-1$$

$$\|f*g\|_{L^r(\Omega)} \leq \|f\|_{L^p(\Omega)}\|g\|_{L^q(\Omega)}$$

CLES.11 Computational Issues in Large Eddy Simulation

Notation concluded, matrix forms, Frobenius norm

$$\text{matrix notation}: \mathbf{x} = (x_i), \quad 1 \le i \le d$$

$$A = (a_{ij}), \quad 1 \le i, j \le d$$

$$\text{inner (dot) product}: \mathbf{x} \bullet \mathbf{y} = \textstyle\sum_i x_i y_i \qquad = \text{ scalar}$$

$$\text{outer (dyadic) product}: \mathbf{x}\mathbf{y}^T = \mathbf{x} \otimes \mathbf{y} = \left(x_i y_j\right)_{i,j} \qquad = \text{matrix}$$

$$\text{matrix dot product}: A : B = \textstyle\sum_{i,j} a_{ij} b_{ij} \qquad = \text{scalar}$$

$$\text{Frobenius norm}: \|A\|_F = \left[\textstyle\sum_{i,j} a_{ij}^{\,2}\right]^{1/2} = \left(A : A\right)^{1/2} = \text{tr}\left(AA^T\right)^{1/2}$$

$$\text{matrix divergence}: \nabla \bullet A = \begin{Bmatrix} \partial/\partial x_1 \\ \partial/\partial x_2 \\ \partial/\partial x_3 \end{Bmatrix} \begin{bmatrix} \mathrm{a}_{11} & \mathrm{a}_{12} & \mathrm{a}_{13} \\ \mathrm{a}_{21} & \mathrm{a}_{22} & \mathrm{a}_{23} \\ \mathrm{a}_{31} & \mathrm{a}_{32} & \mathrm{a}_{33} \end{bmatrix} = \begin{Bmatrix} \mathrm{a}_{11,1} + \mathrm{a}_{12,2} + \mathrm{a}_{13,3} \\ \mathrm{a}_{21,1} + \mathrm{a}_{22,2} + \mathrm{a}_{23,3} \\ \mathrm{a}_{31,1} + \mathrm{a}_{32,2} + \mathrm{a}_{33,3} \end{Bmatrix}$$

$$\text{strain rate tensor}: \mathbf{D}(\mathbf{V}) = \frac{1}{2}\left[\nabla\mathbf{V} + \nabla\mathbf{V}^T\right] = S_{ij}$$

$$\text{rotation tensor}: \Omega(\mathbf{V}) = \frac{1}{2}\left[\nabla\mathbf{V} - \nabla\mathbf{V}^T\right] = \Omega_{ij}$$

$$\text{stress tensor}: \mathbf{S}(\mathbf{V}) = 2\upsilon\mathbf{D}(\mathbf{V}) - p\mathrm{II}$$

CLES.12 Computational Issues in Large Eddy Simulation

Space averaged non-D NS and the commutation error, $\upsilon = Re^{-1}$

$$\mathrm{D}M : \nabla \bullet \mathbf{u} = 0$$

$$\mathrm{D}\mathbf{P} : \mathsf{L}(\mathbf{u}) = \mathbf{u}_t + \mathbf{u} \bullet \nabla \mathbf{u} + \nabla p - 2\upsilon \nabla \bullet \mathrm{D}(\mathbf{u}) - f = 0, \; in \left(0, T\right] \times \Omega$$

$$\text{resolution}: \; \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$$

filtering: linear and assuming operations commute

$$\overline{\mathrm{D}M} : \nabla \bullet \bar{\mathbf{U}} = 0 = \nabla \bullet \mathbf{u}'$$

$$\overline{\mathrm{D}\mathbf{P}} : \mathsf{L}(\bar{\mathbf{U}}) = \bar{\mathbf{u}}_t + \nabla \bullet (\overline{\mathbf{u}\mathbf{u}^{\mathrm{T}}}) + \nabla \bar{p} - 2\upsilon \nabla \bullet \mathrm{D}(\bar{\mathbf{u}}) - \bar{\mathbf{f}} = 0$$

$$\text{linearity}: \; \overline{\mathbf{u}\mathbf{u}^{T}} = \overline{\bar{\mathbf{u}}\bar{\mathbf{u}}^{T}} + \overline{\bar{\mathbf{u}}\mathbf{u}'^{T}} + \overline{\mathbf{u}'\bar{\mathbf{u}}^{T}} + \overline{\mathbf{u}'\mathbf{u}'^{T}}$$

Commutation error associated with tensor S $(\mathbf{u}, p)$ at boundary

analysis framework extends domain beyond $\partial\Omega$, yields $\mathsf{L}^m(\mathbf{u})$ on $\Omega \Rightarrow \mathbb{R}^d$

$$\mathrm{D}\mathbf{P}^m : \mathsf{L}^m(\mathbf{u}) = \mathsf{L}(\mathbf{u}) - \int_{\partial\Omega} \mathbf{S}(\mathbf{u},p)(t,\mathbf{s}) \, \hat{\mathbf{n}}(\mathbf{s})\phi(\mathbf{s}) \, d\mathbf{s}$$

convolution of $\mathrm{D}\mathbf{P}^m$ with filter $g(\mathbf{x},\delta)$ yields

$$\overline{\mathrm{D}\mathbf{P}^m} : \mathsf{L}^m(\bar{\mathbf{u}}) = \mathsf{L}(\bar{\mathbf{u}}) - \int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\mathbf{S}(\mathbf{u},p)(t,\mathbf{s}) \, \hat{\mathbf{n}}(\mathbf{s}) d\mathbf{s}, \; on \left(0,T\right] \times \mathbb{R}^d$$

$$\text{commutation error}: A_\delta(\mathbf{S}(\mathbf{u},p)(t,\mathbf{x}) := \int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\mathbf{S}(\mathbf{u},p)(t,\mathbf{s}) \, \hat{\mathbf{n}}(\mathbf{s}) d\mathbf{s}, \; on \left(0,T\right] \, \mathrm{x}\mathbb{R}^d$$

$$\text{note}: A_\delta = f(\mathbf{u},p, \text{ not } \bar{\mathbf{u}},\bar{p})$$

CLES.13 Computational Issues in Large Eddy Simulation

Error estimates for the commutation error, Gaussian filter

commutation error : $A_\delta(g,\mathbf{u},p) := \int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\mathbf{S}(\mathbf{u},p)(t,\mathbf{s})\,\hat{\mathbf{n}}(\mathbf{s})d\mathbf{s},$

$$\Rightarrow \int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\psi(\mathbf{s})d\mathbf{s}, \quad \psi \in L^q\left(\partial\Omega\right),\ 1 \le q \le \infty$$

comments : $A_\delta(\bullet) \in L^p(\mathbb{R}^d)$, and as $\delta \to 0$ vanishes *only* when

$\mathbf{S}(\bullet)\,\hat{\mathbf{n}}(\mathbf{s}) = 0$ almost everywhere on $\partial\Omega$

rules out *any* practical bounded flow problem!

Asymptotic bounding of this error leading to its neglect

strong form solution (FD) : error is $O(1)$

for $\psi \in L^p(\partial\Omega)$: $\displaystyle\int_{\mathbb{R}^d}\left|\int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\psi(\mathbf{s})d\mathbf{s}\right| d\mathbf{x} \le C\delta^{f(k,d,\theta,q)}\,\|\psi\|^k_{L^p(\partial\Omega)}$

convergence in $\mathsf{H}^{-1}(\Omega)$: for functions in $\mathsf{H} \equiv \left\{\upsilon \in H^{-1}(\mathbb{R}^d) : \upsilon|_{\partial\Omega} = 0\right\}$

$$\left\|\int_{\partial\Omega} g_\delta(\mathbf{x}-\mathbf{s})\psi(\mathbf{s})d\mathbf{s}\right\|_{\mathsf{H}^{-1}_{\mathsf{H}}(\mathbb{R}^d)} \le C\delta^{1/2}\,\|\psi\|_{L^2(\partial\Omega)}$$

weak form convergence: $\displaystyle\left|\int_{\mathbb{R}^d} \upsilon(\mathbf{x}) \int_{\partial\Omega} g(\mathbf{x}-\mathbf{s})\psi(\mathbf{s})d\mathbf{s}\right| d\mathbf{x} \le C\delta^{f(\bullet,\beta)}\,\|\psi\|^k_{L^p(\partial\Omega)}\,\|\upsilon\|_{H^2(\Omega)}$

$\simeq O(\delta^1)$ for $d = 2$

CLES.14 Computational Issues in Large Eddy Simulation

LES models based on approximations in wave number space

approach : $\Omega \in \mathbb{R}^d$, $\delta =$ constant for Gaussian filter

Fourier transform $\overline{\mathbf{u}\mathbf{u}^T}$ for $\mathbf{u} \equiv \overline{\mathbf{u}} + \mathbf{u}'$

express $\mathbf{F}(\mathbf{u}')$ via $\mathbf{F}(\overline{\mathbf{u}})$ to eliminate $\mathbf{u}'$

approximate $\mathbf{F}(g)$ such that $\mathbf{F}^{-1}(g)$ is explicitly available

use $\mathbf{F}^{-1}(g)$ to partially model $\overline{\mathbf{u}\mathbf{u}^T}$

establish a closure model for $\overline{\mathbf{u}'\mathbf{u}'}$

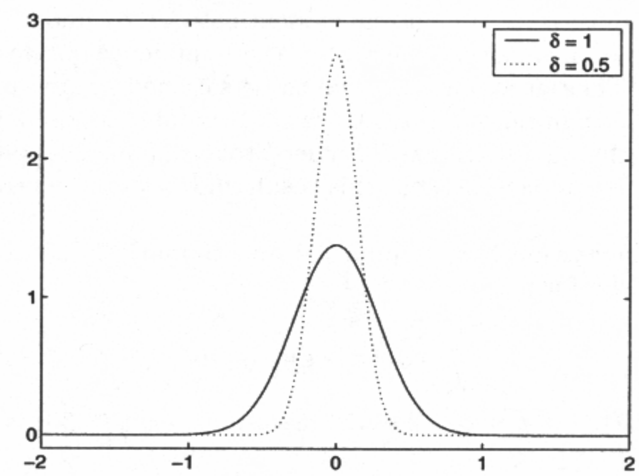
Gaussian filter : $g_\delta(\mathbf{x}) \equiv \Pi_i^d g_i(\mathbf{x}_i)\,, 1 \le i \le d$

$$g_\delta(x_i) = \sqrt{\frac{\gamma}{\pi\delta^2}} \exp\left(-\frac{\gamma}{\delta^2} x_i^2\right), \text{ and assume } \gamma = 6$$

$$g_\delta(\mathbf{x}) = \left(\frac{6}{\pi\delta^2}\right)^{d/2} \exp\left(\frac{-6}{\delta^2}\|\mathbf{x}\|_2^2\right)$$

$$\mathbf{F}(g_\delta)(\mathbf{y}) = \exp\left(-\frac{\delta^2}{24}\|\mathbf{y}\|_2^2\right)$$

$$y_c = \text{cutoff wave number} \equiv 2\pi/\delta$$



Modelling of the large scale and cross terms in $\overline{\mathbf{u}\mathbf{u}^T}$

filtered stress : $\overline{\mathbf{u}\mathbf{u}^T} = \overline{\bar{\mathbf{u}}\bar{\mathbf{u}}^T} + \overline{\bar{\mathbf{u}}\mathbf{u}'^T} + \overline{\mathbf{u}'\bar{\mathbf{u}}^T} + \overline{\mathbf{u}'\mathbf{u}'^T}$

