Isogeometric Variational Multiscale Methods in Turbulence Modeling: Progress and Challenges

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Outline

- Two ways to improve a variational method:
 - Improve the variational formulation, e.g., stabilization, VMS
 - Improve the discrete spaces, e.g., FEM, NURBS
- Isogeometric Analysis
- Incompressible Navier-Stokes Equations:
 - Large Eddy Simulation inspired VMS turbulence theory
 - Residual-based turbulence modeling
- Numerical Examples
 - Forced isotropic turbulence (Re₂=164)
 - Channel flow (Re_{τ}= 395 to 950)
 - Weak versus strong Dirichlet boundary conditions
 - Fluid-structure interaction
- Concluding Remarks

Isogeometric Analysis

- Based on technologies (e.g., NURBS) from computational geometry used in:
 - Design
 - Animation
 - Graphic art
 - Visualization



- Includes standard FEA as a special case, but offers other possibilities:
 - Precise and efficient geometric modeling
 - Simplified mesh refinement
 - Superior approximation properties
 - Integration of design and analysis



Isogeometric Analysis (NURBS, T-Splines, etc.)

FEA

h-, p-refinement

k-refinement

B-Splines

B-spline Basis Functions

•
$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1}, \\ 0 & \text{otherwise} \end{cases}$$

• $N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \xi_i + \xi_i + \xi_i \end{cases}$

$$\frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$



B-spline basis functions of order 0, 1, 2 for a *uniform knot vector:*

 $\Xi = \{0, 1, 2, 3, 4, \dots\}$





Quadratic (*p*=2) basis functions for an *open, non-uniform knot vector:*

 $\boldsymbol{\Xi} = \{0, 0, 0, 1, 2, 3, 4, 4, 5, 5, 5\}$





Cubic *p*-refined Curve



Quartic *p*-refined Curve





Non-Uniform Rational B-splines

Circle from 3D Piecewise Quadratic Curves







Further h-refined Surface Control net



Mesh

Control net







Mesh



Variation Diminishing Property









Finite Element Analysis and Isogeometric Analysis

 Compact support
 Partition of unity
 Affine covariance
 Isoparametric concept
 Patch tests satisfied

Pure Advection

Problem:

$$\begin{cases} \frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} = 0 \quad \text{for} \quad x \in (0, L) \quad (1) \\ \varphi(0, t) = \varphi(L, t) \quad (2) \end{cases}$$

Solutions take the form:

$$\varphi_n(x,t) = A\sin(kx - \omega t) + B\cos(kx - \omega t)$$

(1) $\Rightarrow \omega / k = u$, phase speed is a constant
(2) $\Rightarrow k = 2n\pi / L$, $n = 0, 1, 2, ...$

Pure Advection Phase Error



Pure Diffusion Phase Error



Advection Skew to Mesh: Problem Setup



Advection Skew to Mesh at 45°



Cahn-Hilliard Equation (1957)

• Applications:

- Phase segregation of binary alloys
- Image processing
- Planet formation
- Growth of tumors
- Etc.
- Spatial derivatives of order four

Cahn-Hilliard Equation

$$\boldsymbol{E} = \int_{\Omega} \left(\boldsymbol{f}_0(\boldsymbol{c}) + \kappa \left\| \nabla \boldsymbol{c} \right\|^2 \right) d\boldsymbol{x}, \qquad \dot{\boldsymbol{E}} \leq 0$$

Conservation of mass:

$$\frac{\partial \boldsymbol{c}}{\partial t} + \nabla \cdot \boldsymbol{J} = \boldsymbol{0}$$

Dynamics driven by variational derivative of energy:

$$J = -M_c \nabla \left(\frac{\delta E}{\delta c}\right), \qquad \frac{\delta E}{\delta c} = f_0'(c) - 2\kappa \Delta c = \mu_c - \lambda \Delta c$$

Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla \left(\mu_c - \lambda \Delta c \right) \right), \ M_c = Dc(1-c), \ \mu_c = f'_0, \ \lambda \text{ const.}$$

Cahn-Hilliard Equation

Variational Formulation

Find $c \in V$ such that $\forall w \in V$, B(w, c) = 0 where

$$B(w,c) = \left(w, \frac{\partial c}{\partial t}\right)_{\Omega} + \left(\nabla w, M_c \nabla \mu_c + \lambda \nabla M_c \Delta c\right)_{\Omega} + \left(\Delta w, \lambda M_c \Delta c\right)_{\Omega}$$

Remarks

- 1. Periodic boundary conditions assumed
- 2. Galerkin method
- 3. C^k-continuous B-splines, $k \ge 1$



