A review of mathematical regularization as model for small-scale turbulence

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Multiscale Modeling and Simulation

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Turbulence in physical space
Incompressible flow

Conservation of mass and momentum:

\[ \partial_j u_j = 0 \]

\[ \partial_t u_i + \partial_j (u_i u_j) + \partial_i p - \frac{1}{Re} \partial_{jj} u_i = 0 \]

- **convective flux**: nonlinear, destabilizing
- **viscous flux**: linear, dissipative

Ratio – Reynolds number

\[ Re = \frac{\text{convection}}{\text{dissipation}} = \frac{UL}{\nu} \]

Turbulence requires \( Re \gg 1 \)
Energy cascading process in 3D

I: large-scales stirring at integral length-scale $\ell_i \sim 1/k_i$

II: inviscid nonlinear transfer – inertial range $E \sim k^{-5/3}$

III: viscous dissipation dominant $\ell_d \sim 1/k_d$
Complexity of turbulent flow

Kolmogorov: small scales are **viscous, isotropic and universal**

Proposition: properties depend on viscosity $\nu$ and dissipation rate $\epsilon$

$$[\nu] = \text{length}^2 / \text{time} \quad ; \quad [\epsilon] = \text{length}^2 / \text{time}^3$$

Scales: make length and time

$$\eta = \left( \frac{\nu^3}{\epsilon} \right)^{1/4} \sim \frac{1}{k_d} \quad ; \quad \tau_\eta = \left( \frac{\nu}{\epsilon} \right)^{1/2}$$

Three dimensions:

$$\# \text{dof} \sim \left( \frac{\ell}{\eta} \right)^3 \sim Re^{9/4} \quad ; \quad \# \text{time-steps} \sim \frac{t_{\text{end}}}{\tau_\eta} \sim Re^{1/2}$$

Computationally intensive problem as $Re \gg 1$
Computational challenge

Reynolds scaling of numerical resolution

\[ N = \left( \frac{\ell}{\eta} \right)^3 \sim Re^{9/4} \]

Memory: if \( Re \to Re \times 10 \) then \( N \to 10^{9/4} \times N \approx 175 \times N \)

Reynolds scaling of numerical work

\[ Work \sim Re^{1/2} Re^{9/4} \sim Re^{11/4} \]

CPU: if \( Re \to Re \times 10 \) then \( W \to 10^{11/4} W \approx 560 W \)

Tough simulation problem
- direct approach often impractical
- capture primary features instead
Four themes to be mastered:

- Phenomenology of (coarsened) turbulence
- Turbulence modeling and numerical methods
- Error-assessment for large-eddy simulation
- High-performance computing
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Outline

1. Filtering and closure
2. Regularized Navier-Stokes as turbulence model
3. Model testing
4. Concluding Remarks
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DNS and LES in a picture

- capture both large and small scales: resolution problem
- Coarsening/mathematical modeling instead: LES
Filtering Navier-Stokes equations

\[ \partial_j u_j = 0 \quad ; \quad \partial_t u_i + \partial_j(u_i u_j) + \partial_i \rho - \frac{1}{Re} \partial_{jj} u_i = 0 \]

**Convolution-Filtering:** filter-kernel \( G \)

\[ \bar{u}_i = L(u_i) = \int G(x - \xi) u(\xi) \, d\xi \quad ; \quad L(1) = 1 \]

Large-eddy equations:

\[ \partial_j \bar{u}_j = 0 \]

\[ \partial_t \bar{u}_i + \partial_j(\bar{u}_i \bar{u}_j) + \partial_i \bar{\rho} - \frac{1}{Re} \partial_{jj} \bar{u}_i = -\partial_j(\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) \]

Sub-filter stress tensor

\[ \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j = L(\Pi_{ij}(u)) - \Pi_{ij}(L(u)) = [L, \Pi_{ij}](u) \]

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Spatial filtering, closure problem

After closure - Shorthand notation:

\[ NS(u) = 0 \quad \Rightarrow \quad NS(\bar{u}) = -\nabla \cdot \tau(u, \bar{u}) \iff -\nabla \cdot M(\bar{u}) \]

Basic LES formulation

\[ Find \ v : \quad NS(v) = -\nabla \cdot M(v) \]

What models \( M \) are available/reasonable?