Gaussian(δ) : $\bar{\mathbf{u}}(\mathbf{x},t) = g_\delta * \mathbf{u}(\mathbf{x},t)$

process : compute Fourier transforms
replace $\mathbf{F}(\mathbf{u}')$ as function of $\mathbf{F}(\bar{\mathbf{u}})$
approximate g_δ
neglect higher order terms in δ
compute inverse Fourier transform

large scale : $\mathbf{F}\left(\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}^T}\right) = \mathbf{F}\left(g_\delta * \bar{\mathbf{u}}\bar{\mathbf{u}}^T\right) = \mathbf{F}\left(g_\delta\right)\mathbf{F}\left(\bar{\mathbf{u}}\bar{\mathbf{u}}^T\right)$

cross terms : $\mathbf{F}\left(\overline{\bar{\mathbf{u}}\mathbf{u}'^T}\right) = \mathbf{F}\left(g_\delta\right)\mathbf{F}\left(\bar{\mathbf{u}}\mathbf{u}'^T\right) = \mathbf{F}\left(g_\delta\right)\mathbf{F}\left(\bar{\mathbf{u}}\right) * \mathbf{F}\left(\mathbf{u}'^T\right)$

$\mathbf{F}\left(\overline{\mathbf{u}'\bar{\mathbf{u}}^T}\right) = \mathbf{F}\left(g_\delta\right)\mathbf{F}\left(\mathbf{u}'\bar{\mathbf{u}}^T\right) = \mathbf{F}\left(g_\delta\right)\mathbf{F}\left(\mathbf{u}'\right) * \mathbf{F}\left(\bar{\mathbf{u}}^T\right)$

$\mathbf{F}(g_\delta) \neq 0 : \mathbf{F}(\mathbf{u}) = \dfrac{\mathbf{F}(g_\delta)\mathbf{F}(\mathbf{u})}{\mathbf{F}(g_\delta)} = \dfrac{\mathbf{F}(\bar{\mathbf{u}})}{\mathbf{F}(g_\delta)}$

$\mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}} : \mathbf{F}(\mathbf{u}') = \left[\dfrac{1}{\mathbf{F}(g_\delta)} - 1\right]\mathbf{F}(\bar{\mathbf{u}})$

hence : $\mathbf{F}\left(\overline{\bar{\mathbf{u}}\mathbf{u}'^T}\right) = \mathbf{F}\left(g_\delta\right)\left[\mathbf{F}(\bar{\mathbf{u}}) * \left(\dfrac{1}{\mathbf{F}(g_\delta)} - 1\right)\mathbf{F}(\bar{\mathbf{u}})\right]$

$\mathbf{F}\left(\overline{\mathbf{u}'\bar{\mathbf{u}}^T}\right) = \mathbf{F}\left(g_\delta\right)\left[\left(\dfrac{1}{\mathbf{F}(g_\delta)} - 1\right)\mathbf{F}(\bar{\mathbf{u}}) * \mathbf{F}\left(\bar{\mathbf{u}}^T\right)\right]$

Approximations to $\mathsf{F}(g_\delta)$ lead to $\overline{\mathrm{DP}}$ modification

TS approximations : $\mathbf{F}(g_\delta)(\delta,\mathbf{y}) = 1 - (4\gamma)^{-1}\|\mathbf{y}\|_2^2 + O(\delta^4)$

$$\frac{1}{\mathbf{F}(g_\delta)}(\delta,\mathbf{y}) = 1 + (4\gamma)^{-1}\|\mathbf{y}\|_2^2 + O(\delta^4)$$

second order $\mathbf{F}(g_\delta)$ approximations yield

$$\mathbf{F}(\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}^T}) = \mathbf{F}(\overline{\mathbf{u}}\,\overline{\mathbf{u}}^T) + \frac{\delta^2}{4\gamma}\mathbf{F}\left(\Delta(\overline{\mathbf{u}}\,\overline{\mathbf{u}}^T)\right) + O\left(\delta^4, \overline{\mathbf{u}}(\delta^\alpha)\right)$$

$$\mathbf{F}(\overline{\overline{\mathbf{u}}\mathbf{u}'^T}) = -\frac{\delta^2}{4\gamma}\mathbf{F}\left(\overline{\mathbf{u}}\Delta(\overline{\mathbf{u}}^T)\right) + O\left(\delta^4, \overline{\mathbf{u}}(\delta^\alpha)\right)$$

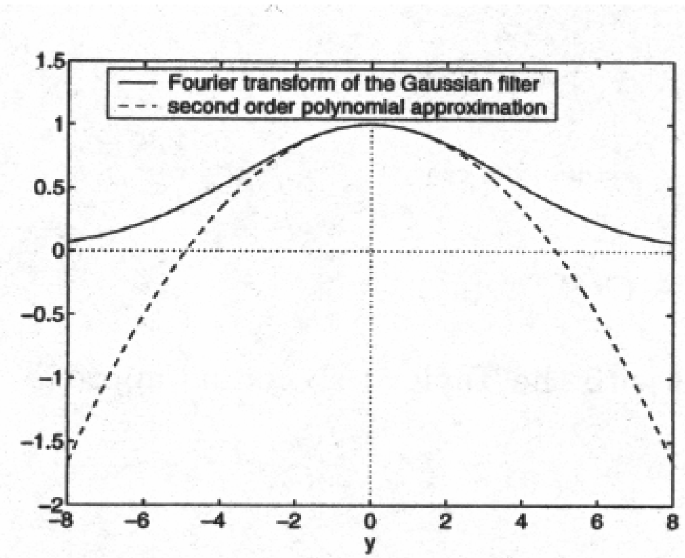
$$\mathbf{F}(\overline{\mathbf{u}'\overline{\mathbf{u}}^T}) = -\frac{\delta^2}{4\gamma}\mathbf{F}\left(\Delta(\overline{\mathbf{u}})(\overline{\mathbf{u}}^T)\right) + O\left(\delta^4, \overline{\mathbf{u}}(\delta^\alpha)\right)$$

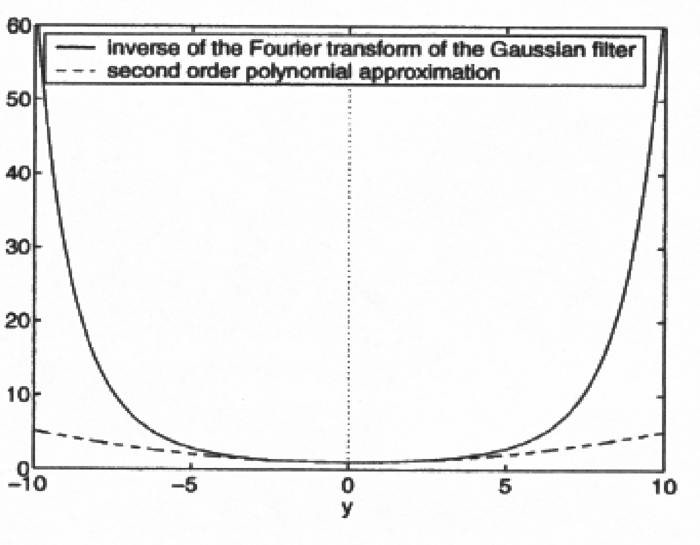
apply inverse Fourier transforms, $(\Delta = \nabla^2)$

$$\overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}^T} = \overline{\mathbf{u}}\,\overline{\mathbf{u}}^T + \frac{\delta^2}{4\gamma}\nabla^2\left(\overline{\mathbf{u}}\,\overline{\mathbf{u}}^T\right) + O(\bullet)$$

$$\overline{\overline{\mathbf{u}}\mathbf{u}'^T} = -\frac{\delta^2}{4\gamma}\overline{\mathbf{u}}\nabla^2\left(\overline{\mathbf{u}}^T\right) + O(\bullet)$$

$$\overline{\mathbf{u}'\overline{\mathbf{u}}^T} = -\frac{\delta^2}{4\gamma}\nabla^2(\overline{\mathbf{u}})\,\overline{\mathbf{u}}^T + O(\bullet)$$





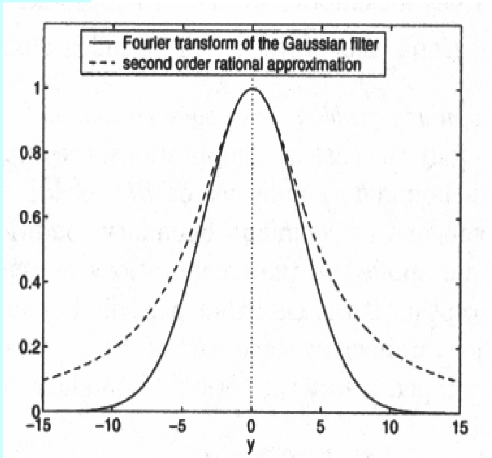
CLES.17 Computational Issues in Large Eddy Simulation

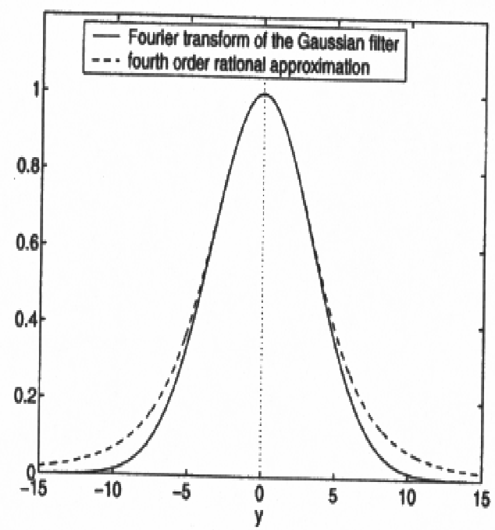
Filtered stress via TS and rational Pade′ approximations

TS :
$$\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}^T} + \overline{\bar{\mathbf{u}}\mathbf{u}'^T} + \overline{\bar{\mathbf{u}}\mathbf{u}'^T}$$
$$\approx \bar{\mathbf{u}}\bar{\mathbf{u}}^T + \frac{\delta^2}{4\gamma}\left[\nabla^2(\bar{\mathbf{u}}\bar{\mathbf{u}}^T) - \bar{\mathbf{u}}\nabla^2(\bar{\mathbf{u}}^T) - \nabla^2(\bar{\mathbf{u}})\bar{\mathbf{u}}^T\right]$$
$$= \bar{\mathbf{u}}\bar{\mathbf{u}}^T + \frac{\delta^2}{2\gamma}\nabla\bar{\mathbf{u}}\nabla\bar{\mathbf{u}}^T + O\left(\delta^4, \bar{\mathbf{u}}(\delta^\alpha)\right)$$

Pade2 :
$$\mathbf{F}(g_\delta)(\delta,\mathbf{y}) = \left[1 + \frac{\delta^2}{4\gamma}\|\mathbf{y}\|_2^2\right]^{-1} + O\left(\delta^4\right)$$
$$\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}}^T + \overline{\bar{\mathbf{u}}\mathbf{u}'^T} + \overline{\mathbf{u}'\bar{\mathbf{u}}^T}$$
$$\approx \left[I - \frac{\delta^2}{4\gamma}\nabla^2\right]^{-1}\left[\bar{\mathbf{u}}\bar{\mathbf{u}}^T - \frac{\delta^2}{4\gamma}(\bullet)\right]$$
$$= \bar{\mathbf{u}}\bar{\mathbf{u}}^T + \frac{\delta^2}{2\gamma}\left[I - \frac{\delta^2}{4\gamma}\nabla^2\right]^{-1}\nabla\bar{\mathbf{u}}\bullet\nabla\bar{\mathbf{u}}^T + O\left(\delta^4, \bar{\mathbf{u}}(\delta^\alpha)\right)$$