Numerical Results: α = 3000, \overline{c} = 0.63

C¹-continuous quadratics (64²)





Numerical Results: $\alpha = 6000$, $\overline{c} = 0.63$

C³-continuous quartics (64²)





3D Numerical Results (128³)



 $\bar{c} = 0.63$

 $\bar{c} = 0.75$





Incompressible Navier-Stokes Equations

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) + \nabla \boldsymbol{p} = \boldsymbol{v} \Delta \boldsymbol{u} + \boldsymbol{f} \quad \text{in } \boldsymbol{Q}$$

$$\nabla \cdot \boldsymbol{u} = 0 \qquad \text{in } \boldsymbol{Q}$$

$$\boldsymbol{u} = \boldsymbol{0} \qquad \text{on } \boldsymbol{P}$$

$$\boldsymbol{u}(t = 0^{+}) = \boldsymbol{u}(t = 0^{-}) \quad \text{on } \boldsymbol{\Omega}$$

$$T$$

$$Q = \Omega \times (0, T)$$

$$P = \Gamma \times (0, T)$$

$$\Gamma = \partial \Omega$$

$$0$$

Variational Space-Time Formulation

Find
$$\boldsymbol{U} = \left\{ \boldsymbol{u}, \boldsymbol{p} \right\} \in \boldsymbol{V}$$
 such that $\forall \boldsymbol{W} = \left\{ \boldsymbol{w}, \boldsymbol{q} \right\} \in \boldsymbol{V}$

$$B(\boldsymbol{W},\boldsymbol{U}) = B_1(\boldsymbol{W},\boldsymbol{U}) + B_2(\boldsymbol{W},\boldsymbol{U},\boldsymbol{U}) = (\boldsymbol{W},\boldsymbol{F})$$

where

$$B_{1}(\boldsymbol{W},\boldsymbol{U}) = \left(\boldsymbol{w}(T^{-}),\boldsymbol{u}(T^{-})\right)_{\Omega} - \left(\frac{\partial \boldsymbol{w}}{\partial t},\boldsymbol{u}\right)_{\Omega} + \left(\nabla^{s}\boldsymbol{w},2v\,\nabla^{s}\boldsymbol{u}\right)_{\Omega} + \left(q,\nabla\cdot\boldsymbol{u}\right)_{\Omega} - \left(\nabla\cdot\boldsymbol{w},\boldsymbol{p}\right)_{\Omega}$$
$$B_{2}(\boldsymbol{W},\boldsymbol{U},\boldsymbol{U}) = -\left(\nabla\boldsymbol{w},\boldsymbol{u}\otimes\boldsymbol{u}\right)_{\Omega} + \left(\boldsymbol{w}(0^{+}),\boldsymbol{u}(0^{-})\right)_{\Omega}$$

Variational Multiscale Formulation

Split



Finite dimensional subspace Standard FE, spectral or NURBS space, etc.

Original problem becomes:

Find $U = \overline{U} + U'$, $\overline{U} \in \overline{V}$, $U' \in V'$, such that $(\overline{U}) \qquad B(\overline{W}, \overline{U} + U') = (\overline{W}, F) \qquad \forall \overline{W} \in \overline{V}$ $(U') \qquad B(W', \overline{U} + U') = (W', F) \qquad \forall W' \in V'$

Variational Multiscale Method

Exact Theory

$$(\overline{U}) \qquad B(\overline{W}, \overline{U} + U') = (\overline{W}, F)$$
$$(U') \qquad \begin{cases} B(W', \overline{U} + U') = (W', F) \\ \overline{U'} = \mathfrak{F}'(\overline{u}, R'(\overline{U})) \\ (W', R'(\overline{U})) = B(W', \overline{U}) - (W', F) \\ R'(\overline{U}) = \text{Residual of coarse scales} \end{cases}$$

Turbulence Modeling Theory

Set $\overline{U} \equiv U^h$ and $\overline{W} \equiv W^h$ in (\overline{U}) , $(U^h) \qquad B(W^h, U^h + \widetilde{\mathfrak{F}'}(u^h, R'(U^h))) = (W^h, F)$ where $\widetilde{\mathfrak{F}'} \approx \mathfrak{F}'$ is the only approximation. The projector $\overline{P} : U \to \overline{U}$ is fundamental; see H.-Sangalli, *SIAM J. Num. Anal.*, 2007.