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Eddy-viscosity modeling

Obtain smoothing via increased dissipation:

\[
\partial_t \bar{u}_i + \partial_j(\bar{u}_j \bar{u}_i) + \partial_i \bar{p} - \left( \frac{1}{Re} + \nu_t \right) \partial_{jj} \bar{u}_i = 0
\]

Damp large gradients: dimensional analysis

\[
\nu_t = \text{length} \times \text{velocity} \sim \Delta \times \Delta |\partial_x \bar{u}|
\]

Effect: Strong damping at large filter-width and/or gradients
Some explicit subgrid models

Popular models:

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

  \[ \tau_{ij} \to -\nu_t S_{ij} = -(C_S \Delta)^2 |S| S_{ij} \quad ; \quad \text{effect} \quad \frac{1}{Re} \to \left( \frac{1}{Re} + \nu_t \right) \]

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

  \[ \tau_{ij} \to [L, \Pi_{ij}](\overline{u}) = \overline{u_i} \overline{u_j} - \overline{u_i} \overline{u_j} \]

- **Mixed models:**

  \[ m_{ij} = \text{Bardina} + C_d \text{Smagorinsky} \]

  \[ C_d \text{ via dynamic Germano-Lilly procedure} \]
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Dissipation or regularization?

Capture turbulence with eddy-viscosity or, with mathematics?

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More regularization in LES

Ciprian Foias — Darryl Holm — Edriss Titi

Models with rigorously established existence, uniqueness, regularity, convergence to NS, transformation, symmetries, ...
Mathematical regularization as subgrid model

Dynamic models popular in LES but:
- expensive; ad hoc implementation features (‘clipping’)
- still limited accuracy; complex flow extension difficult

Regularization principle directly altering the nonlinearity

- Systematically obtain implied subgrid closure
- ‘Inherit’ rigorous mathematical properties
- Maintain transport structure and transformation properties of equations

Consider two examples: Leray and NS-$\alpha$
From Leray regularization to SFS model

Proposal:

\[ \partial_t v_i + \vec{V}_j \partial_j v_i + \partial_i q - \frac{1}{Re} \partial_{jj} v_i = 0 \]

Convolution filtering Leray: use \( \partial_j \vec{V}_j = 0 \)

\[ \partial_t \vec{V}_i + \partial_j (\vec{V}_j \vec{V}_i) + \partial_i \vec{q} - \frac{1}{Re} \partial_{jj} \vec{V}_i = 0 \]

Rewrite into LES template:

\[ \partial_t \vec{V}_i + \partial_j (\vec{V}_j \vec{V}_i) + \partial_i \vec{q} - \frac{1}{Re} \partial_{jj} \vec{V}_i = -\partial_j (\vec{V}_j \vec{V}_i - \vec{V}_j \vec{V}_i) \]

Implied Leray model:

\[ m_{ij} = \vec{V}_j \vec{V}_i - \vec{V}_j \vec{V}_i = L(\vec{V}_j L^{-1}(\vec{V}_i)) - \vec{V}_j \vec{V}_i \]

with \( L^{-1} \) formally inverting \( L \)
Regularization requires filter-inversion

Geometric series: repeated filtering

\[ L^{-1} = (I - (I - L))^{-1} \rightarrow \sum_{n=0}^{N} (I - L)^n \]

For example:

\[ N = 0 : \quad u = L_0^{-1}(u) = \bar{u} \]
\[ N = 1 : \quad u = L_1^{-1}(u) = \bar{u} + (I - L)\bar{u} = 2\bar{u} - \bar{u} \]
\[ N = 2 : \quad u = L_2^{-1}(u) = \bar{u} + (I - L)\bar{u} + (I - L)(I - L)\bar{u} \]
\[ = 3\bar{u} - 3\bar{u} + \bar{u} \]
Regularization requires filter-inversion
**Alternative regularizations**

