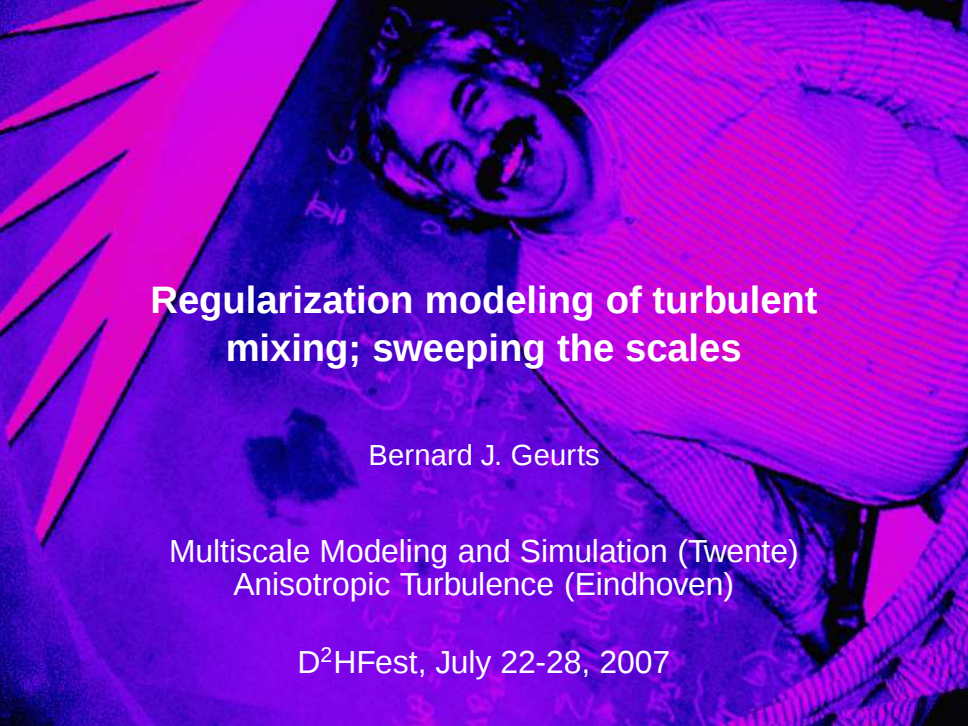




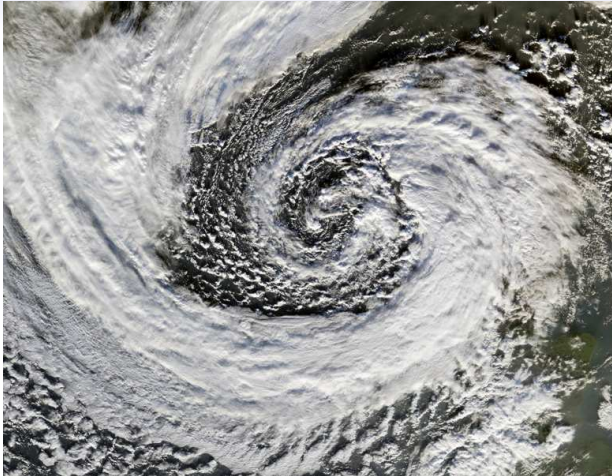
Regularization modeling of turbulent mixing; sweeping the scales

Bernard J. Geurts

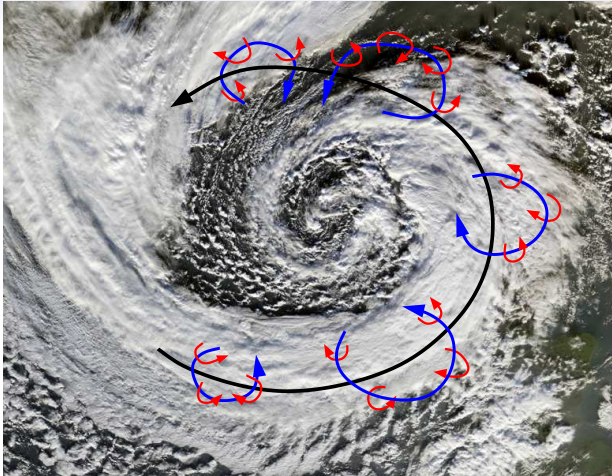
Multiscale Modeling and Simulation (Twente)
Anisotropic Turbulence (Eindhoven)

D²HFest, July 22-28, 2007

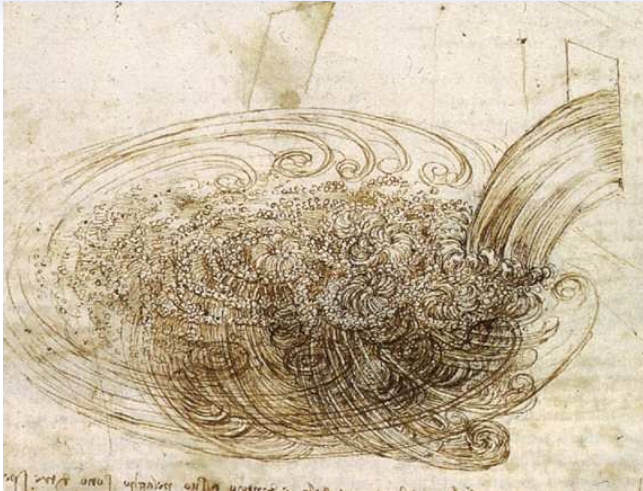
Turbulence — sweeping scales?



Cyclone near Iceland



Cyclone near Iceland



Early impression of swept scales - Da Vinci



Practical relevance - weather dynamics



Vortices in the far wake - airport congestion

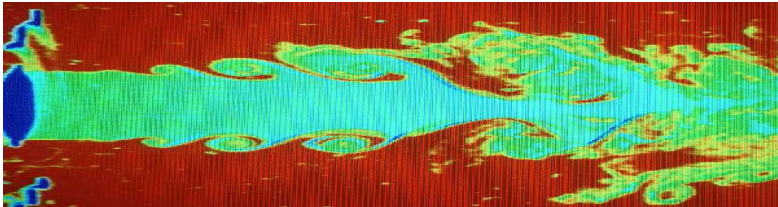
Outline

- 1 Turbulence and filtering
- 2 Regularization modeling of small scales
- 3 Numerics: friend or foe?
- 4 Mixing: combustion and stratification
- 5 Concluding remarks

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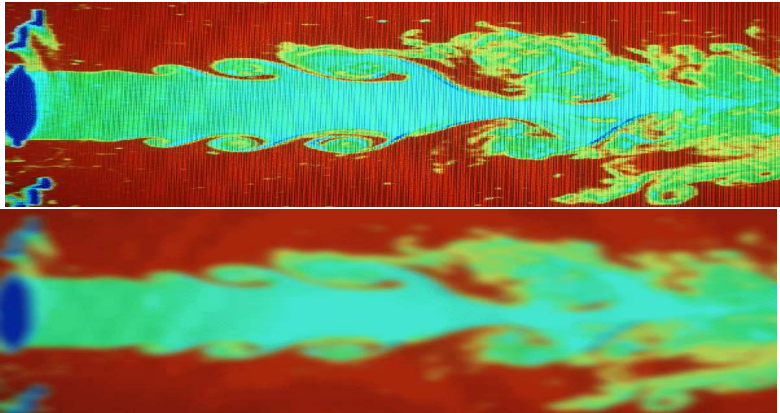
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DNS and LES in a picture



- capture both large and small scales: $W \sim Re^3 \sim N^4$
- Coarsening/mathematical modeling instead: LES

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Filtering Navier-Stokes equations

Convolution-Filtering: filter-kernel G , width Δ

$$\bar{u}_i = L(u_i) = \int G(x - \xi) u(\xi) d\xi$$

Application of filter:

$$\partial_t \bar{u}_i + \partial_j (\bar{u}_i \bar{u}_j) + \partial_i \bar{p} - \frac{1}{Re} \partial_{jj} \bar{u}_i = -\partial_j (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)$$

Turbulent stress tensor:

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j = L(u_i u_j) - L(u_i) L(u_j) = [L, \Pi_{ij}](\mathbf{u})$$

Properties τ :

- fully specified by filter L and NS-dynamics
- depends on u and $\bar{u}$ – closure problem

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Heuristic: Eddy-viscosity modeling

Obtain smoothing via increased dissipation:

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Damp large gradients: dimensional analysis

$$\nu_t = \text{length} \times \text{velocity} \sim \Delta \times \Delta |\partial_x v|$$

Effect: Strong damping at large filter-width and/or gradients

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Some explicit subgrid models

Popular models:

- **Dissipation:** Eddy-viscosity models, e.g., Smagorinsky

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- **Similarity:** Inertial range, e.g., Bardina

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- **Mixed models ?**

$$m_{ij} = \text{Bardina} + \mathbf{C}_d \text{Smagorinsky}$$

$\mathbf{C}_d$ via dynamic Germano-Lilly procedure

Are these models any good?