Pade4 :
$$\mathbf{F}(g_\delta)(\delta,\mathbf{y}) = \left[1 + \frac{\delta^2}{4\gamma}\|\mathbf{y}\|_2^2 + \frac{\delta^4}{32\gamma^2}\|\mathbf{y}\|_2^4\right]^{-1} + O\left(\delta^6\right)$$
$$\overline{\bar{\mathbf{u}}\bar{\mathbf{u}}}^T + \overline{\bar{\mathbf{u}}\mathbf{u}'^T} + \overline{\mathbf{u}'\bar{\mathbf{u}}^T}$$
$$\approx \bar{\mathbf{u}}\bar{\mathbf{u}}^T + \frac{\delta^2}{2\gamma}\left[I - \frac{\delta^2}{4\gamma}\nabla^2 + \frac{\delta^4}{32\gamma^2}\|\mathbf{y}\|_2^4\right]^{-1}$$
$$\left[\nabla\bar{\mathbf{u}}\nabla\bar{\mathbf{u}}^T - \frac{\delta^2}{8\gamma}\left[\Delta\bar{\mathbf{u}}\Delta\bar{\mathbf{u}}^T + \nabla(\Delta\bar{\mathbf{u}})\nabla\bar{\mathbf{u}}^T + \nabla\bar{\mathbf{u}}\nabla(\Delta\bar{\mathbf{u}}^T) + \Delta(\nabla\bar{\mathbf{u}}\nabla\bar{\mathbf{u}}^T)\right]\right]$$





CLES.18 Computational Issues in Large Eddy Simulation

Pade′ approximations to $\mathsf{F}(g_\delta)$ introduce inverse Laplacian operators

$$\text{Pade 2}: \left[\mathrm{I} - (\delta^2/4\gamma)\nabla^2\right]^{-1}, \text{ elliptic second order PDE}$$

$$\text{auxilliary problem : on bounded domain } \Omega,\ \nabla^2 \text{ requires BCs on } \partial\Omega$$

$$\text{Galdi \& Layton}: \left[\mathrm{I}- \ \bullet\right]^{-1} \Rightarrow \mathbf{v}_t - \nabla^2\mathbf{v} = \frac{4\gamma}{\delta^2}\mathbf{f}\ ,\ on\ \left(0,T\right]\times\Omega$$

$$\text{BCs}: \hat{\mathbf{n}}\bullet\nabla\mathbf{v} = 0,\ on\ \left(0,T\right]\times\partial\Omega$$

$$\text{IC}: \mathbf{v}(\mathbf{x},0) = 0,\ on\ (0)\times\Omega\cup\partial\Omega$$

$$\text{GWS}^h + \theta\text{TS}: \{F(\mathbf{V})\} = [M]\ \{\mathbf{V}(T)\} + \Delta t\left(\left[\text{DIFF}\right]\{\mathbf{V}\} - \{\mathrm{b}(\mathbf{f})\}\right)$$

$$\text{choose}: \theta\equiv 1,\ \Delta t = T = 4\gamma/\delta^2,\ \mathbf{f} = \nabla\mathbf{u}\nabla\mathbf{u}^T$$

$$\text{auxilliary problem : alternative is to handle as convolution}$$

$$\mathsf{F}(g_\delta * \mathbf{u}) = \mathsf{F}(g_\delta)\ \mathsf{F}(\mathbf{u}) \approx \left[1 + \frac{\delta^2}{4\gamma}\|\mathbf{y}\|_2^2\nabla^2\right]^{-1}\mathsf{F}(\mathbf{u}) = \mathsf{F}\left(\left[\mathrm{I} - (\delta^2/4\gamma)\nabla^2\right]^{-1}\mathbf{u}\right)$$

$$\text{thereby}: g_\delta * \mathbf{u} \approx \left[\mathrm{I} - \frac{\delta^2}{4\gamma}\nabla^2\right]^{-1}\mathbf{u}$$

$$\text{hence}: \overline{\bar{\mathbf{u}}\bar{\mathbf{u}}^T} + \overline{\bar{\mathbf{u}}\mathbf{u}'^T} + \overline{\mathbf{u}'\bar{\mathbf{u}}^T} \approx \bar{\mathbf{u}}\bar{\mathbf{u}}^T + \frac{\delta^2}{2\gamma} g_\delta * (\nabla\mathbf{u}\nabla\mathbf{u}^T)$$

CLES.19 Computational Issues in Large Eddy Simulation

Gaussian filter approximation closure models for $\overline{\mathbf{u}'\mathbf{u}'^T}$

$$\text{transform}: \mathsf{F}(\overline{\mathbf{u}'\mathbf{u}'^T}) = \mathsf{F}(g_\delta * \mathbf{u}'\mathbf{u}'^T) = \mathsf{F}(g_\delta)\mathsf{F}(\mathbf{u}'\mathbf{u}'^T)$$

$$= \mathsf{F}(g_\delta)\left[\mathsf{F}(\mathbf{u}') * \mathsf{F}(\mathbf{u}')\right]$$

$$= \mathsf{F}(g_\delta)\left[\left(\frac{1}{\mathsf{F}(g_\delta)} - 1\right)\mathsf{F}(\mathbf{u}) * \left(\frac{1}{\mathsf{F}(g_\delta)} - 1\right)\mathsf{F}(\mathbf{u}^T)\right]$$

$$= \left(1 - \mathsf{F}(g_\delta)\right)\mathsf{F}(\mathbf{u}) * \left(1 - \mathsf{F}(g_\delta)\right)\mathsf{F}(\mathbf{u}^T)$$

$$\text{TS}: \mathsf{F}(\overline{\mathbf{u}'\mathbf{u}'^T}) \approx \ldots = (\delta^2/4\gamma)^2 \mathsf{F}(\Delta\mathbf{u}\Delta\mathbf{u}^T) + O\left(\delta^6, \mathbf{u}(\delta^\alpha)\right)$$

$$\overline{\mathbf{u}'\mathbf{u}'^T} \approx (\delta^2/4\gamma)^2\, \Delta\mathbf{u}\Delta\mathbf{u}^T + O\left(\delta^6, \mathbf{u}(\delta^\alpha)\right)$$

$$\text{Pade2}: \overline{\mathbf{u}'\mathbf{u}'^T} \approx (\delta^2/4\gamma)^2\left[I - (\delta^2/4\gamma)\Delta\right]\Delta\mathbf{u}\Delta\mathbf{u}^T + O\left(\delta^6, \bullet\right)$$

$$\text{Pade4}: \overline{\mathbf{u}'\mathbf{u}'^T} \approx g_\delta * (\delta^2/4\gamma)^2 \Delta\mathbf{u}\Delta\mathbf{u}^T + O\left(\delta^6, \bullet\right)$$

observations : all approximations lead to $\overline{\mathbf{u}'\mathbf{u}'^T}$ of order δ^4

only Pade4 retains this order

requires $\overline{\mathbf{u}}^h \in H^3$ which is impractical

Alternative approaches to closure models for $\overline{\mathbf{u}'\mathbf{u}'^T}$

Smagorinsky : published developments are $O(\delta^2)$

inconsistent with theory predicted $O(\delta^4)$

generates excessive level of δ-scale dissipation

Iliescu & Layton : propose δ-scale dissipation ~ kinetic energy of $\mathbf{u}'$

$$\upsilon_T \equiv \upsilon_T\left(\|\mathbf{u}'\|_2^2\right) \Rightarrow c l_m \|\mathbf{u}'\|_2, \; l_m \equiv \delta$$

from Fourier representations

$$\mathbf{u}' \approx -(\delta^2/4\gamma)\Delta\mathbf{u} + O(\delta^4)$$

$$\therefore \upsilon_T = c(\delta^3/\gamma)\|\Delta\bar{\mathbf{u}}\|_2$$

assuming $g_\delta \approx g_\delta^2$ leads to

$$\upsilon_T = c(\delta^3/\gamma)\|g_\delta * \bar{\mathbf{u}}\|_2$$

$$\upsilon_T = c\delta\|\bar{\mathbf{u}} - g_\delta * \bar{\mathbf{u}}\|_2$$

approximating convolution as auxiliary problem

$$\upsilon_T = c\delta\left\|\bar{\mathbf{u}} - \left[\mathrm{I} - (\delta^2/4\gamma)\Delta\right]^{-1}\bar{\mathbf{u}}\right\|_2$$

Grubert & Baker : $\upsilon_T = \left[\dfrac{\mathrm{Re}\, h^2(\delta)}{12}\right]\bar{\mathbf{u}}\bar{\mathbf{u}}^T$

CLES.21 Computational Issues in Large Eddy Simulation

Weak form solution process, $(\bar{\mathbf{u}}, \bar{p}) \Rightarrow (\mathbf{w}, r)$, Ω bounded by $\partial\Omega$

$$\overline{\mathrm{D}M} : \nabla \bullet \mathbf{w} = 0$$

$$\overline{\mathrm{D}\mathbf{P}} : \mathsf{L}^m(\mathbf{w}) = \mathbf{w}_t + (\mathbf{w}\bullet\nabla)\mathbf{w} + \nabla r - \nabla\bullet((2\upsilon + \upsilon_T)\mathbf{D}(\mathbf{w}))$$

$$+\nabla\bullet\frac{\delta^2}{2\gamma}\left[A(\nabla\mathbf{w}\nabla\mathbf{w}^T)\right] - \bar{\mathbf{f}} = 0 \ \ on \ \left(0,T\right]\times\Omega$$

$$\text{weak form : WF} \equiv \int_0^T\int_\Omega \mathbf{v}\mathsf{L}^m(\mathbf{w},r)\,\mathrm{d}\mathbf{x}\mathrm{d}t \equiv 0$$

$$= \int_0^T\int_\Omega \mathbf{v}\Big(\mathsf{L}^m(\bullet) - \nabla\bullet(\text{terms})\Big)\,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T\int_\Omega \nabla\mathbf{v}\bullet(\text{terms})\,\mathrm{d}\mathbf{x}\mathrm{d}t$$

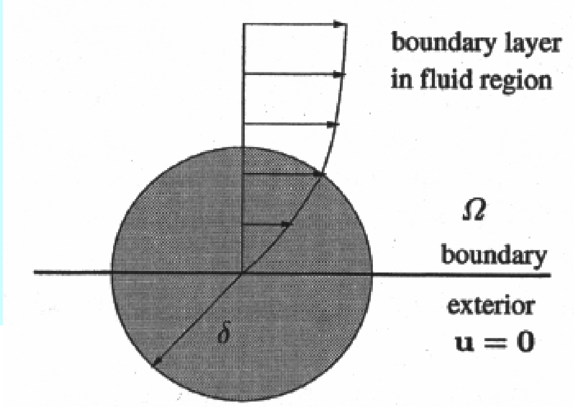
$$+\int_0^T\int_{\partial\Omega}\mathbf{v}\left[(2\upsilon+\upsilon_T)\mathbf{D}(\mathbf{w}) - \frac{\delta^2}{2\gamma}A(\nabla\mathbf{w}\nabla\mathbf{w}^T)\right]\bullet\hat{\mathbf{n}}\,\mathrm{d}s\,\mathrm{d}t$$

$$\text{with } (\nabla\bullet\mathbf{w}, q) = 0, \ \forall\ \mathbf{v},\mathbf{w}\in H^1(\Omega)$$

BCs on $\partial\Omega$: slip with linear friction

$$\mathbf{w}\bullet\hat{\mathbf{n}} = 0$$

$$l(\mathbf{w}) = \hat{\mathbf{n}}\bullet\nabla\mathbf{w} + g(\mathbf{D}(\mathbf{w}), A, \upsilon_T) = 0$$