Consider \( a - b \) models: \( \partial_j v_j = 0 \) and

\[
\partial_t v_i + \partial_j (a_j b_i) + \partial_i q - \frac{1}{Re} \partial_{jj} v_i = 0
\]

Then

- Choose: \( a_j = v_j; b_i = v_i \) to obtain NS
- Choose: \( a_j = \overline{v}_j; b_i = v_i \) to obtain Leray
- Choose: \( a_j = v_j; b_i = \overline{v}_i \) to obtain modified Leray
- Choose: \( a_j = \overline{v}_j; b_i = \overline{v}_i \) to obtain modified Bardina

Or, implied models: \( m_{ij}^R = a_j b_i - \overline{v}_j \overline{v}_i \), i.e.,

\[
\text{Leray : } m_{ij}^L = \overline{v}_j \overline{v}_i - \overline{v}_j v_i \\
\text{Modified Leray : } m_{ij}^{mL} = \overline{v}_j v_i - \overline{v}_j \overline{v}_i \\
\text{Modified Bardina : } m_{ij}^{mB} = \overline{v}_j \overline{v}_i - \overline{v}_j \overline{v}_i
\]
NS-α regularization

Kelvin’s circulation theorem

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

Filtered Kelvin theorem (\(\Gamma(u) \rightarrow \Gamma(\overline{u})\)) extends Leray
**NS-$\alpha$ regularization**

Filtered Kelvin circulation theorem

\[
\frac{d}{dt} \left( \int_{\Gamma(u)} u_j \, dx_j \right) - \frac{1}{Re} \int_{\Gamma(u)} \partial_{kk} u_j \, dx_j = 0
\]

Euler-Poincaré

\[
\partial_t u_j + \bar{u}_k \partial_k u_j + u_k \partial_j \bar{u}_k + \partial_j \rho - \partial_j \left( \frac{1}{2} \bar{u}_k u_k \right) - \frac{1}{Re} \partial_{kk} u_j = 0
\]

Rewrite into LES template: Implied subgrid model

\[
\partial_t \bar{u}_i + \partial_j (\bar{u}_j \bar{u}_i) + \partial_i \bar{\rho} - \frac{1}{Re} \partial_{jj} \bar{u}_i = -\partial_j \left( \bar{u}_j u_i - \bar{u}_j \bar{u}_i \right) - \frac{1}{2} \left( u_j \partial_i \bar{u}_j - \bar{u}_j \partial_i u_j \right)
\]
Cascade-dynamics – computability

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

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A posteriori testing

Filtered NS eqs. \(\rightarrow\) DNS \(\rightarrow\) \(p, u_i\) \(\rightarrow\) filtered DNS eqs. \(\rightarrow\) LES \(\rightarrow\) \(\bar{p}, \bar{u}_i\)

Error-sources:
- subgrid-model
- numerical algorithm

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HIT at $Re_\lambda = 50, 100$

Pseudo-spectral method and explicit time-stepping

Range: $\Delta = \ell/64, \ell/32, \ell/16, \ell/8, \ell/4, \ell/2$ at $N = 32, 64, 128, 256, 512$
Smagorinsky
Error-landscape: Definition

Framework for collecting error information:

\[
\frac{l_s}{\delta E} \quad N
\]

Each Smagorinsky LES corresponds to single point:

\[
(N, \frac{l_s}{h}) \quad \text{error} : \delta_E
\]

Contours of energy error $\delta_E$ — fingerprint of LES

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Interacting simulation errors

Computational model limited by numerical and modeling errors

HIT error landscape
Iterative optimization?
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: $\circ \rightarrow \star \rightarrow \diamond \rightarrow \square \rightarrow \dagger$

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Flow-structures: DNS, Leray, modified Leray

\[ \Delta = \ell/64 \quad \Delta = \ell/32 \quad \Delta = \ell/16 \quad \Delta = \ell/8 \]

(a) (b) (c) (d)

(e) (f) (g) (h)

(i) (j) (k) (l)