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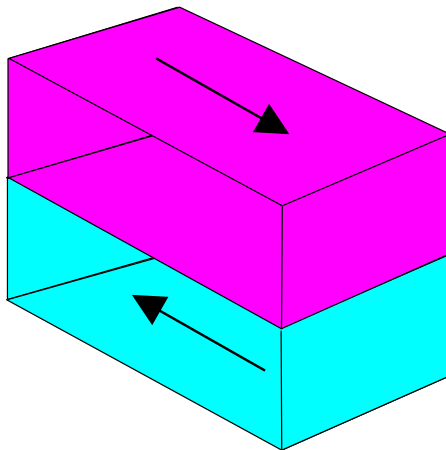
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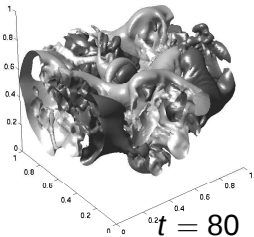
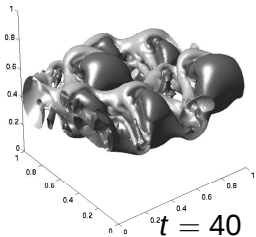
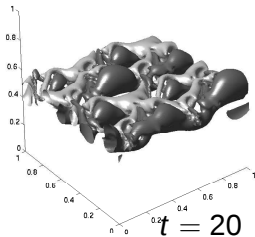
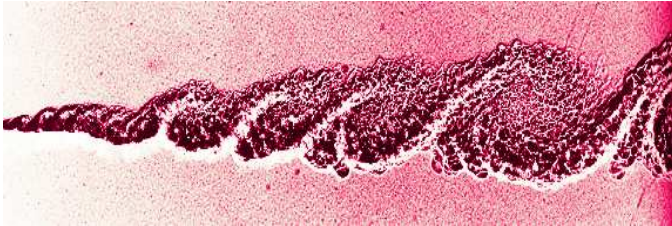
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Mixing layer: testing ground for models



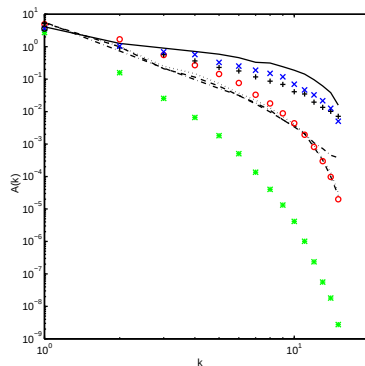
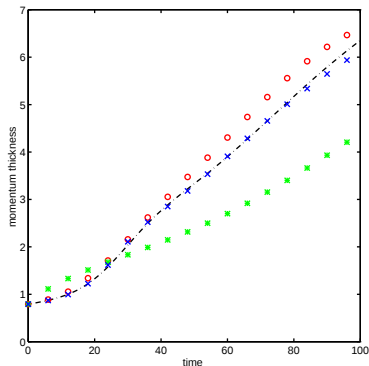
Temporal model for mixing layer

Mixing layer: testing ground for models



Temporal at different $t \approx$ Spatial at different x

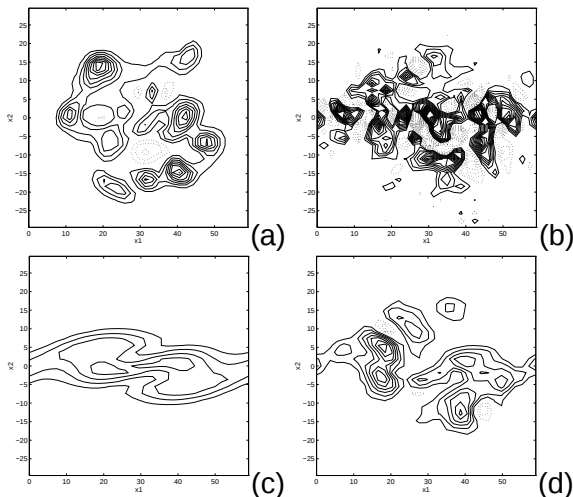
Some basic flow properties



Momentum thickness and energy spectrum

- Smagorinsky too dissipative, Bardina not enough
- dynamic models quite accurate
- problems, e.g., intermediate and smallest scales

Instantaneous snapshots of spanwise vorticity



a: $\overline{DNS}$, b: Bardina, c: Smagorinsky, d: dynamic
Accuracy limited: regularization models better?

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Models and connection to filter

Central role of filter identified, but ...
... modeling rather heuristically, and ...
... connection with filter is only partial ..

Alternative – regularization models:

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- derive implied subgrid model
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Example: Leray regularization

Alter convective fluxes: sweeping by large scales

$$\partial_t u_i + \overline{u_j} \partial_j u_i + \partial_i p - \frac{1}{Re} \Delta u_i = 0$$

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Approximate inversion procedures

- Geometric series: repeated filtering

$$L^{-1}(v) = (I - (I - L))^{-1}(v) \approx \sum_{n=0}^N (I - L)^n(v)$$

For example:

$$N = 0 : \quad u = L_1^{-1}(v) = v$$

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- Exact inversion of Simpson-top-hat: 3-point filters
(a, 1 - 2a, a)

$$L^{-1}(v_m) \approx \sum_{j=-n}^n \left(\frac{a - 1 + \sqrt{1 - 2a}}{a} \right)^{|j|} \frac{v_{m+rj/2}}{(1 - 2a)^{1/2}}$$

Use: $a = 1/3$ and $r = \Delta/h = 2, 4, \dots$ Convergence?

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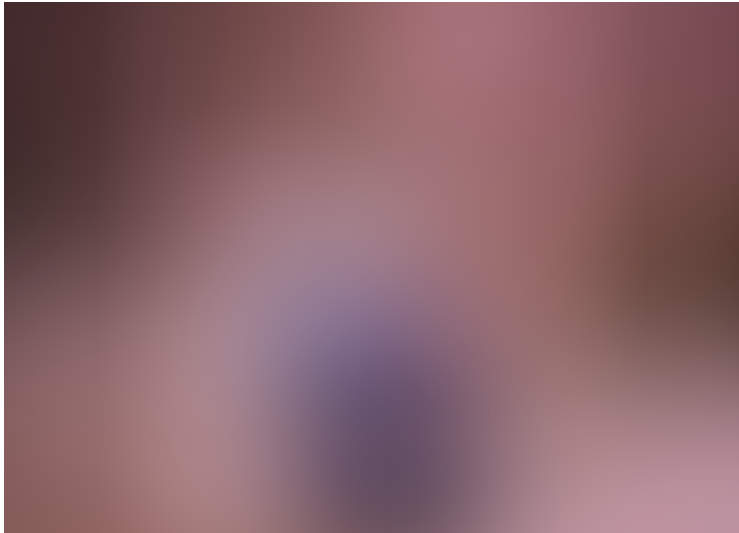
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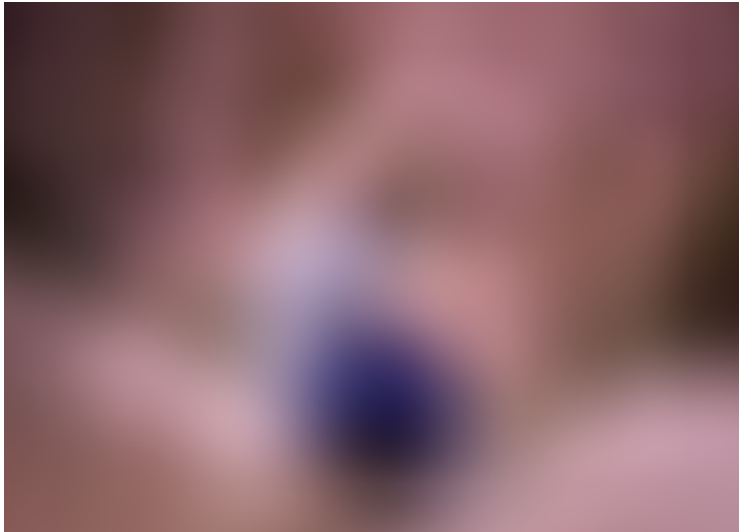
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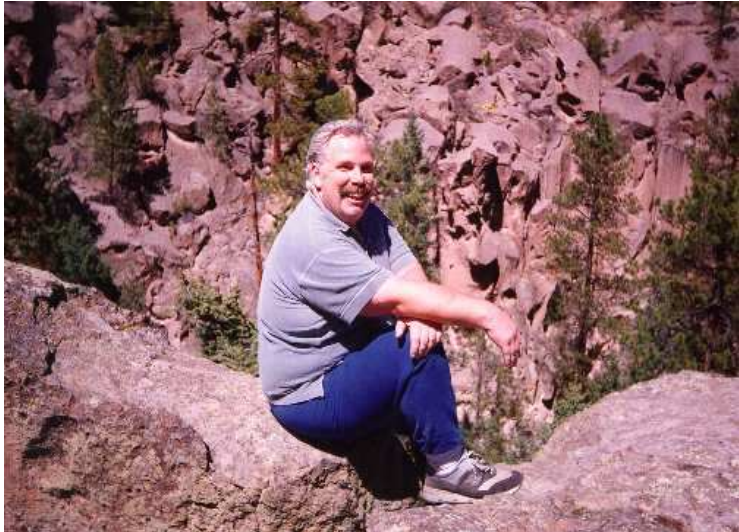
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NS- α regularization