Weak form solution, auxiliary problem, rational LES model

$$\text{auxiliary}: \frac{-\delta^2}{4\gamma}\nabla^2\mathbf{X} + \mathbf{X} = \nabla\mathbf{w}\nabla\mathbf{w}^T \text{ in } \Omega$$

$$\hat{\mathbf{n}}\bullet\left(\nabla\mathbf{X}\right)\equiv 0 \qquad \text{on } \partial\Omega$$

weak form : find $\mathbf{X}\in H^1(\Omega)$, for all $\mathbf{Y}\in H^1(\Omega)$ such that

$$\frac{\delta^2}{4\gamma}\left(\nabla\mathbf{X}\bullet\nabla\mathbf{Y}\right) + \left(\mathbf{X}\mathbf{Y}\right) = \left(\nabla\mathbf{w}\nabla\mathbf{w}^T, \mathbf{Y}^h\right)$$

linearization : evaluate $\mathbf{w}$ at previous timestation or iteration

Direct implementation of the convolution, rational LES model

$$\text{convolution}: A(\nabla\mathbf{w}\nabla\mathbf{w}^T) = g_\delta * (\nabla\mathbf{w}\nabla\mathbf{w}^T)$$

$$= \int_\Omega g_\delta(\mathbf{y}\text{-}\mathbf{x})(\bullet)(\mathbf{x})d\mathbf{x}$$

comment : theory enforcement via auxilliary PDE is much more efficient

CLES.23 Computational Issues in Large Eddy Simulation

LES weak solutions, existence and uniqueness, discrete implementation

rigorous mathematical analyses are exceedingly difficult

non-linearity, domain boundedness

monotonocity issues, NS dispersive instability

Smagorinsky : uniqueness proved for weak solution for "small data"

due to model stabilizing numerical diffusion

Taylor LES : Smagorinsky term dominates Taylor LES term

contradicts formal ordering, δ^2 versus δ^4

rational LES : existence and uniqueness confirmed for $\upsilon_T = 0$, $T = O(\delta^4)$

numerical tests refute this for nominal Re

unstable to small perturbations

discrete form : $(\mathbf{w}, r) \in H^1(\Omega) \Rightarrow (\mathbf{w}^h, r^h) \subset \mathbf{V}^h \in H^1(\Omega)$

TP bases : Q_1/Q_0, Q_2/P_1^{disc}, Q_2/Q_1,....

natural : P_1/P_0, P_2/P_1,....

use of upwind stabilization, Vanka smoothers

Asymptotic error estimates for the discrete weak form solutions

Smagorinsky : natural regularity requires $\nabla \mathbf{w} \in L^3(0,T;L^3(\Omega))$

Re-independence requires addition of $a_0(\delta) > 0$

splitting error $\mathbf{e} \equiv (\mathbf{w}\text{-}\tilde{\mathbf{w}}) - (\mathbf{w}^h\text{-}\tilde{\mathbf{w}})$, then

$$\left\|\mathbf{e}^h(T)\right\| \equiv \left\|\mathbf{w}\text{-}\mathbf{w}^h\right\|^2_{L^\infty(0,T;L^2(\Omega))} + \delta^2 \left\|\mathsf{D}(\mathbf{w}\text{-}\mathbf{w}^h)\right\|^3_{L^3(0,T;L^3(\Omega))}$$

$$+ \left(\mathrm{Re}^{-1} + c a_0(\delta)\right)\left\|\mathsf{D}(\mathbf{w}\text{-}\mathbf{w}^h)\right\|^2_{L^2(0,T;L^2(\Omega))} + \ldots$$

$$\leq C \inf \mathsf{F}(\mathbf{w}\text{-}\tilde{\mathbf{w}}, r\text{-}q^h, \delta) + C\left\|(\mathbf{w}\text{-}\mathbf{w}^h)(\mathbf{x},0)\right\|^2_{L^2(\Omega)}$$

Taylor LES: $$\left\|\mathbf{e}^h(T)\right\| \equiv \left\|\mathbf{w}\text{-}\mathbf{w}^h\right\|^2_{L^\infty(0,T;L^2(\Omega))} + c_s\delta^2 \left\|\nabla(\mathbf{w}\text{-}\mathbf{w}^h)\right\|^3_{L^3(0,T;L^3(\Omega))}$$

$$+ \mathrm{Re}^{-1}\left\|\nabla(\mathbf{w}\text{-}\mathbf{w}^h)\right\|^2_{L^2(0,T;L^2(\Omega))}$$

$$\leq C \inf \mathsf{F}(\mathbf{w}\text{-}\tilde{\mathbf{w}}, r\text{-}q^h, \mathrm{Re}, \delta, c_s, T) + C\left\|\mathbf{w}(\mathbf{x},0) - \mathbf{w}^h(\mathbf{x},0)\right\|^2_{L^2(\Omega)}$$

Asymptotic error estimates for the discrete weak form solutions

error : $f\left(\left\|\mathbf{w}\text{-}\mathbf{w}^h\right\|_p\right) < C$ (data, Ω^h, $\mathbf{V}^h$...) in appropriate L^p norms

key results : $\left\|\mathbf{e}^h\right\|_p$ bound independent of Re for fixed δ and h

for fixed δ, h-convergence predicted as $f(p)$

bounded by interpolation, time truncation errors

Verification, Chorin's vortex decay problem (Chorin, 1968)

$w_1 = -\cos(n\pi x)\sin(n\pi y)\exp(-2n^2\pi^2 t/\tau)$

$w_2 = \sin(n\pi x)\cos(n\pi y)\exp(-2n^2\pi^2 t/\tau)$

$r = -(1/4)(\cos(2n\pi x) + \cos(2n\pi y))\exp(-4n^2\pi^2 t/\tau)$

solution : for decay time $\tau = \upsilon^{-1}$, this is a solution to NS PDE system

decay of array of oppositely signed vortices

IC, BCs : NS $\mathbf{f}, \mathbf{w}_0$, Dirichlet BCs chosen such that $(\mathbf{w}, r)$ is NS solution

data : $\tau = 1000$, $T = 8$, $c_s = 0.05$

$n = 4$, $\delta = 0.1$, $\upsilon_{art} = 0.$

time : $\Delta t = 0.001$, θ fractional step

domain: $\Omega = (0,1)^2$, Ω^h uniform, $h/2 \Leftrightarrow h/128$

CLES.26 Computational Issues in Large Eddy Simulation

Table 8.2. Example 8.19, $\|\mathbf{w} - \mathbf{w}^h\|_{L^\infty(0,T;L^2(\Omega))}$, Q_2/P_1^{disc} finite element discretisation, error and order of convergence with respect to h (in parentheses)

ν^{-1}	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$	$h = 1/128$
10^2	2.20176-2	2.76780-3 (2.992)	3.47796-4 (2.992)	4.35185-5 (2.999)	5.43988-6 (3.000)
10^3	3.19389-2	3.50372-3 (3.188)	4.81015-4 (2.865)	4.86864-5 (3.304)	5.50381-6 (3.145)
10^4	5.97051-2	7.01100-3 (3.090)	1.00294-3 (2.805)	1.39466-4 (2.846)	1.44706-5 (3.269)
10^5	7.67057-2	7.73782-3 (3.309)	1.09801-3 (2.817)	1.62252-4 (2.758)	1.92552-5 (3.075)
10^6	7.86394-2	7.81755-3 (3.330)	1.10830-3 (2.818)	1.64891-4 (2.749)	1.98664-5 (3.053)
10^7	7.88349-2	7.82560-3 (3.333)	1.10934-3 (2.818)	1.65161-4 (2.748)	1.99288-5 (3.051)
10^8	7.88545-2	7.82641-3 (3.333)	1.10945-3 (2.819)	1.65188-4 (2.748)	1.99371-5 (3.051)
10^9	7.88564-2	7.82649-3 (3.333)	1.10946-3 (2.819)	1.65190-4 (2.748)	1.99377-5 (3.051)
10^{10}	7.88566-2	7.82650-3 (3.333)	1.10946-3 (2.819)	1.65191-4 (2.748)	1.99380-5 (3.051)

Table 8.3. Example 8.19, $\|\mathbb{D}(\mathbf{w} - \mathbf{w}^h)\|_{L^2(0,T;L^2(\Omega))}$, Q_2/P_1^{disc} finite element discretisation, error and order of convergence with respect to h (in parentheses)

ν^{-1}	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$	$h = 1/128$
10^2	1.248279	3.13720-1 (1.992)	7.84736-2 (1.999)	1.96114-2 (2.000)	4.90234-3 (2.000)
10^3	1.569352	3.60470-1 (2.122)	8.42787-2 (2.097)	2.00913-2 (2.069)	4.93406-3 (2.026)
10^4	2.351005	4.66554-1 (2.333)	1.05387-1 (2.146)	2.34301-2 (2.169)	5.28506-3 (2.148)
10^5	2.681270	4.98844-1 (2.426)	1.14609-1 (2.122)	2.61063-2 (2.134)	5.79700-3 (2.171)
10^6	2.720373	5.02793-1 (2.436)	1.15920-1 (2.117)	2.66473-2 (2.121)	5.96091-3 (2.160)
10^7	2.724344	5.03197-1 (2.437)	1.16058-1 (2.116)	2.67093-2 (2.119)	5.98435-3 (2.158)
10^8	2.724742	5.03237-1 (2.437)	1.16072-1 (2.116)	2.67156-2 (2.119)	5.98686-3 (2.158)
10^9	2.724782	5.03241-1 (2.437)	1.16073-1 (2.116)	2.67162-2 (2.119)	5.98711-3 (2.158)
10^{10}	2.724786	5.03242-1 (2.437)	1.16073-1 (2.116)	2.67163-2 (2.119)	5.98714-3 (2.158)

CLES.27 Computational Issues in Large Eddy Simulation

Verification, duct flow LES solution energy bounded on $\Omega \cup \partial\Omega$

channel flow : $E(\mathbf{u}) \equiv \frac{1}{2}\int_\Omega \mathbf{u}^T\mathbf{u}\,d\mathbf{x} = 2.667$

$E(\mathbf{w}^h) < \infty$, for $t \in [0, T]$

data for $\overline{\mathrm{D}M} + \overline{\mathrm{D}\mathbf{P}}$: $\Omega = (1,1,10)$

$\upsilon^{-1} = 10^5$, $\overline{\mathrm{Re}} = 66{,}667$

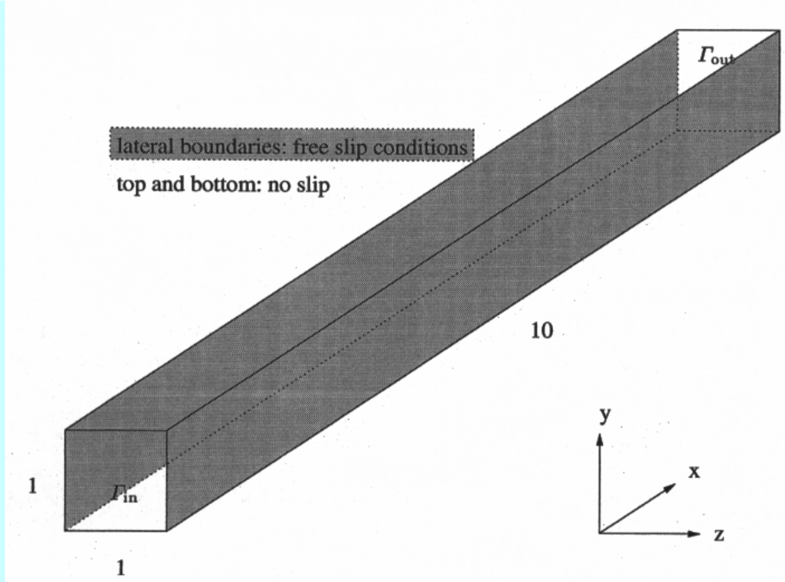
$\Delta t = 0.01\mathrm{s}$, $T = 20$

$\delta = 0.5$

BCs : $\mathbf{w}\bullet\hat{\mathbf{i}} = 4\mathrm{y}(1\text{-}y)$ *on* $(0,y,z)$

$\hat{\boldsymbol{n}}\bullet\nabla\mathbf{w} = 0$ *on* $(x,y,z = \pm 0.5)$, $(10,y,z)$