Variational Multiscale Method





Exact Solution for the Fine Scales

Assumption (inspired by LES)

 $\mathfrak{F}'(\boldsymbol{u}^h, \boldsymbol{0}) = \boldsymbol{0}$, and if $\boldsymbol{R}'(\boldsymbol{U}^h)$ is "small", $\mathfrak{F}'(\boldsymbol{u}^h, \boldsymbol{R}'(\boldsymbol{U}^h))$ is "small"

Perturbation series

$$\begin{aligned} \boldsymbol{U}' &= \sum_{k=1}^{\infty} \varepsilon^{k} \, \boldsymbol{U}'_{k} = \varepsilon \, \boldsymbol{U}'_{1} + \varepsilon^{2} \, \boldsymbol{U}'_{2} + \dots, \qquad \varepsilon = \left\| \boldsymbol{R}'(\boldsymbol{U}^{h}) \right\| \\ \varepsilon \, \boldsymbol{U}'_{1} &= \boldsymbol{G}'_{\boldsymbol{u}^{h}}(\boldsymbol{R}'(\boldsymbol{U}^{h})) \qquad \qquad \left(\boldsymbol{G}'_{\boldsymbol{u}^{h}} = \text{Green's operator} \right) \\ \varepsilon^{2} \, \boldsymbol{U}'_{2} &= \boldsymbol{G}'_{\boldsymbol{u}^{h}}(\nabla \cdot (\varepsilon \, \boldsymbol{u}'_{1} \otimes \varepsilon \, \boldsymbol{u}'_{1})) \\ \vdots \end{aligned}$$

$$\varepsilon^{j} \boldsymbol{U}_{j}^{\prime} = \boldsymbol{G}_{\boldsymbol{u}^{h}}^{\prime} (\nabla \cdot (\sum_{k=1}^{j-1} \varepsilon^{k} \boldsymbol{u}_{k}^{\prime} \otimes \varepsilon^{j-k} \boldsymbol{u}_{j-k}^{\prime}))$$

Residual-Driven Turbulence Modeling

Green's operator approximation

$$\varepsilon \, \boldsymbol{U}_{1}^{\prime} \approx \tilde{\boldsymbol{G}}_{\boldsymbol{u}^{h}}^{\prime}(\boldsymbol{R}^{\prime}(\boldsymbol{U}^{h})) \qquad \left(\tilde{\boldsymbol{G}}_{\boldsymbol{u}^{h}}^{\prime} \approx \boldsymbol{M}_{\boldsymbol{u}^{h}}^{\prime}\right) \\ \varepsilon^{2} \, \boldsymbol{U}_{2}^{\prime} \approx \tilde{\boldsymbol{G}}_{\boldsymbol{u}^{h}}^{\prime}(\nabla \cdot (\varepsilon \, \boldsymbol{u}_{1}^{\prime} \otimes \varepsilon \, \boldsymbol{u}_{1}^{\prime} \,)) \\ \vdots \\ \varepsilon^{j} \, \boldsymbol{U}_{j}^{\prime} \approx \tilde{\boldsymbol{G}}_{\boldsymbol{u}^{h}}^{\prime}(\nabla \cdot (\sum_{k=1}^{j-1} \varepsilon^{k} \boldsymbol{u}_{k}^{\prime} \, \otimes \varepsilon^{j-k} \boldsymbol{u}_{j-k}^{\prime}))$$

Inspiration from Stabilized Methods

 $\tilde{G}'_{\mu^h} = \tau$ (selected by scaling arguments)

Residual-Driven Turbulence Modeling

Fine-scale approximation:

$$\boldsymbol{u'} = -\boldsymbol{\tau}_{M}\boldsymbol{r}_{M} \quad \text{and} \quad \boldsymbol{p'} = -\boldsymbol{\tau}_{C} \boldsymbol{r}_{C}$$
$$\boldsymbol{\tau}_{M} = \left(\left(\frac{2}{\Delta t} \right)^{2} + \boldsymbol{u}^{h} \cdot \boldsymbol{G} \boldsymbol{u}^{h} + \boldsymbol{C}_{i} \boldsymbol{v}^{2} \operatorname{tr} \left(\boldsymbol{G} \cdot \boldsymbol{G} \right) \right)^{-1/2}$$
$$\boldsymbol{\tau}_{C} = \left(\boldsymbol{g} \cdot \boldsymbol{\tau}_{M} \boldsymbol{g} \right)^{-1}$$
where
$$\boldsymbol{G} = \frac{\partial \boldsymbol{\xi}^{T}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{x}} \quad \text{and} \quad \boldsymbol{g}_{i} = \sum_{j=1}^{3} \boldsymbol{G}_{jj}$$