Kelvin's circulation theorem

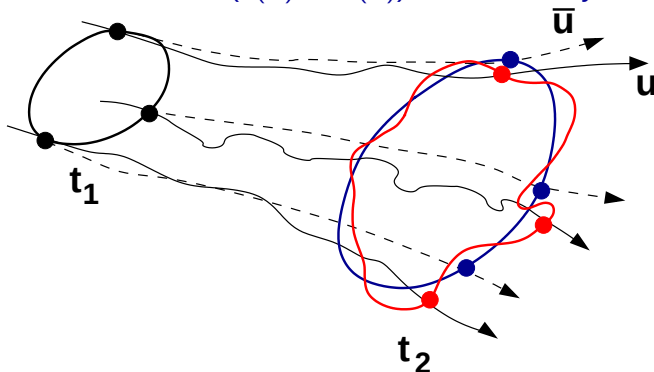
$$\frac{d}{dt} \left(\oint_{\Gamma(\mathbf{u})} u_j \, dx_j \right) - \frac{1}{Re} \oint_{\Gamma(\mathbf{u})} \partial_{kk} u_j \, dx_j = 0 \quad \Rightarrow \quad \text{NS} - \text{eqs}$$

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Filtered Kelvin theorem ($\Gamma(\mathbf{u}) \rightarrow \Gamma(\bar{\mathbf{u}})$) extends Leray



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α -principle: $\Gamma(\mathbf{u}) \rightarrow \Gamma(\bar{\mathbf{u}}) \Rightarrow$ Euler-Poincaré

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Rewrite into LES template: Implied subgrid model

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Alternative expression of large-scale sweeping

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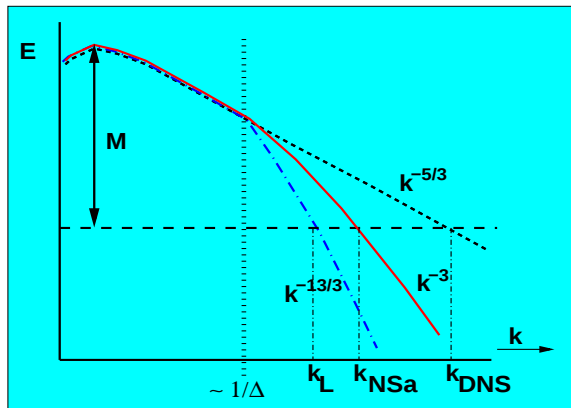
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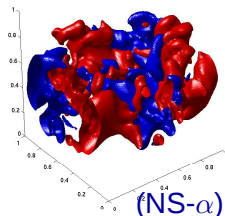
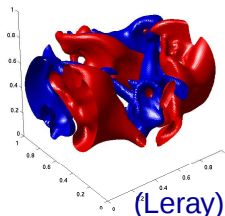
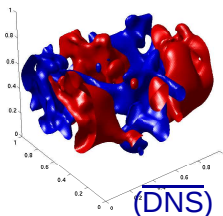
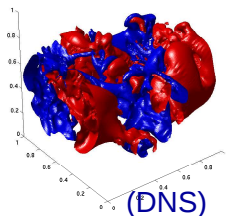
Alternative expression of large-scale sweeping

Cascade-dynamics – computability



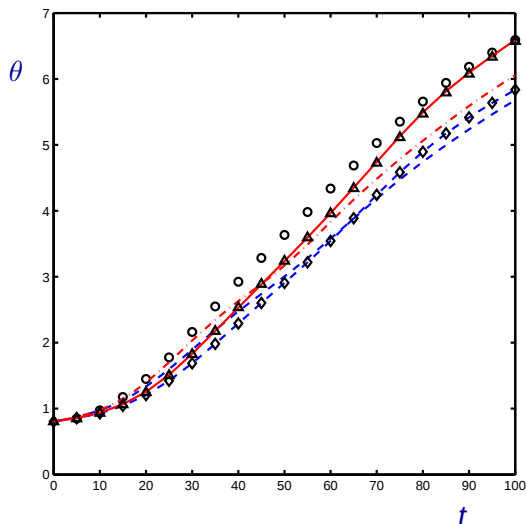
- $NS-\alpha$, Leray are dispersive
- Regularization alters spectrum – controllable cross-over as $k \sim 1/\Delta$: steeper than $-5/3$

Leray and NS- α predictions: $Re = 50$, $\Delta = \ell/16$



Snapshot u_2 : red (blue) corresponds to up/down

Momentum thickness θ as $\Delta = \ell/16$



Filtered DNS ($\circ$)

Leray-model

32^3 : dash-dotted

64^3 : solid

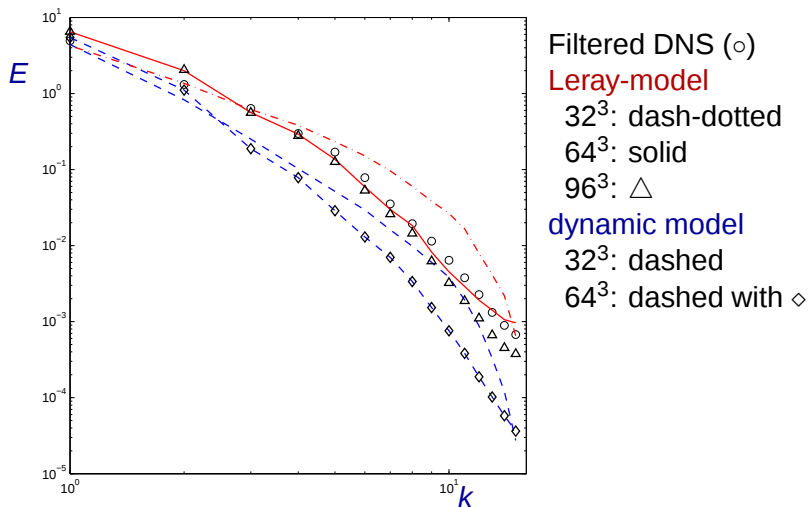
96^3 : $\triangle$

dynamic model

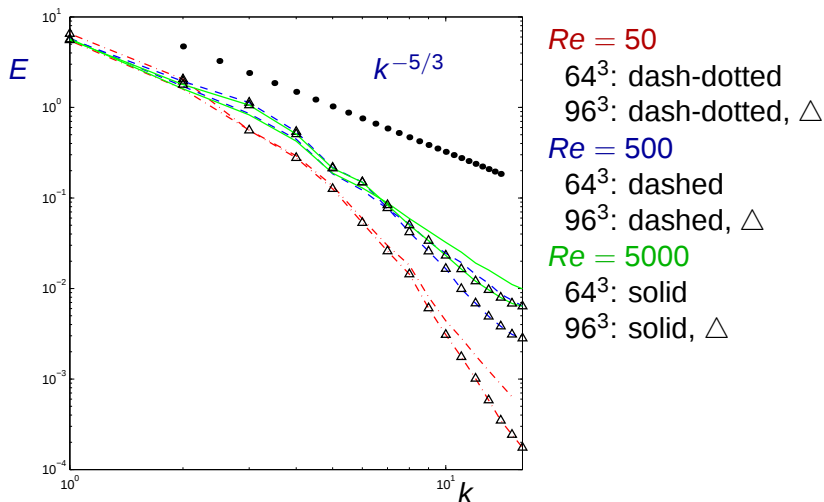
32^3 : dashed

64^3 : dashed with $\diamond$

Streamwise kinetic energy E as $\Delta = \ell/16$

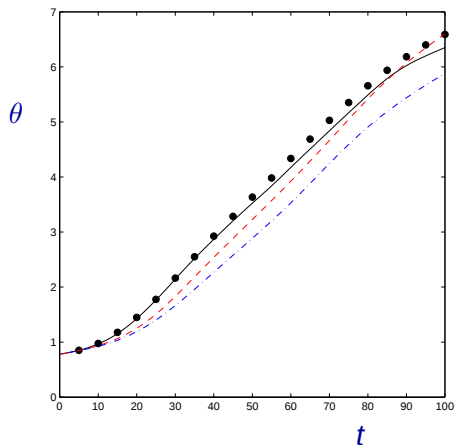


Robustness at arbitrary Reynolds number



What about improvements arising from NS- α ?