DNS at $512^3$ and LES at $128^3$
Skewness prediction

Grid-independent LES: $N = 128$

Figure: Filtered DNS (solid), Leray (dash), NS-$\alpha$ (dash-dot), Modified Leray (dot) and Modified Bardina (solid with ∗). From bottom to top: $\Delta = \ell/64$, $\ell/32$, $\ell/16$, $\ell/8$, $\ell/4$ and $\Delta = \ell/2$ – curves are shifted
Numerical contamination Leray: $Re_\lambda$

Figure: $N = 128$ (dash), $N = 64$ (dash-dot), $N = 32$ (dot) and $N = 16$ (solid) (bottom to top) $\Delta = \ell/64$, $\ell/32$ and $\ell/16$. 
Is regularization modeling practical?

Computational speed-up

\[ W \approx \left( \frac{N_{DNS}}{N_{LES}} \right)^4 \]

Increased \( Re \): factor \( \approx W^{1/3} \) since complexity \( \sim Re^3 \)

General impression:

- ‘very accurate’ predictions at small filter-widths: \( \Delta/\ell \lesssim 1/64 \), requiring \( N \approx 128 \)
  \[ W \approx 256 \quad \text{allows factor} \quad \approx 6 \text{ in } Re \]

- ‘quite accurate’ predictions as \( 1/32 \lesssim \Delta/\ell \lesssim 1/16 \), requiring \( N = 32 \) to \( N = 64 \) provided proper SFS model
  \[ W \approx 4096 - 65536 \quad \text{allows factor} \quad \approx 16 \text{ to } \approx 40 \text{ in } Re \]

- ‘sometimes still OK’ as \( \Delta/\ell \approx 1/8 \), requiring \( N \approx 16 \):
  \[ W \approx 10^6, \text{ i.e., factor } \approx 100 \text{ in } Re \]
- considerable errors at very large filter-widths: \( \Delta/\ell \gtrsim 1/4 \)
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**Mixing**
Mixing layer: testing ground for LES

(a): Flow domain mixing layer
(b): Spark shadow photograph

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Basic mixing layer configuration
Some mean flow properties

Kinetic energy and momentum thickness

- Smagorinsky too dissipative
- Bardina, dynamic models preferred

Filtering  Regularization  Testing  Conclusion

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Closer look: Streamwise energy spectrum

- Dissipation: Smagorinsky too much, Bardina not enough
- Dynamic models quite acceptable
- ‘Middle range’ wavenumbers much too high
Instantaneous snapshots of spanwise vorticity

(a) DNS, (b) Bardina, (c) Smagorinsky, (d) dynamic

Accuracy limited: regularization models better?
Leray and NS- α predictions: $Re = 50, \Delta = \ell/16$

Snapshot $u_2$: red (blue) corresponds to up/down
Momentum thickness $\theta$ as $\Delta = \ell/16$

**Filtered DNS ($\circ$)**
- $32^3$: dash-dotted
- $64^3$: solid
- $96^3$: $\triangle$

**Leray-model**
- $32^3$: solid
- $64^3$: $\triangle$

**Dynamic model**
- $32^3$: dashed
- $64^3$: dashed with $\diamond$
Streamwise kinetic energy $E$ as $\Delta = \ell/16$

Filtered DNS (○)

**Leray-model**
- $32^3$: dash-dotted
- $64^3$: solid
- $96^3$: △

**Dynamic model**
- $32^3$: dashed
- $64^3$: dashed with ◇
Robustness at arbitrary Reynolds number

\[ Re = 50 \]
- 64\(^3\): dash-dotted
- 96\(^3\): dash-dotted, △

\[ Re = 500 \]
- 64\(^3\): dashed
- 96\(^3\): dashed, △

\[ Re = 5000 \]
- 64\(^3\): solid
- 96\(^3\): solid, =△
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Concluding remarks

Does mathematical regularization imply accurate SFS model?

- reviewed coarsened turbulence
- closure problem: eddy-viscosity and regularization
- illustrated a posteriori testing for HIT and mixing layer
- Leray and NS-$\alpha$ are accurate and Leray is more robust

open challenge:
- what fluid-mechanical properties should be included for successful NS regularization?
- what is needed to assure/predict simulation reliability?