$\mathbf{w} = 0$ *on* $(x, y = \pm 0.5, z)$



$$\mathrm{IC} : \mathbf{w}(0,\mathbf{x}) = (\mathbf{w}\bullet\mathbf{i})\hat{\mathbf{i}} + c_{noise}\begin{Bmatrix} -4\pi\sin(4\pi y)\hat{\mathbf{i}} \\ -3\pi\sin(3\pi z)\hat{\mathbf{j}} \\ 3\pi\cos(3\pi x)\hat{\mathbf{k}} \end{Bmatrix}, \; c_{noise} = 0.01$$

$r(0,x) = -8(x-10)/\mathrm{Re}$

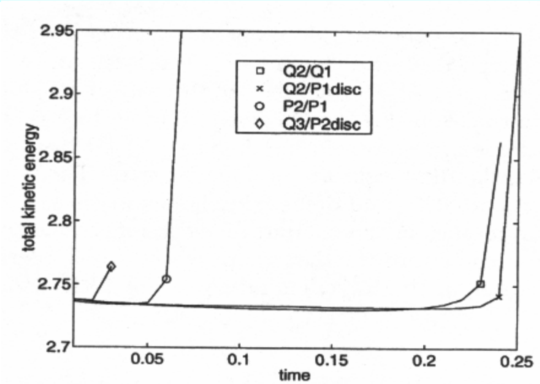
FE spaces : Q_2/Q_1, Q_2/P_1^{disc}, Q_3/P_2^{disc}, P_2/P_1

discretization Ω^h: Q (80 cubes at h=0.5 $\Rightarrow$ 480 cubes at h=0.25)

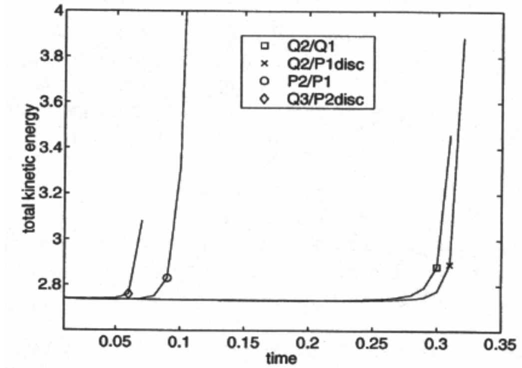
P (each cube bisected into 6 tetrahedra)

CLES.28 Computational Issues in Large Eddy Simulation

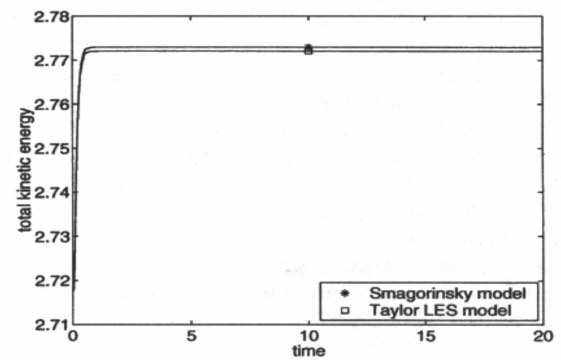
Duct flow verification, Taylor LES with Smagorinsky subgrid model



$c_s = 0.01$, fractional θ



$c_s = 0.01$, θCN

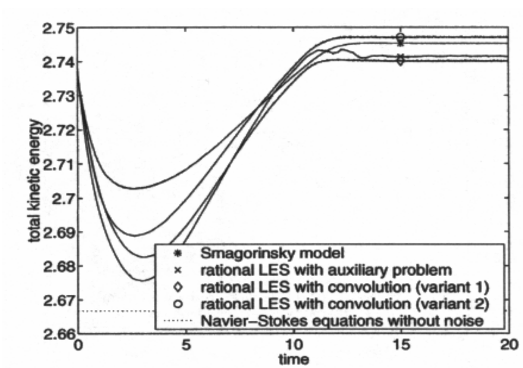


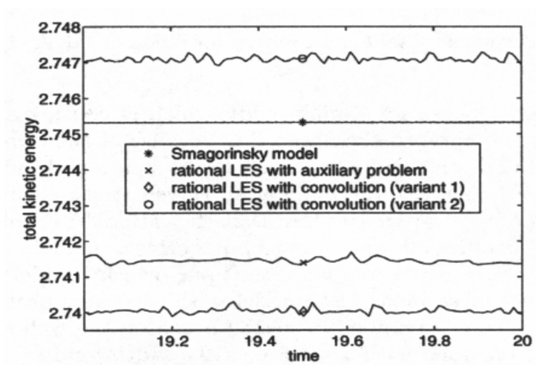
$c_s = 1/3$, f θ, Q_2/P_1^d

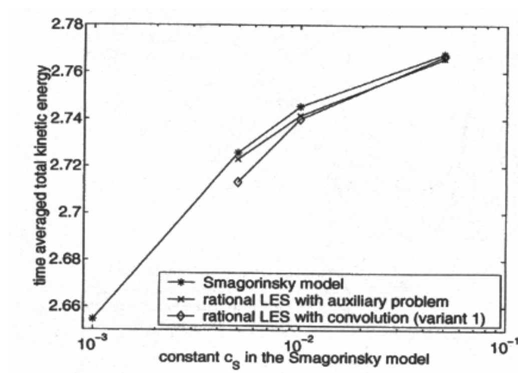
conclusion :failure due to poor $F(g_\delta)$ approximation

not influenced by boundary conditions

Duct, rational LES with Smagorinsky subgrid model, $c_s = 0.01$, Q_2/P_1^d

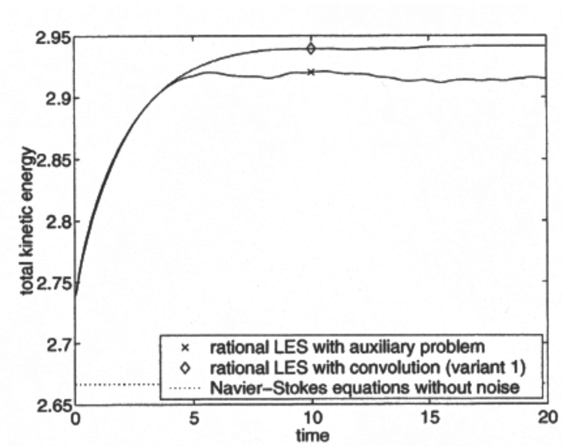




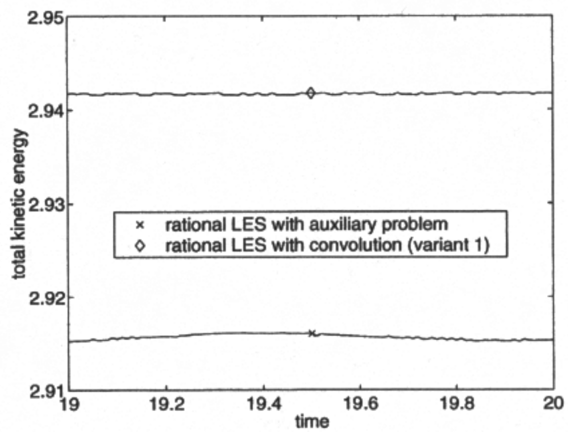


CLES.29 Computational Issues in Large Eddy Simulation

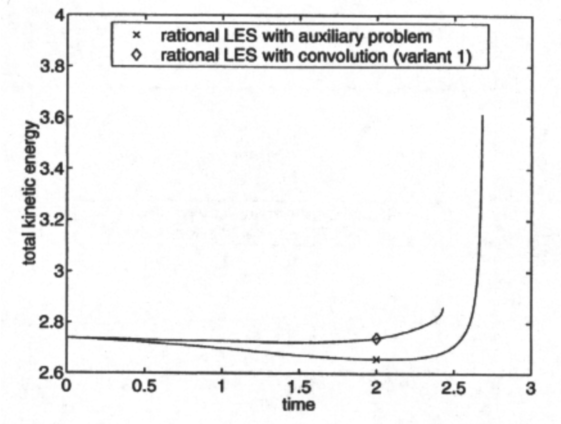
Duct, rational LES with Iliescu-Layton subgrid model, Q_2/P_1^{disc}, fractional θ



c_s=0.17



c_s=0.17



c_s=0

Conclusions, weak solution boundedness, duct flow, $\text{Re} \approx 10^5$

Smagorinsky : $\upsilon_T = c_s \delta^2 \|D(\bar{\mathbf{u}})\|_F$

Iliescu-Layton : $\upsilon_T = c_s \delta^3 \|\Delta(\bar{\mathbf{u}})\|_2$

Taylor LES + Smagorinsky, for standard c_s $\Rightarrow$ divergent solution

rational LES + Smagorinsky or I-L $\Rightarrow$ bounded solution for sufficient c_s

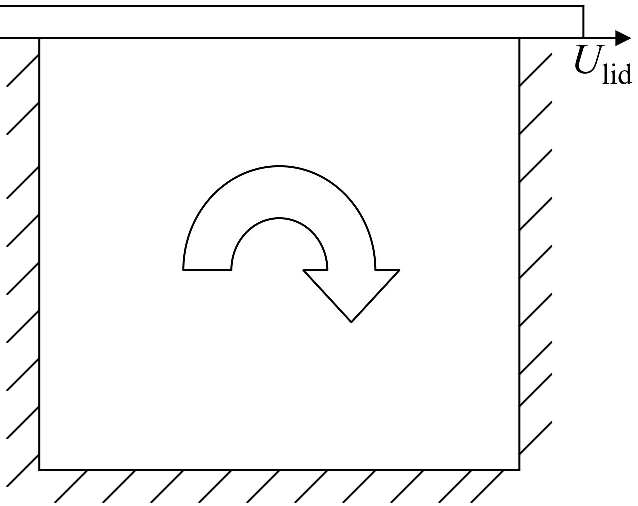
rational LES + no subgrid term $\Rightarrow$ divergent solution

for various FE spaces and 2nd order θ-schemes

CLES.30 Computational Issues in Large Eddy Simulation

Benchmark, driven cavity LES solution

domain : $\Omega = (0,1)^2$
BCs : no slip for NS
data : lid velocity U
$\upsilon = \mathrm{Re}^{-1}$



Iliescu, John, Layton, et al (2003)

LES should replicate NS solution for small enough Re

$E(\mathbf{w}^h_{\text{LES}} - \mathbf{w}^h_{\text{NSE}})$, Re = 400, Q_2/P_1^{disc}

Model	h = 1/16	h = 1/32	h = 1/64
Taylor LES	1.19E-03	1.67E-04	1.47E-05
rational LES + aux	1.29E-03	0.97E-04	0.17E-05
rational LES + conv	1.60E-03	1.24E-04	1.06E-05

LES solution must be bounded in total energy
Taylor LES solutions, Re = 10,000
IC = Galerkin FEM
h = 1/64, $\delta = \sqrt{2}/64$

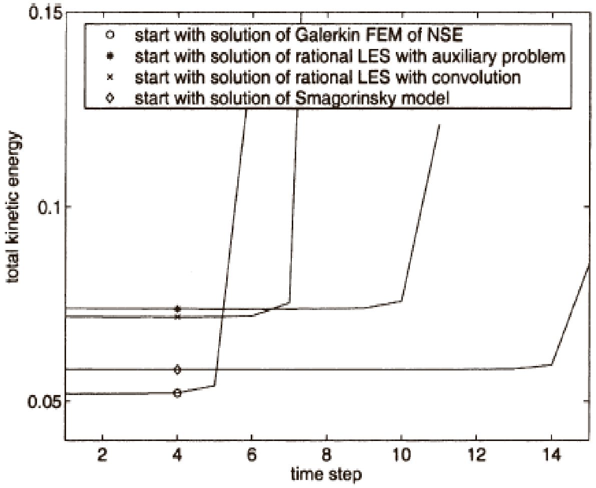


FIGURE 2 2D driven cavity problem, blow up of the Taylor LES model starting with various fully developed flow fields as starting conditions at $t = 1000$, $h = 1/64$, $\delta = \sqrt{2}/64$, $Re = 10{,}000$. Note that the blow up does not depend on using an impulsive start.