Momentum thickness θ as $\Delta = \ell/16$



- NS- α (solid), Leray (dash), dynamic (dash-dotted), DNS •
- approximately grid-independent at 96^3

NS- α accurate but converges slowest

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Numerics in academic LES setting

Goal: approximate the unique solution to system of PDE's resulting after adopting explicit closure model

General requirements:

- Filter separates scales $> \Delta$ from scales $< \Delta$
- Computational grid provides additional length-scale h
- Require Δ/h to be sufficiently large ($\Delta/h \rightarrow \infty$)
- Good numerics: $v(x, t : \Delta, h) \rightarrow v(x, t : \Delta, 0)$ rapidly

However:

- computational costs $\sim N^4$: implies modest Δ/h
- potentially large role of numerical method in computational dynamics because of marginal resolution

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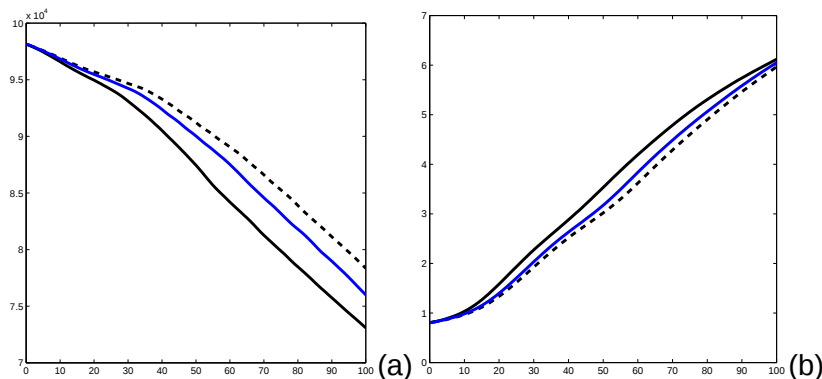
Numerical aspects

Study influence of:

- Filter inversion
- Spatial discretization method

Also study error interactions/cancellations ...

Quality of filter-inversion – Leray

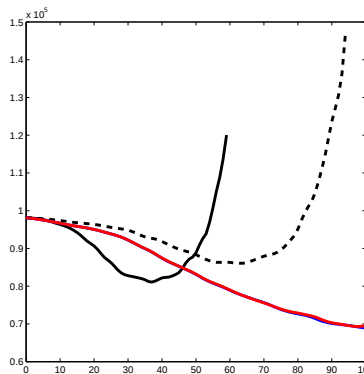


Inversion of Simpson top-hat filter:

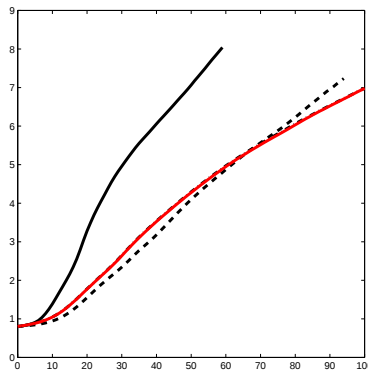
- Kinetic energy (a) and momentum thickness (b)
- $n = 1$ (solid), $n = 2$ (dash), $n \geq 5$

Quality of filter-inversion – LANS- α

Kinetic energy E and momentum thickness D



(a)



(b)

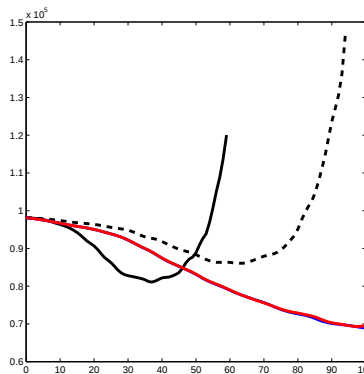
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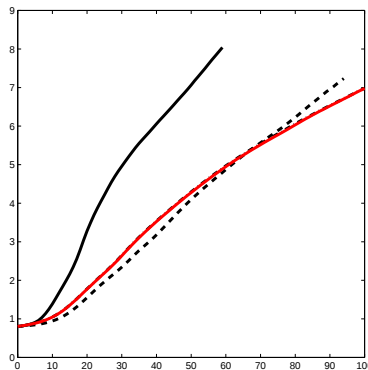
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Spatial discretization

Discretization induces spatial filter:

$$\delta_x f(x) = \partial_x(\hat{f})$$

- modified mean flux
- modified turbulent stress tensor

Compare:

- Second order FV: $\delta_x^{(2)}(f(u))$
- Fourth order FV: $\delta_x^{(4)}(f(u))$
- Combination treats small scales at second order

$$\delta_x(f(u)) = \delta_x^{(4)}(f(\bar{u})) + \delta_x^{(2)}(f(u) - f(\bar{u}))$$

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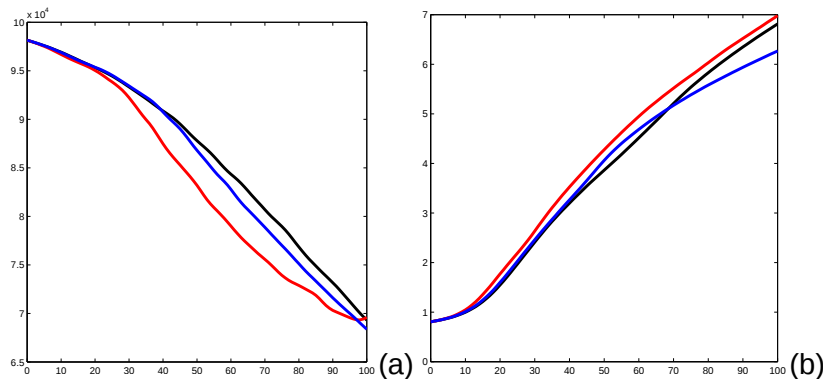
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LANS- α : sensitive to discretization

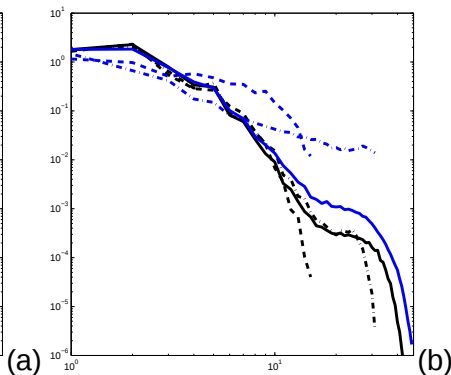
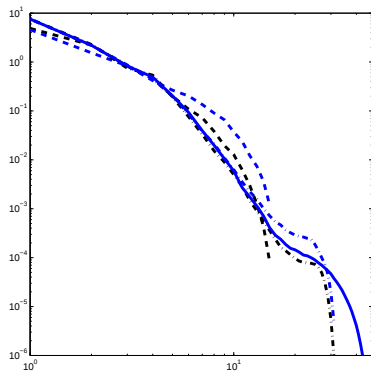
$N = 32$: Kinetic energy E and momentum thickness D



● Second order, Fourth order, (4-2) method

Spectral signature of numerics

Leray and LANS- α spectra:



- Second order, **Fourth order**
- $N = 32$ (dash), $N = 64$ (dash-dot), $N = 96$ (solid)

Numerics or modeling or both ?