Discrete "Conservative" Form

$$\begin{pmatrix} \boldsymbol{w}^{h}(T^{-}), \boldsymbol{u}^{h}(T^{-}) \end{pmatrix}_{\Omega} - \begin{pmatrix} \frac{\partial \boldsymbol{w}^{h}}{\partial t}, \boldsymbol{u}^{h} \end{pmatrix}_{\Omega} \\ + \left(\nabla^{s} \boldsymbol{w}^{h}, 2v \nabla^{s} \boldsymbol{u}^{h} \right)_{\Omega} + \left(q^{h}, \nabla \cdot \boldsymbol{u}^{h} \right)_{\Omega} - \left(\nabla \cdot \boldsymbol{w}^{h}, p^{h} \right)_{\Omega} \\ - \left(\nabla \boldsymbol{w}^{h}, \boldsymbol{u}^{h} \otimes \boldsymbol{u}^{h} \right)_{\Omega} \\ - \left(\nabla \boldsymbol{w}^{h}, \boldsymbol{u}^{h} \otimes \boldsymbol{u}^{h} \right)_{\Omega} - \left(\boldsymbol{w}^{h}, \boldsymbol{f} \right)_{\Omega} \\ - \left(\frac{\partial \boldsymbol{w}^{h}}{\partial t} + \nabla \cdot \left(2v \nabla^{s} \boldsymbol{w}^{h} \right) + \nabla q^{h}, \boldsymbol{u}' \right)_{\Omega} - \left(\nabla \cdot \boldsymbol{w}^{h}, p' \right)_{\Omega} \\ - \left(\nabla \boldsymbol{w}, \boldsymbol{u}' \otimes \boldsymbol{u}^{h} + \boldsymbol{u}^{h} \otimes \boldsymbol{u}' + \boldsymbol{u}' \otimes \boldsymbol{u}' \right)_{\Omega} \\ \end{pmatrix}$$

Fine-scale approximation: $\mathbf{u}' = -\tau_{M} \mathbf{r}_{M}$ and $p' = -\tau_{C} \mathbf{r}_{C}$

Comparison with Classical Stabilized Methods

Coarse-scale equation

$$0 = B(\boldsymbol{W}^{h}, \boldsymbol{U}^{h}) - (\boldsymbol{W}^{h}, \boldsymbol{F}) \qquad \leftarrow \text{Galerkin terms} \\ + B_{1}(\boldsymbol{W}^{h}, \boldsymbol{U}') + B_{2}(\boldsymbol{W}^{h}, \boldsymbol{U}', \boldsymbol{U}^{h}) \qquad \leftarrow \text{Classical stabilization} \\ + B_{2}(\boldsymbol{W}^{h}, \boldsymbol{U}^{h}, \boldsymbol{U}') + B_{2}(\boldsymbol{W}^{h}, \boldsymbol{U}', \boldsymbol{U}') \qquad \leftarrow \text{Non-classical stabilization}$$

Remarks

- These terms omitted in classical stabilized methods
- Extension of the ideas of SUPG, GLS and MS
- No eddy viscosity

Forced Isotropic Turbulence

- NURBS (B-splines)
 - Linears (standard hexahedral finite elements), C⁰
 - Meshes: 32³, 64³, 128³, 256³
 - Quadratics, C¹
 - Meshes: 32³, 64³, 128³
 - Cubics, C²
 - Meshes: 32³, 64³
- Uniform mesh in all three directions
- Statistics:
 - Energy spectra
 - Third-order structure functions $S_3 = \langle (u(x + r) u(x))^3 \rangle$
 - Forcing of three lowest modes of the velocity field at each instant
- Power input kept constant (P_{input} = 62.8)
- Samples taken ~0.4 T_{eddy} apart

Periodic NURBS (B-spline) Basis Functions













Energy Spectra Re_{λ} =164 (*h*-refinement)



Energy Spectra Re_{λ} =164 (*k*-refinement)



Energy Spectra and Third-order Structure Function

*Re*_λ=164



Turbulent Channel Flow at Re=395

- Meshes of 32³ and 64³ elements
- Hyperbolic tangent stretching
- NURBS
- *h*-and *k*-refinement
- Domain size: 2π x 2 x 2π/3
- Comparison with DNS of Moser, Kim, and Mansour (1999)
 - Used 256 x 193 x 192 spectral functions