CLES.31 Computational Issues in Large Eddy Simulation

Driven cavity benchmark (IJL[+]03)

$\mathrm{Re} = 10{,}000$, $t = 1000$

$h = 1/16$, $\delta = \sqrt{2}/16$

$\upsilon_T = c_s \delta^2 \|D(\bar{\mathbf{u}})\|_F$

UL : rational LES+ aux

UR : rational LES + conv

LL : Smagorinsky (A=0)

LR : Galerkin DNS, h = 1/64

Comments

h/16 mesh is coarse!
- representative of LES model meshes
- cannot resolve small structures

rational LES + Smagorinsky υ_T
- bounded energy
- can only resolve main eddy
- "good" agreement with NS on *h*/64

rational LES without Smagorinsky υ_T
- blows up

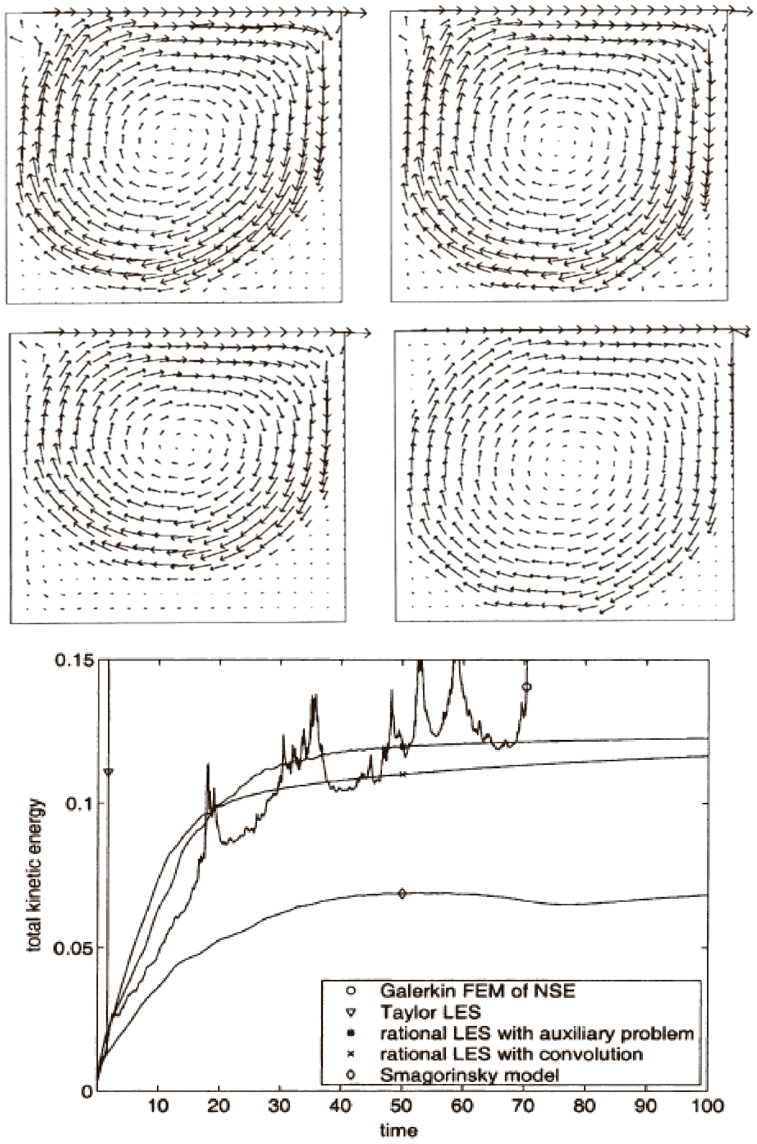


FIGURE 4 2D driven cavity problem, total kinetic energy, $Re = 10{,}000$, $h = 1/16$, $\delta = \sqrt{2}/16$.

Validation exercise, mixing layer on d=2

domain : $\Omega = (-1,1)^2$

BCs : $\hat{\mathbf{n}}\bullet\nabla(\bullet)=0,\ y = -1,1$

periodic, $x = -1,1$

$$\text{IC} : \mathbf{w}_0 = \begin{Bmatrix} W_\infty \tanh(2y/\sigma_0) \\ 0 \end{Bmatrix} + c_{\text{noise}} W_\infty \begin{Bmatrix} \partial\psi/\partial y \\ -\partial\psi/\partial x \end{Bmatrix}$$

$$\psi = \exp(-(2y/\sigma_0)^2)(\cos(8\pi x)+\cos(20\pi x))$$

data : $\eta = 4$ vortices expected, hence $\sigma_0 = 1/14$

$W_\infty = 1$, $c_{\text{noise}} = 0.001$, $\text{Re} = W_\infty\sigma_0/\upsilon = 10{,}000$

time algorithm : fractional θ, $\bar{t} \equiv \sigma_0/W_\infty$, $\Delta t = 0.1\bar{t} = (140)^{-1}\text{s}$

$$T = 200\bar{t} \sim 14.285\text{s}$$

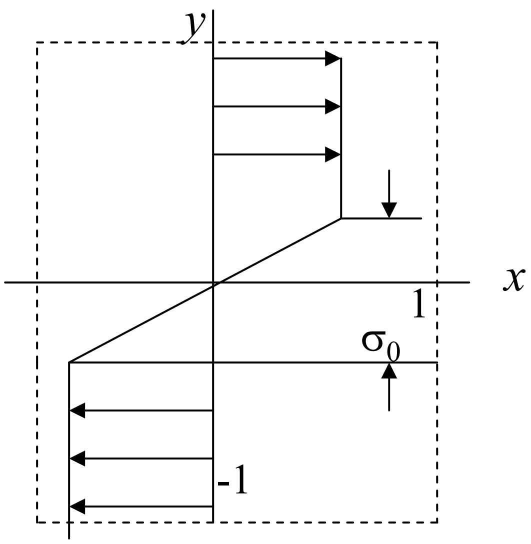
weak solution : Q_2/P_1^{disc} on 8 multi-grid levels, $h_0 = 1/1$, $h_8 = 1/256$

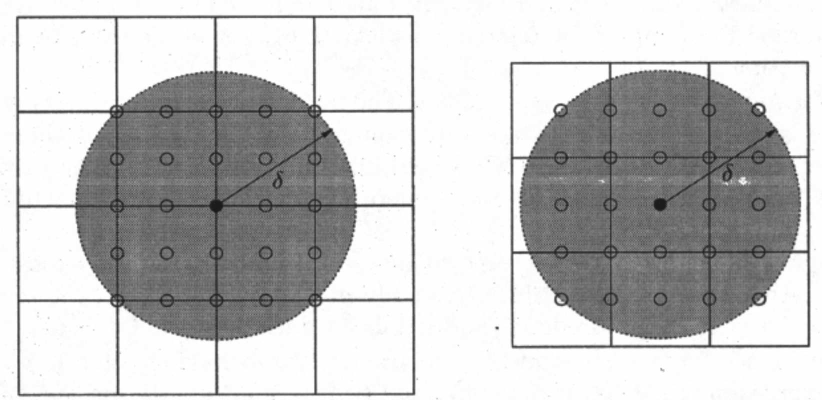
filter : $\delta = h$, $h = \rho(\Omega_e)$

algorithm : rational LES

SGS models : $\upsilon_T = c_s\delta^2\left\|D(\bar{\mathbf{u}})\right\|_F$

$$\upsilon_T = c_s\delta\left\|\bar{\mathbf{u}} - (I - \frac{\delta^2}{4\gamma}\Delta)^{-1}\bar{\mathbf{u}}\right\|_2$$





CLES.33 Computational Issues in Large Eddy Simulation

Galerkin FEM (DNS) on level 8

Filtered Galerkin DNS, δ = √2/32

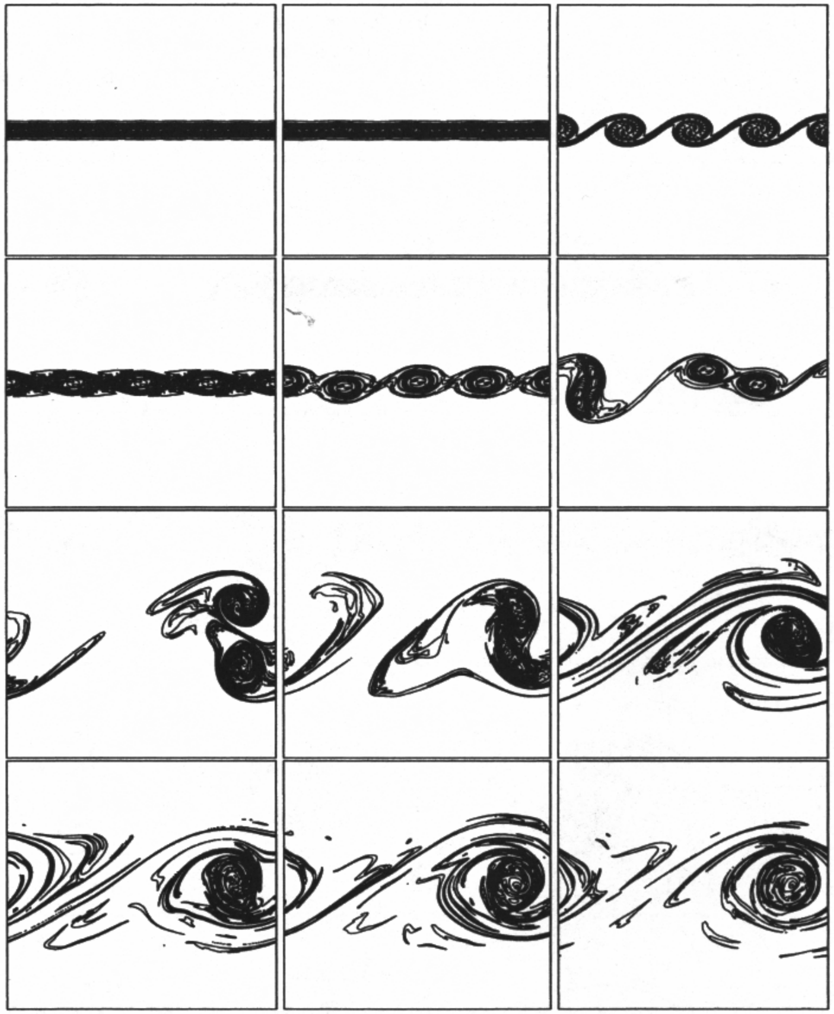


Fig. 11.3. Galerkin FEM, vorticity on level 8, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