Observe:

- At marginal resolution numerics modifies the equations
- Likewise, a subgrid model modifies these equations

Dilemma: which is to be preferred

- Not just best numerics/best model ... LES paradoxes
- Governed by error-interactions: nonlinear error-accumulation

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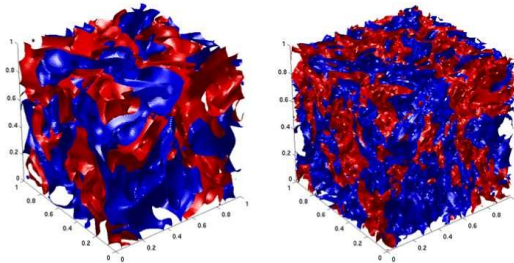
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Smagorinsky fluid

Homogeneous decaying turbulence at $Re_\lambda = 50, 100$



- Smagorinsky fluid — subgrid model:

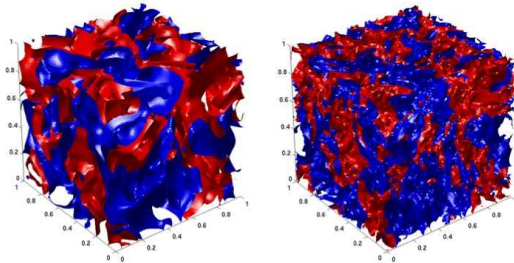
$$m_{ij}^S = -2(C_S \overline{\Delta})^2 |\overline{S}| \overline{S}_{ij} = -2\ell_S^2 |\overline{S}| \overline{S}_{ij}$$

introduces Smagorinsky-length ℓ_S

- Also dynamic Smagorinsky fluid with length-scale ℓ_d

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Experimental error-assessment

Pragmatic: minimal total error at given computational costs

Discuss:

- error-landscape/optimal refinement strategy
- LES-specific error-minimization: SIPI

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Accuracy measures

Monitor resolved kinetic energy

$$E = \frac{1}{|\Omega|} \int_{\Omega} \frac{1}{2} \bar{\mathbf{u}} \cdot \bar{\mathbf{u}} d\mathbf{x} = \frac{1}{2} \langle \bar{\mathbf{u}} \cdot \bar{\mathbf{u}} \rangle$$

Measure relative error: top-hat filter Δ , grid $h = \Delta/r$

$$\delta_E(\Delta, r) = \left\| \frac{E_{LES}(\Delta, r) - E_{DNS}(\Delta, r)}{E_{DNS}(\Delta, r)} \right\|$$

with error integrated over time

$$\|f\|^2 = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} f^2(t) dt$$

- each simulation represented by **single** number
- concise representation facilitates comparison

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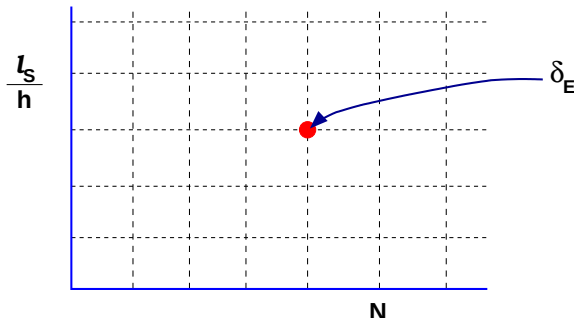
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Error-landscape: Definition

Framework for collecting error information:



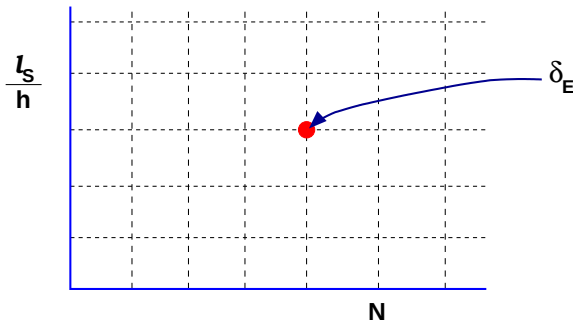
Each Smagorinsky LES corresponds to **single** point:

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Contours of δ_E — fingerprint of LES

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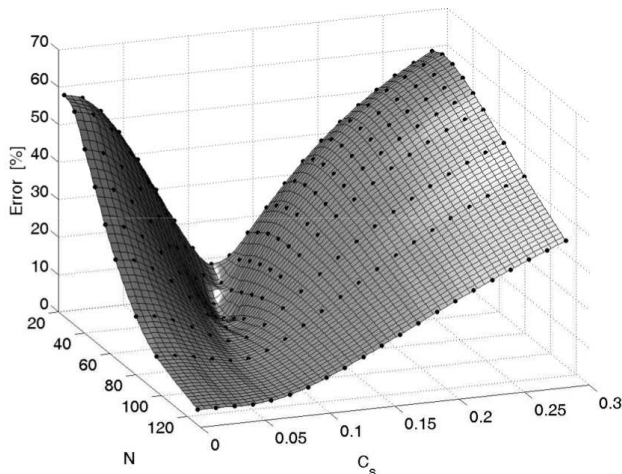


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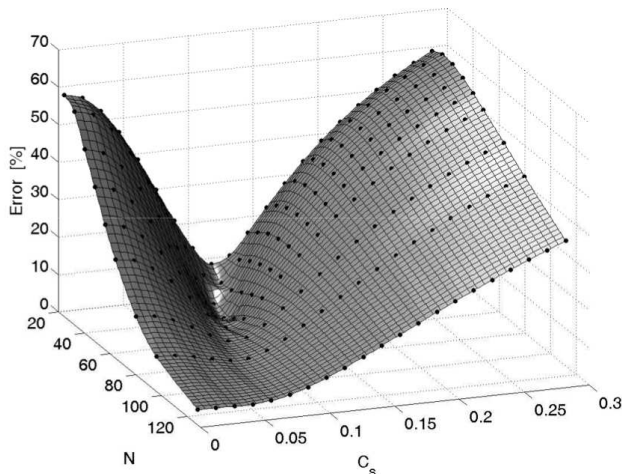
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Total error-landscape



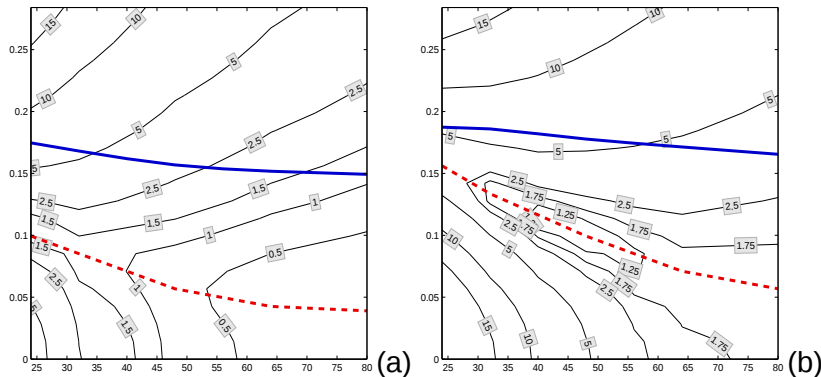
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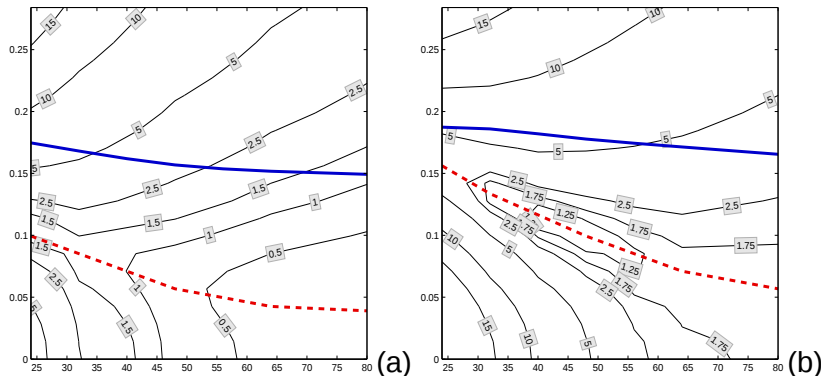
Error-landscape: optimal refinement



Optimal trajectory for $Re_\lambda = 50$ (a) and $Re_\lambda = 100$ (b)

- Under-resolution leads to strong error-increase
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MILES philosophy

Observation:

- practical LES implies marginal resolution
- which implies large role of specific numerical discretization
- next to dynamics due to subgrid model
- and leads to strong interactions and complex error-accumulation

Proposal:

- obtain smoothing via appropriate numerical method alone
- accept that there is no grid-independent solution, other than DNS
- accept that predictions become discretization dependent

Is 'no-model/just numerics' option optimal/viable ?