NURBS (B-spline) Basis Functions Normal to Wall





Turbulent channel flow at Re=395

Quadratic NURBS

h-refinement



Turbulent channel flow at Re=395

Cubic NURBS

h-refinement



Turbulent channel flow at Re=395

32³ mesh

k-refinement

Note the increase in accuracy from linear to quadratic



Turbulent channel flow at Re=395

64³ mesh

k-refinement

Both quadratics and cubics are very accurate

Turbulent channel flow at Re=590, 64³ mesh



Balloon Containing an Incompressible Fluid



From Wall '06, Tezduyar '07

Balloon Containing an Incompressible Fluid

- Quadratic NURBS for both solid and fluid
- Boundary layer meshing









Balloon Containing an Incompressible Fluid



Weak Boundary Conditions

- Wall-bounded turbulent flows
- Discontinuous Galerkin methodology used to enforce no-slip Dirichlet conditions weakly
- Turbulent channel flow
 - Quadratic NURBS
 - Re = 395
 - 32³ mesh, stretched and uniform, $2\pi \times 2 \times 2\pi/3$
 - DNS: 256 x 193 x 192, spectral, $2\pi \times 2 \times \pi$
 - Re = 950
 - 64³ mesh, stretched and uniform, $4\pi \times 2 \times 4\pi/3$
 - DNS: 3072 x 385 x 2304, spectral, 8π x 2 x 3π

Weak Dirichlet BC Formulation

Find $\{u^h, p^h\}$, $u^h \cdot n = 0$ on Γ , s.t. $\forall \{w^h, q^h\}$, $w^h \cdot n = 0$ on Γ ,

$$B^{MS}(\{w^{h},q^{h}\},\{u^{h},p^{h}\}) - F^{MS}(\{w^{h},q^{h}\})$$

$$-(w^{h},2v\nabla^{s}u^{h}\cdot n)_{\tilde{\Gamma}}$$

$$-(2v\nabla^{s}w^{h}\cdot n,u^{h}-0)_{\tilde{\Gamma}}$$

$$-(w^{h}\tau_{B},u^{h}-0)_{\tilde{\Gamma}}$$

$$Adjoint-consistency term$$

$$Penalty term$$

Penalty Term

Original formulation (purely numerical):

 $\tau_{B} = \frac{C_{B}' v}{h}$ $C_{B}' \ge C > 0 \quad \text{(stability)}$ h - element size in the wall-normal direction

New formulation (based on *wall function* ideas):

$$\tau_{B} = \frac{\boldsymbol{u}^{*2}}{\left\|\boldsymbol{u}^{h}\right\|_{l_{2}}}$$

 $u^* =$ wall friction velocity, satisfying

"law of the wall," $y^+ = f(u^+)$, where

 $y^{+} = \frac{yu^{*}}{v}, \ u^{+} = \frac{\left\|u^{h}\right\|_{l_{2}}}{u^{*}}, \ y = \text{normal distance from the wall}$



Turbulent channel flow at Re=395

Stretched mesh of 32³ elements

Weak approaches strong in the limit of vanishing wall-normal mesh size, thus results are similar



100 200 300 400 500 600 700 800 900 1000

y+

0.5 0

0

Turbulent channel flow at Re=395

Uniform mesh of 32³ elements

Weak attains accuracy in the core of the flow despite the coarseness of the boundary layer mesh

Turbulent channel flow at Re=950

Stretched mesh of 64³ elements

Weak approaches strong in the limit of vanishing wall-normal mesh size, thus results are similar



Turbulent channel flow at Re=950

Uniform mesh of 64³ elements

Weak is a considerable improvement over strong when the boundary layer is not resolved

Conclusions: Weak BC

- Weak BC
 - At least as accurate as strong in all cases
 - Much more accurate mean flow velocity than strong when the boundary layer is under-resolved
 - Should be the default strategy
- The law of the wall version is slightly more accurate than the purely numerical version
- It may be possible to improve the weak BC further

Conclusions: VMS

- VMS is a *rational framework* for LES turbulence modeling
 - Fine-scale fields are approximated
 - No eddy viscosities
 - Numerics and modeling are inextricably interlinked
- Very good results in all cases
- Approximation properties of NURBS appear to be partially responsible for accuracy of results
 - C¹ quadratic NURBS are a good combination of accuracy and efficiency

VMS: The Future

- Stabilized methods may be viewed as historical stepping stones leading to VMS
- A *mathematical theory* of fine-scale approximations is needed
- Each fine-scale approximation is a *new and different* turbulence model
 - Even the *simplest* seems effective
 - It should get better
- *Extending* the VMS formulation of turbulence modeling to other situations, such as RANS, etc.
- How far can it go?

Latest Research

• Google "UT Austin ICES" and click on "Research" to find all my preprints.



Turbulent Flow in an Asymmetric Diffuser



- Uniform 302 x 64 x 64 mesh (i.e., no stretching)
- Weakly enforced no-slip boundary condition





(b) Mean stream-wise velocity at x = 22.4



(d) Mean stream-wise velocity at x = 58.4