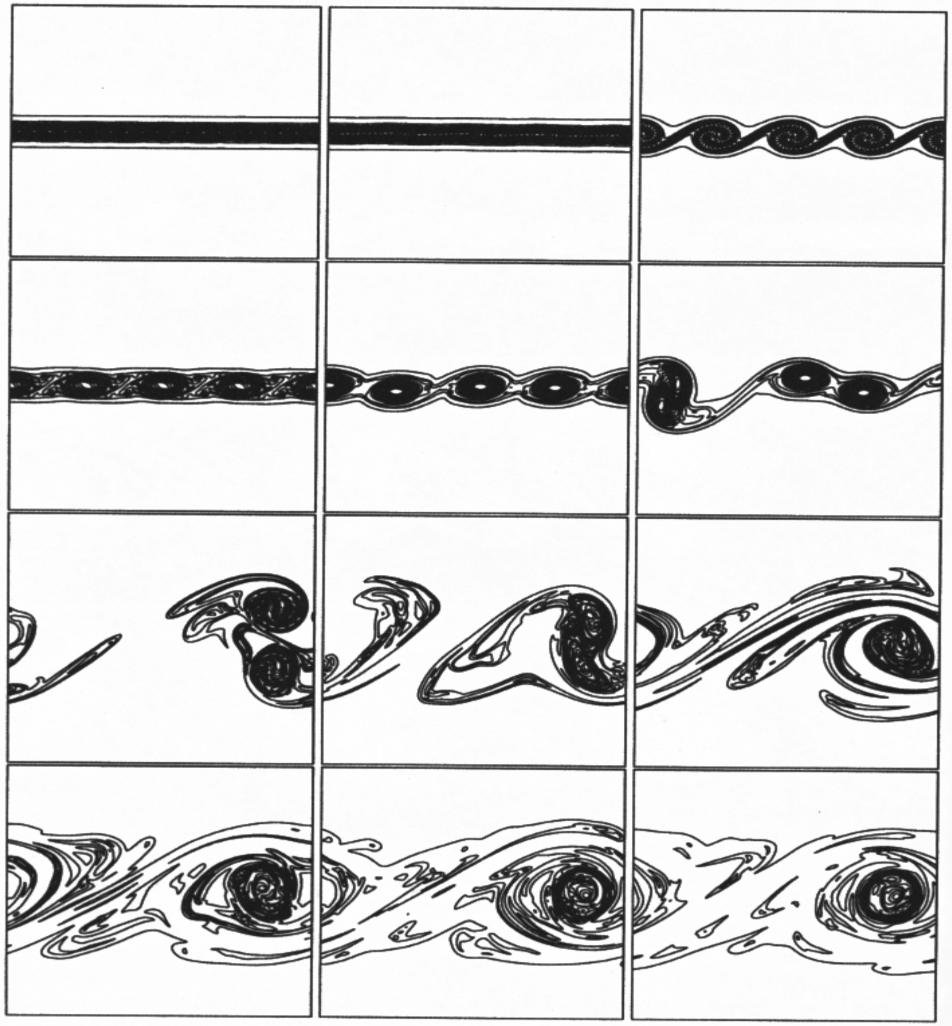


Fig. 11.4. Vorticity of $\overline{\mathbf{u}^h}$, level 8, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

CLES.34 Computational Issues in Large Eddy Simulation

Smagorinsky model, $c_s = 0.01$

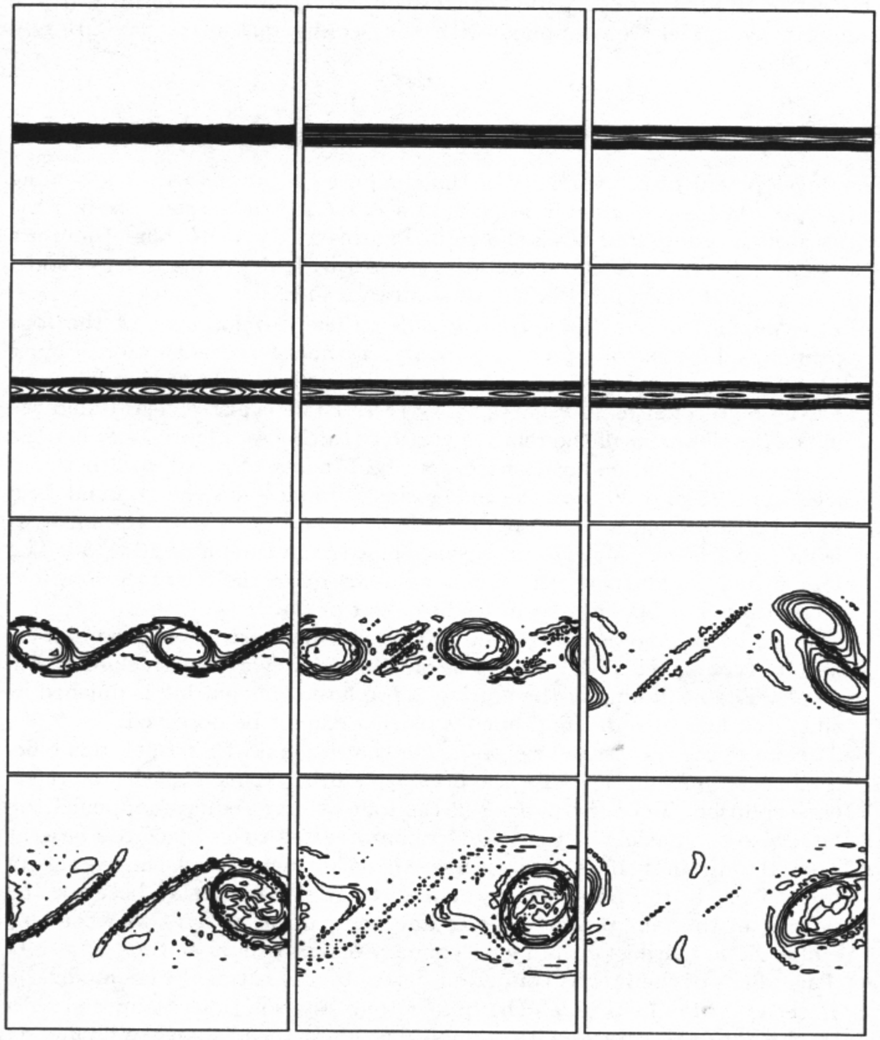


Fig. 11.5. Smagorinsky model (4.3), $c_S = 0.01$, vorticity on level 5, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

rational LES + aux, Smagorinsky SGS

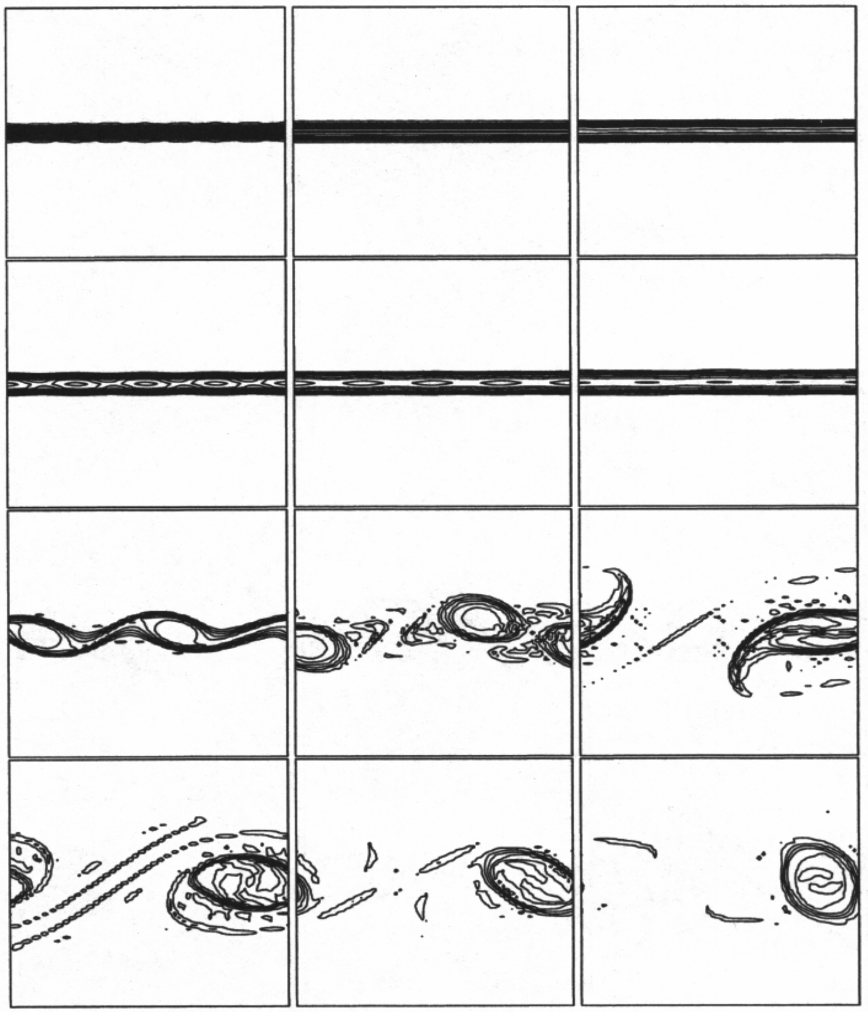


Fig. 11.6. Rational LES model with auxiliary problem, Smagorinsky model (4.3) as subgrid scale model with $c_S = 0.01$, vorticity on level 5, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

CLES.35 Computational Issues in Large Eddy Simulation

normalized vorticity span, $c_s = 0.01$
Smagorinsky SGS, *h*/32

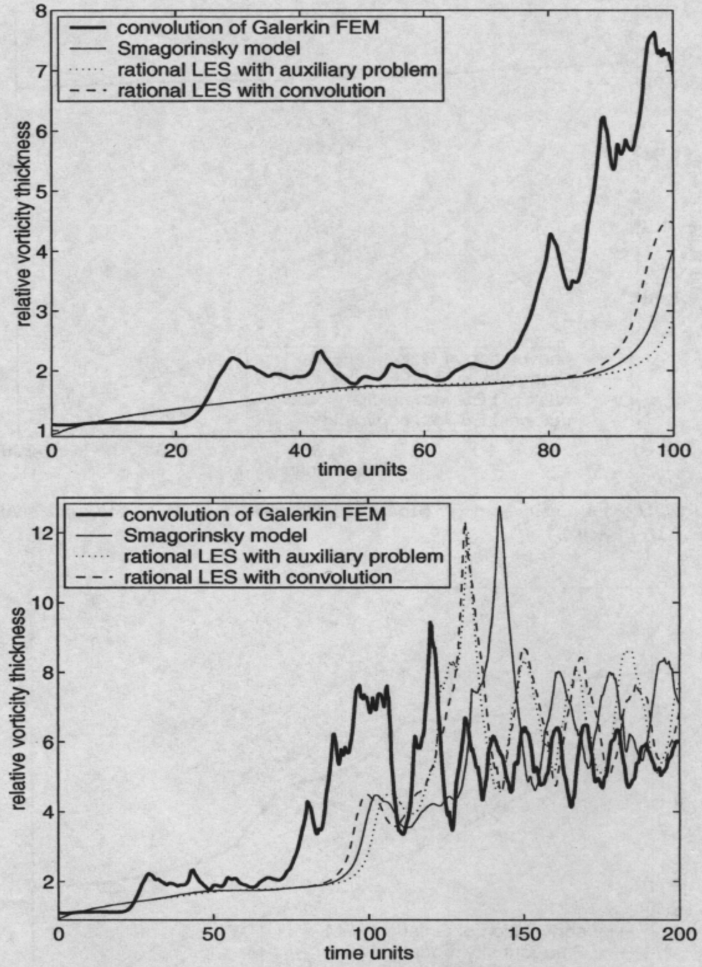


Fig. 11.8. Relative vorticity thickness to σ_0, Smagorinsky model (4.3) as subgrid scale model with $c_S = 0.01$, level 5

E_{tot}, $\left\| w^h \right\|_2$ evolution,
Smagorinsky SGS, *h*/32

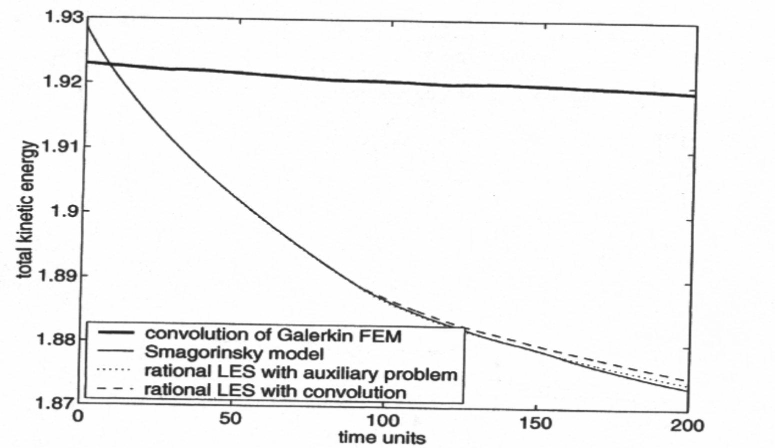


Fig. 11.9. Total kinetic energy, Smagorinsky model (4.3) as subgrid scale model with $c_S = 0.01$, level 5