Consider example: DG-FEM and homogeneous turbulence

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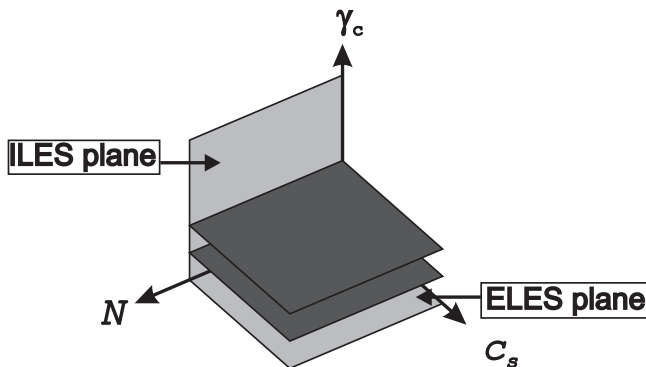
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DG-FEM of homogeneous turbulence

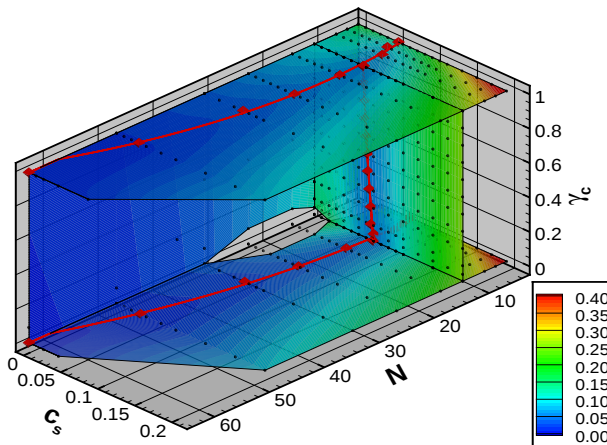
Discretization: Approximate Riemann solver

$$F = F_{central} + \gamma F_{dissipative} \quad ; \quad HLLC - flux$$



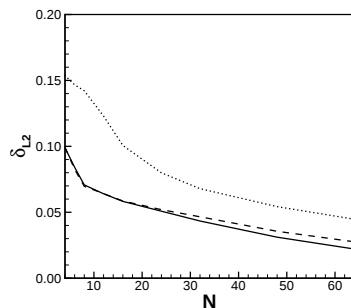
Three-dimensional accuracy charts

LES with DG-FEM: dissipative numerics

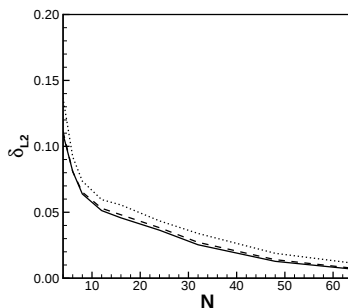


Third order DG-FEM at $Re_\lambda = 100$: red symbols - optimal setting

Optimality of MILES ?



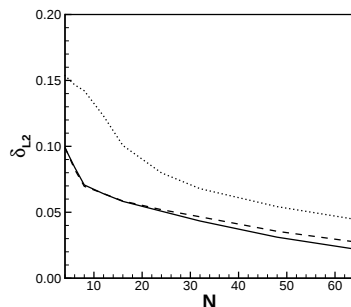
(a)



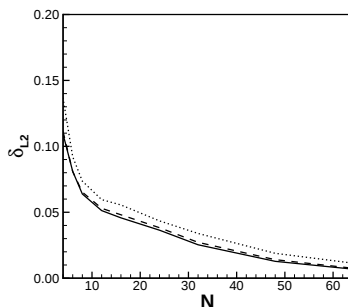
(b)

- (a): 2nd order ; (b): 3rd order
- $\gamma_c = 1.00$ (dot), $\gamma_c = 0.10$ (dash) and $\gamma_c = 0.01$ (—)
- MILES-error larger than with explicit SGS model
- Exchange of dissipation in optimum ...
- Option: directly optimize total simulation error - SIPI

Optimality of MILES ?



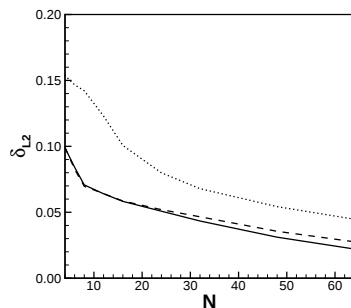
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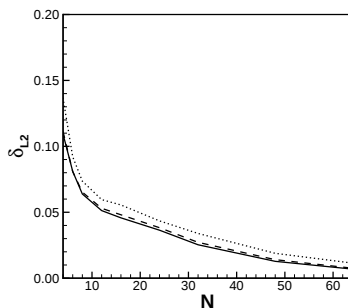
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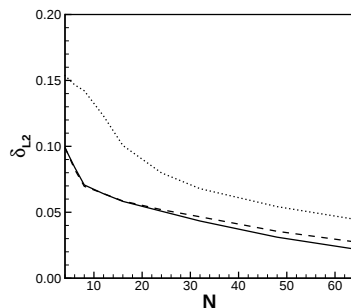
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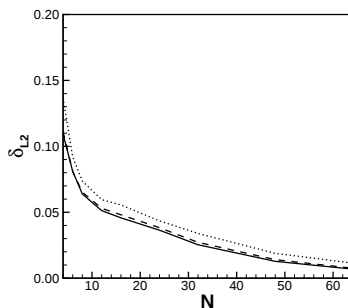
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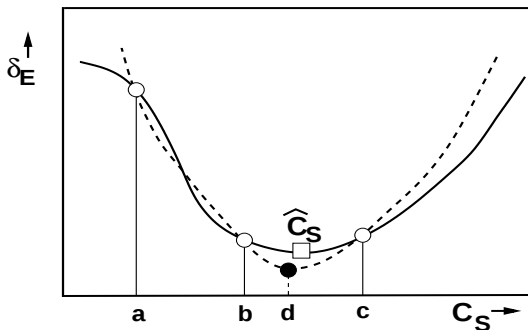


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SIPI - basic algorithm

Goal: minimize total error at given N



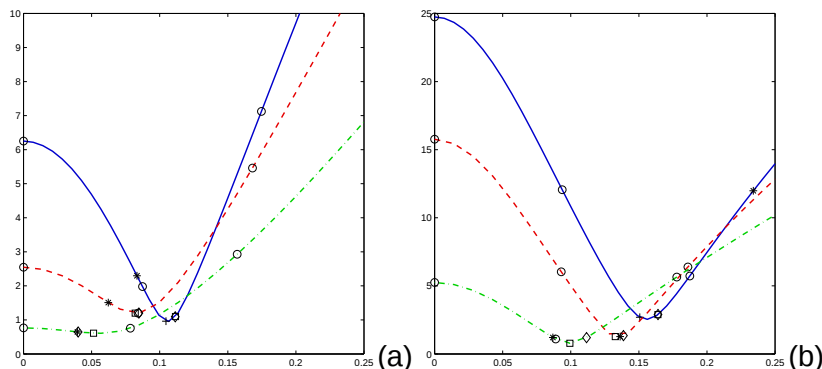
Initial triplet: no-model, dynamic and half-way

New iterand

$$d = b - \frac{1}{2} \frac{(b-a)^2[\delta_E(b) - \delta_E(c)] - (b-c)^2[\delta_E(b) - \delta_E(a)]}{(b-a)[\delta_E(b) - \delta_E(c)] - (b-c)[\delta_E(b) - \delta_E(a)]}$$

SIPI applied to homogeneous turbulence

Each iteration = separate simulation



$Re_\lambda = 50$ (a) and $Re_\lambda = 100$ (b). Resolutions $N = 24$ (solid),
 $N = 32$ (dashed) and $N = 48$ (dash-dotted)

Iterations: $\circ \rightarrow * \rightarrow \diamond \rightarrow \square \rightarrow +$

Convergence example

$Re_\lambda = 50$			$Re_\lambda = 100$	
n	$C_S^{(n)}(24)$	$C_S^{(n)}(48)$	$C_S^{(n)}(24)$	$C_S^{(n)}(48)$
2	0.17470000	0.15690000	0.18740000	0.17780000
3	0.08735000	0.07845000	0.09370000	0.08890000
4	0.08330619	0.03959082	0.23399921	0.08686309
5	0.11142326	0.04010420	0.16404443	0.11154788
6	0.11156545	0.05141628	0.16400079	0.09935076
7	0.10461386	0.05283713	0.15068033	0.09947629
8	0.10508422	0.05468589	0.15445586	0.09926872
9	0.10602797	0.05504089	0.15600828	0.09938967

- **Computational overhead SIPI:** CPU-time $T \sim N^4$ implies approximate optimization at N can be (almost) completed within cost of one simulation at $3N/2$

Outline

- 1 Turbulence and filtering
- 2 Regularization modeling of small scales
- 3 Numerics: friend or foe?
- 4 Mixing: combustion and stratification**
- 5 Concluding remarks

Application to complex physics

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- collection of assumptions/parameters increases
- consistency becomes problem
- predictive power ?

Can first principles approach be extended?