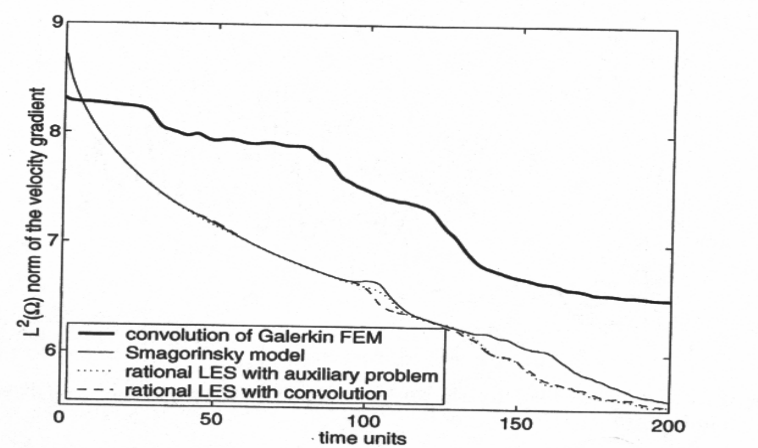


Fig. 11.10. $L^2(\Omega)$ norm of the gradient of the velocity, Smagorinsky model (4.3) as subgrid scale model with $c_S = 0.01$, level 5

CLES.36 Computational Issues in Large Eddy Simulation

Rational LES + auxiliary problem, Iliescu-Layton SGS closure, c_s = 0.5, 0.17

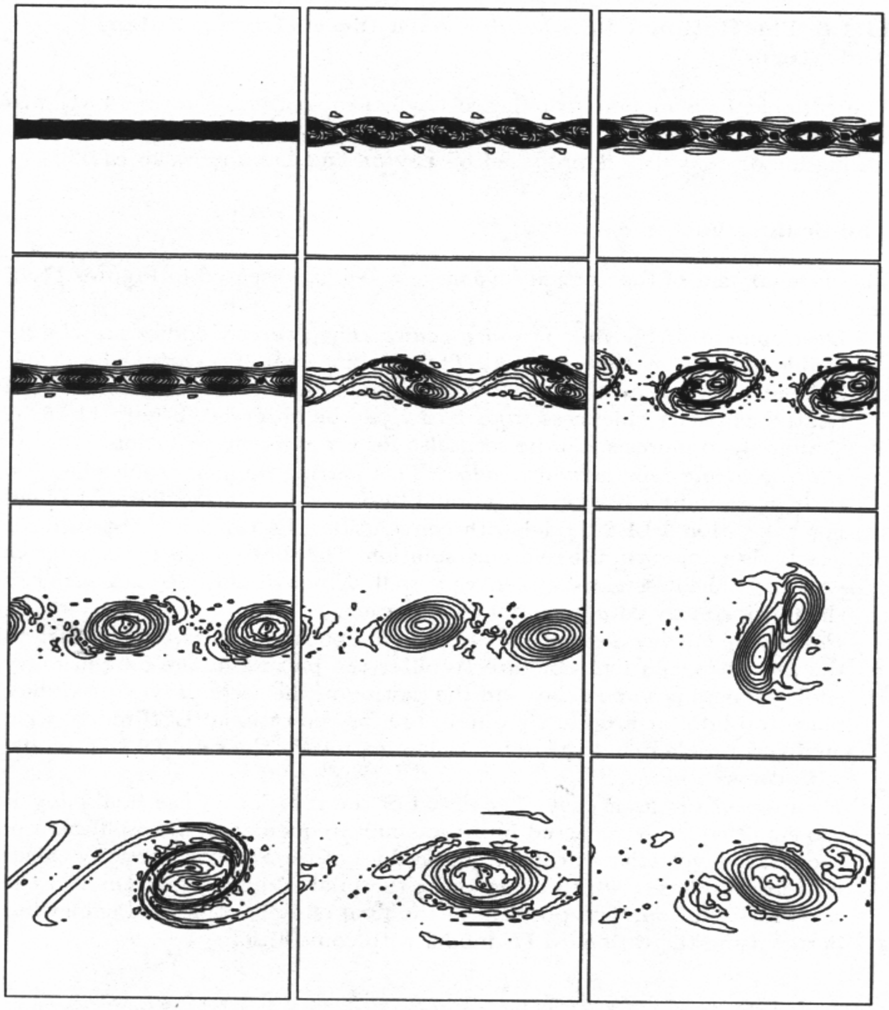


Fig. 11.17. Rational LES model with auxiliary problem, Iliescu-Layton model (4.31) as subgrid scale model with $c_S = 0.5$, vorticity on level 5, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

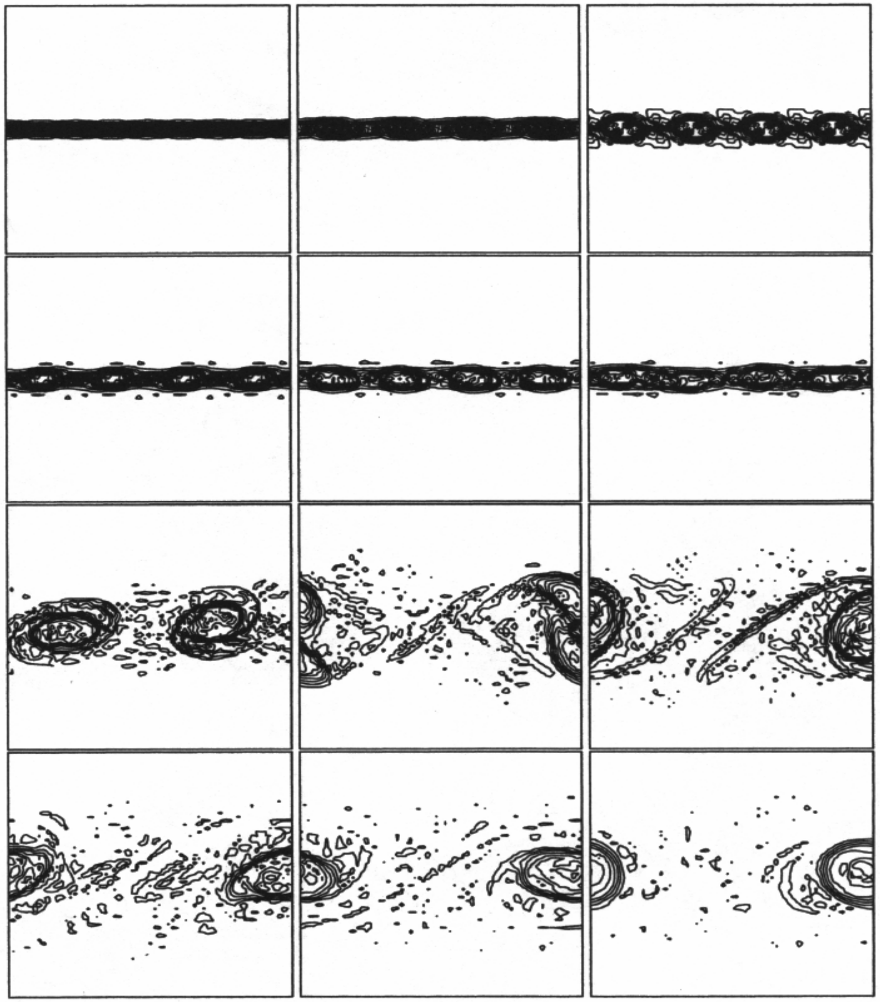
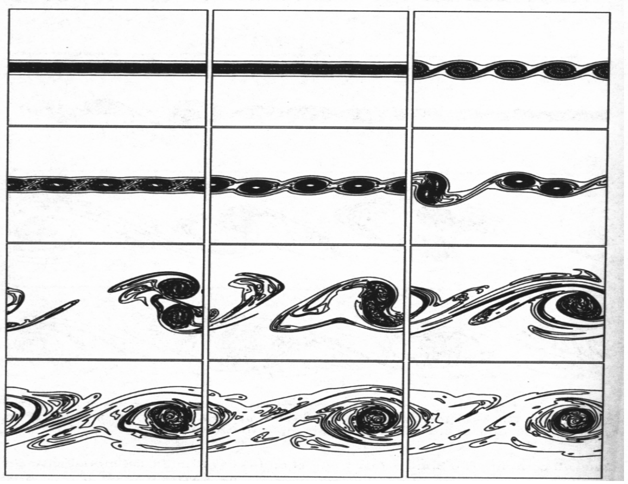


Fig. 11.22. Rational LES model with auxiliary problem, Iliescu-Layton model (4.31) as subgrid scale model with $c_S = 0.17$, vorticity on level 5, at time units 0, 20, 30, 50, 70, 80, 100, 120, 140, 160, 180, 200 (left to right, top to bottom)

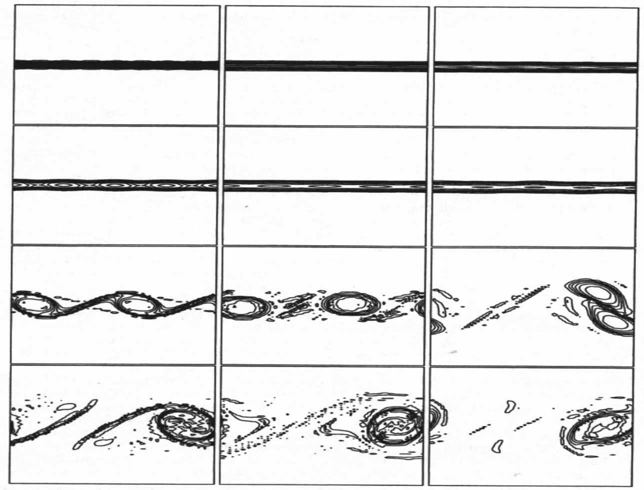
CLES.37 Computational Issues in Large Eddy Simulation

Rational LES with aux validation, *d* =2 mixing layer, $h/32$, $\delta = \sqrt{2}/32$

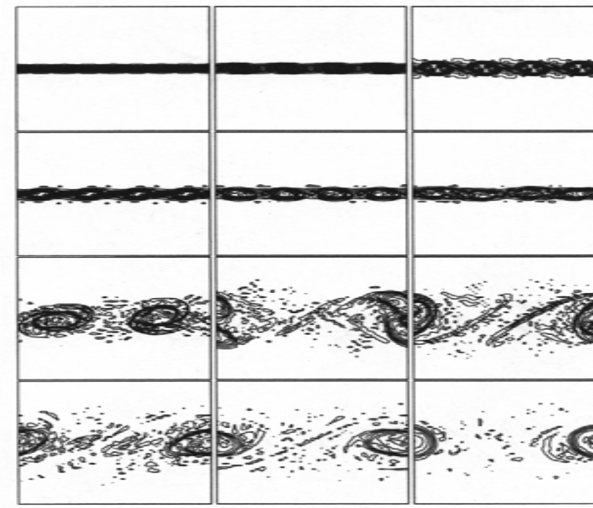
Galerkin DNS



Smagorinsky SGS, c_s=0.01



Iliescu-Layton SGS, c_s=0.17



SGS closure	c_s	vortex pairing	steady solution comparison
Smagorinsky	0.01	very delayed	quantitative
	0.005	less delayed	qualitative but "trashy"
		auxiliary problem preferable to convolution	
Iliescu-Layton	0.5	too fast	quantitative
	0.17	a little slow	qualitative but "trashy"
	0.18	auxiliary problem preferable to convolution	