Consider combustion and stratified mixing

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Example: Turbulent combustion

Computational model:

$$\partial_t \rho + \partial_j(\rho u_j) = 0$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) + \partial_i p - \partial_j \sigma_{ij} = 0$$

$$\partial_t \mathbf{e} + \partial_j((\mathbf{e} + p)u_j) - \partial_j(\sigma_{ij}u_i) + \partial_j q_j - h_k \omega_k = 0$$

$$\partial_t(\rho c_k) + \partial_j(\rho c_k u_j) - \partial_j(\pi_{kj}) - \omega_k = 0 \quad ; \quad k = 1, \dots, N_s$$

F-O-P flame: Arrhenius law $F + O \rightarrow P$

$$\omega_F = -(\rho c_F)(\rho c_O) \frac{Da}{W_O} \exp\left(-\frac{Ze}{T}\right)$$

$$\omega_O = \alpha \omega_F \quad ; \quad \omega_P = -(1 + \alpha) \omega_F$$

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- weight-ratio $\alpha = W_O/W_F$

Energy equation source term: $h_j \omega_j = Q \omega_F$

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Spatial filtering and subgrid closure

Filtered model equations: $(\bar{\rho}, \tilde{u}_j, \bar{p}$ and $\tilde{c}_k)$

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$$\partial_t \check{e} + \partial_j ((\check{e} + \bar{p}) \tilde{u}_j) - \partial_j (\check{\sigma}_{ij} \tilde{u}_i) + \partial_j \check{q}_j = \overline{h_k \omega_k} + \mathcal{A}$$

$$\partial_t (\bar{\rho} \tilde{c}_k) + \partial_j (\bar{\rho} \tilde{c}_k \tilde{u}_j) - \partial_j (\check{\pi}_{kj}) = -\partial_j (\bar{\rho} \zeta_{jk}) + \bar{\omega}_k + \partial_j (\bar{\pi}_{kj} - \check{\pi}_{kj})$$

Terms requiring closure:

- Turbulent stress tensor: τ_{ij}
- Velocity-species stress tensor: ζ_{jk}
- Chemical source terms

Many more contributions - systematic approach needed

Investigate extended Leray approach

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$$\partial_t (\bar{\rho} \tilde{c}_k) + \partial_j (\bar{\rho} \tilde{c}_k \tilde{u}_j) - \partial_j (\check{\pi}_{kj}) = -\partial_j (\bar{\rho} \zeta_{jk}) + \bar{\omega}_k + \partial_j (\bar{\pi}_{kj} - \check{\pi}_{kj})$$

Terms requiring closure:

- Turbulent stress tensor: τ_{ij}
- Velocity-species stress tensor: ζ_{jk}
- Chemical source terms

Many more contributions - systematic approach needed
Investigate extended Leray approach

Spatial filtering and subgrid closure

Filtered model equations: $(\bar{\rho}, \tilde{u}_j, \bar{p}$ and $\tilde{c}_k)$

$$\partial_t \bar{\rho} + \partial_j (\bar{\rho} \tilde{u}_j) = 0$$

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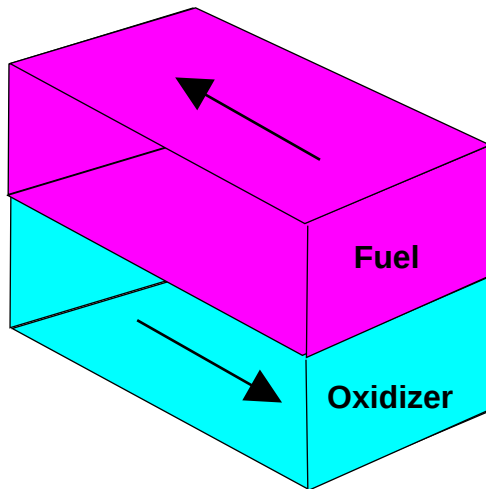
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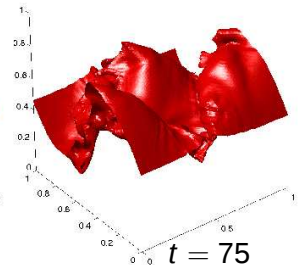
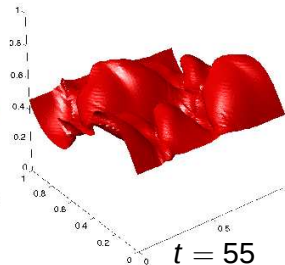
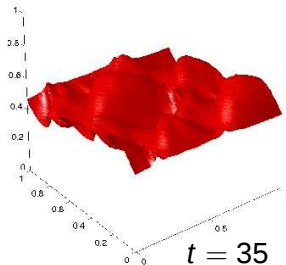
Investigate extended Leray approach

Combustion-modulated turbulence



Stoichiometric surface

Surface $c_F = c_O$



- DNS at 256^3 resolution
- modest heat-release $Q = -1$

Turbulence combustion interaction

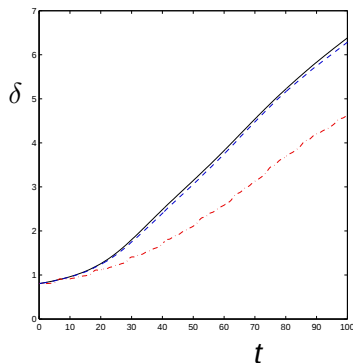
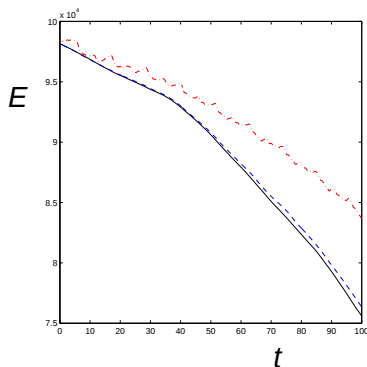
Leray predictions: 32^3 and $\Delta = \ell/16$

$$E(t) = \int_{\Omega} \frac{1}{2} \bar{u}_i \bar{u}_i \, d\mathbf{x} \quad ; \quad \delta = \frac{1}{4} \int_{-\ell/2}^{\ell/2} \left(1 - \langle \bar{u}_1 \rangle\right) \left(\langle \bar{u}_1 \rangle + 1\right) dx_2$$

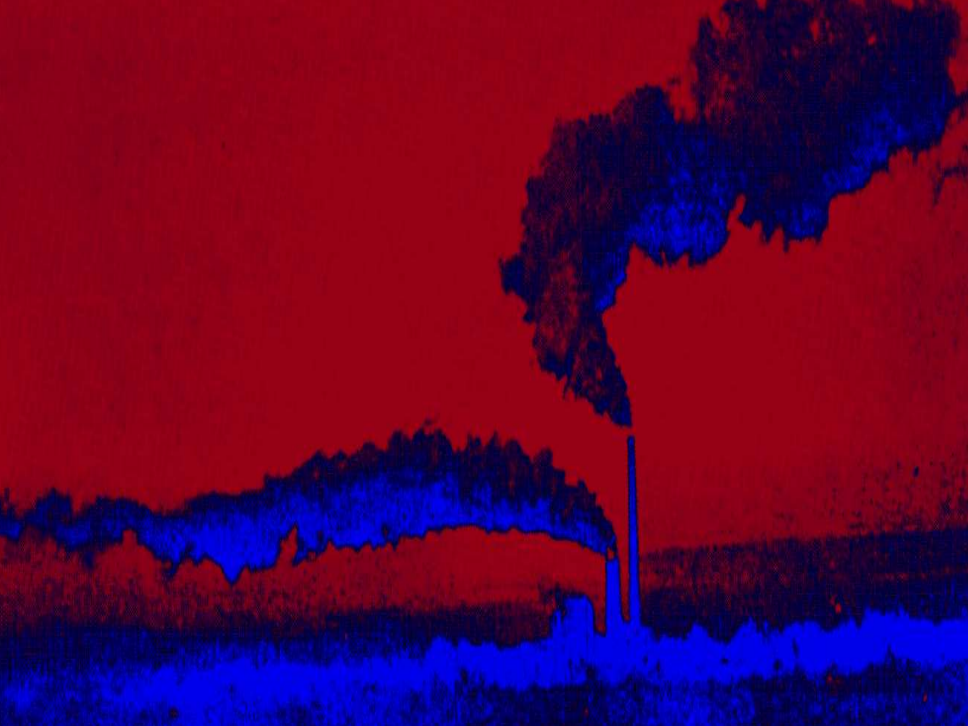
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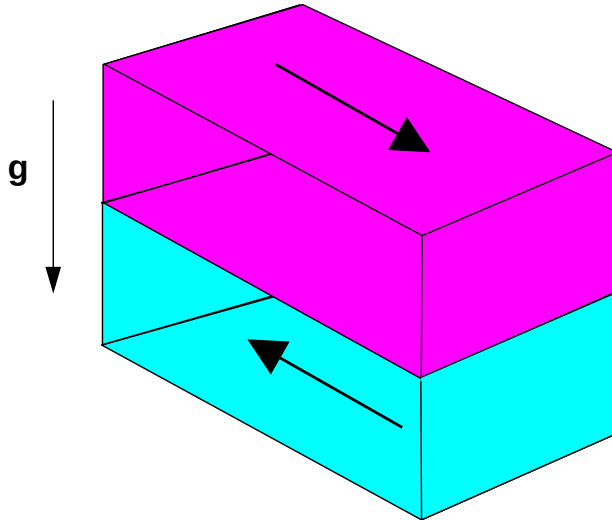
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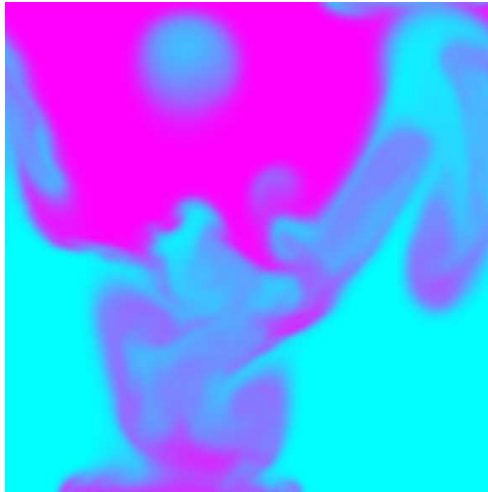
- $Q = -1$ (solid), $Q = -10$ (dash), $Q = -100$ (dash-dot)



Model: Stratified mixing layer



Turbulent plumes



- Unstable, anisotropic, inhomogeneous: [▶ go](#)

Stratification: DNS and LES

Stratification:

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \frac{1}{Re} \nabla^2 \mathbf{u} = -\frac{1}{Fr^2} (c \mathbf{e}_g)$$

Advection-diffusion for scalar c

$$\partial_t c + \mathbf{u} \cdot \nabla c - \frac{1}{Re Sc} \nabla^2 c = 0$$

Characteristic numbers: (Re, Fr, Sc)

LES: subgrid modeling in momentum and scalar equations

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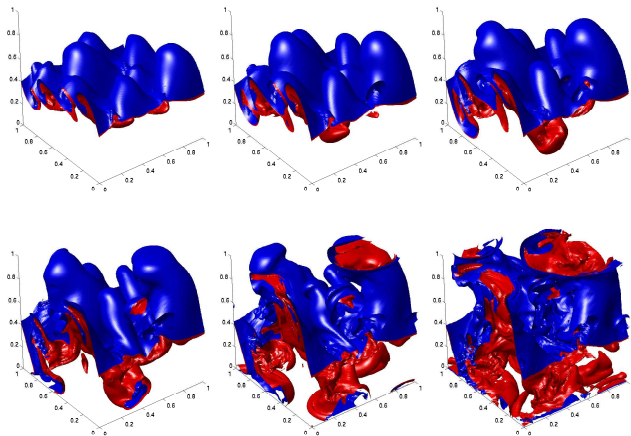
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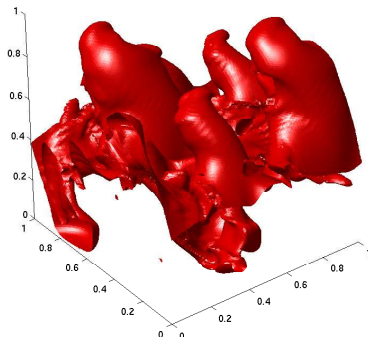
LES: subgrid modeling in momentum and scalar equations

Unstable stratification at $Fr = 2$, $Re = 50$

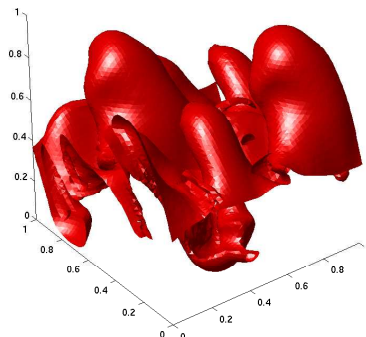


- mixing of **heavy** fluid on top of **lighter** fluid: $t = 30, \dots, 55$

LES capturing of plumes



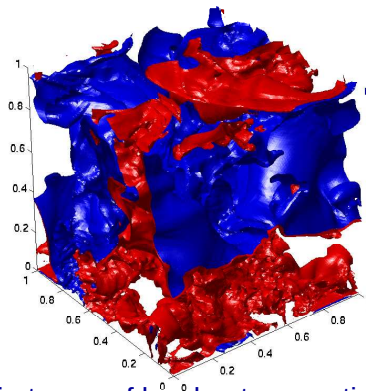
DNS ($t = 40$)



Leray LES ($t = 40$)

- Case: $Fr = 2$ and $Sc = 10$ at $\Delta = \ell/16$
- What about prediction mixing efficiency?

Level-set: surface-area and wrinkling



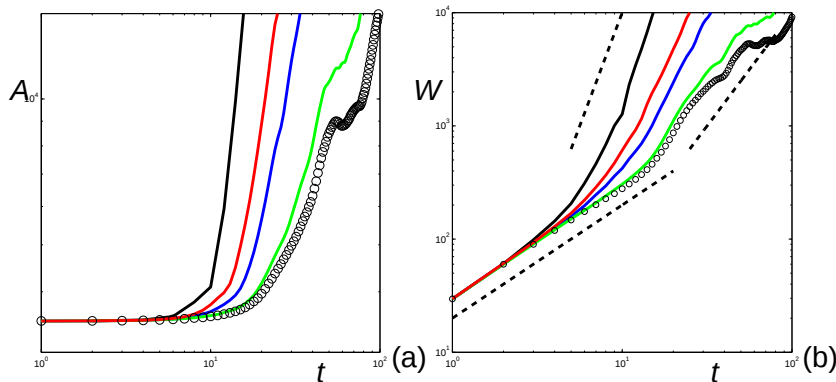
Measure mixing in terms of level-set properties

$$I = \int_{S(a,t)} dA f(\mathbf{x}, t) = \int_V d\mathbf{x} \delta(c(\mathbf{x}, t) - a) |\nabla c(\mathbf{x}, t)| f(\mathbf{x}, t)$$

where $S(a, t) = \{\mathbf{x} \in \mathbb{R}^3 \mid c(\mathbf{x}, t) = a\} \subset V$ – Laplace transform

Effect of Fr on surface area and wrinkling

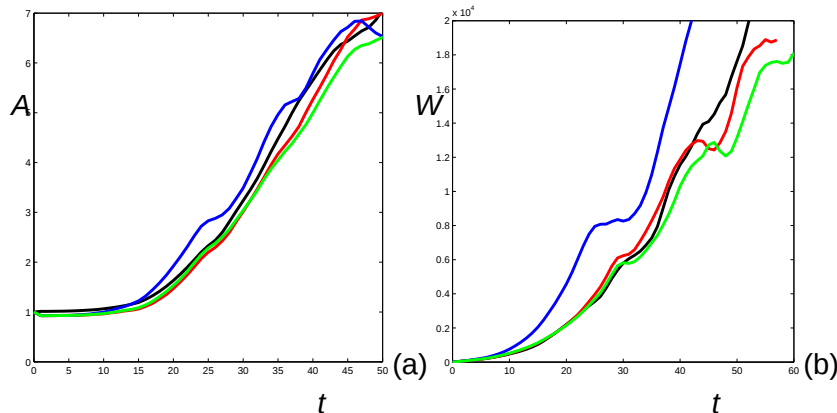
Area ($f = 1$) and wrinkling ($f = |\nabla \cdot \mathbf{n}|$)



- DNS: $Sc = 10$ and $Fr = 1, 1.5, 2, 4, 8$
- W : Initially $\sim t$ then from $\sim t^3$ to $\sim t^4$
- global features captured well with LES

Surface-area and wrinkling: LES

Localized wrinkling more difficult to capture with LES



● $Fr = 2$ and $Sc = 10$: DNS, Leray, NS- α , Dynamic

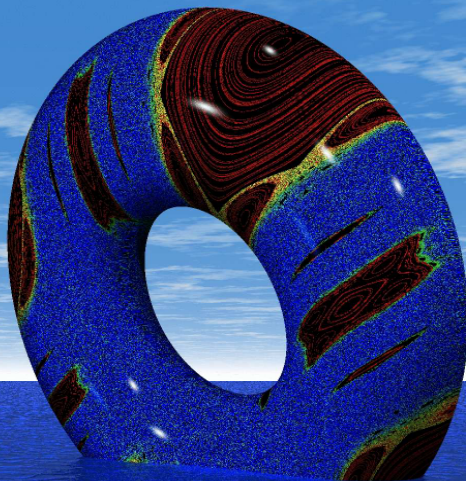
Outline

- 1 Turbulence and filtering
- 2 Regularization modeling of small scales
- 3 Numerics: friend or foe?
- 4 Mixing: combustion and stratification
- 5 Concluding remarks**

Concluding Remarks

Discussed:

- turbulence and coarsening – closure problem
- heuristic modeling – eddy-viscosity
- regularization approach – large-scale sweeping
- role of spatial discretization
- Leray approach robust and generally accurate
- under-resolved LANS- α exaggerates small scales
- extended to complex flows - combustion, stratification (separation, rotation, particles, electromagnetism, ...)



Any questions?