Large scale Finite Element solvers for the large eddy simulation of incompressible turbulent flows

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Motivation

Thesis motivation

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  - Many industrial applications
  - Understanding the phenomena (physics)

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  - Many industrial applications
  - Understanding the phenomena (physics)
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- Take advantage of increasing computational capacity (High-performance Computing (HPC))
- In a Finite Element (FE) framework

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Thesis goal

Highly scalable Finite Element (FE) framework for Large Eddy Simulations (LES) of incompressible turbulent flows

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2. Time integration schemes with velocity-pressure segregation

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Highly scalable Finite Element (FE) framework for Large Eddy Simulations (LES) of incompressible turbulent flows

How to get there?

1. Variational MultiScale (VMS) methods as LES models
2. Time integration schemes with velocity-pressure segregation
3. Highly scalable algorithms based on Domain Decomposition (DD) and block preconditioners

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Step by step...

- Residual-based VMS as LES models

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- Mixed FE formulations as LES models

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1. Motivation

2. Residual-based VMS
   - Formulation
   - Numerical experiments
   - Conclusions

3. Mixed FE VMS

4. Segregated Runge-Kutta

5. Segregated VMS

6. Conclusions

Rb-VMS

Implicit LES

ILES: only numerical dissipation (for stabilization) acts as turbulent model

- Not based on filtering of the Navier-Stokes equations
- Rely on numerical artifacts, no modification at the continuous level

Incomp. Navier Stokes equations

Find $\mathbf{u}$ and p defined in Ω

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nu \nabla^2 \mathbf{u} = \mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

with appropriate boundary conditions on Γ

Incomp. Navier Stokes equations

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with appropriate boundary conditions on Γ

The weak problem is: $\forall \mathbf{v} \in \mathcal{V}_0$ and $\forall q \in \mathcal{Q}_0$, find $\mathbf{u} \in \mathcal{V}$ and $p \in \mathcal{Q}$ such that

$$\begin{aligned} (\mathbf{v}, \partial_t \mathbf{u})_\Omega + (\nabla \mathbf{v}, \nu \nabla \mathbf{u})_\Omega + b(\mathbf{u}, \mathbf{u}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, p)_\Omega &= \langle \mathbf{v}, \mathbf{f} \rangle_\Omega \\ (q, \nabla \cdot \mathbf{u})_\Omega &= 0 \end{aligned}$$

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where

$$b(\mathbf{a}, \mathbf{u}, \mathbf{v}) = \quad \langle \mathbf{v}, \mathbf{a} \cdot \nabla \mathbf{u} \rangle_\Omega$$

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where

$$b(\mathbf{a}, \mathbf{u}, \mathbf{v}) = \frac{1}{2} \langle \mathbf{v}, \mathbf{a} \cdot \nabla \mathbf{u} \rangle_\Omega - \frac{1}{2} \langle \mathbf{a} \cdot \nabla \mathbf{v}, \mathbf{u} \rangle_\Omega + \frac{1}{2} \langle \mathbf{v}, \mathbf{n} \cdot \mathbf{a} \mathbf{u} \rangle_\Gamma$$

VMS decomposition (Hughes 1995)

A decomposition of spaces $\mathcal{V}$ and $\mathcal{Q}$ given by

$$\mathcal{V} = \mathcal{V}_h \oplus \widetilde{\mathcal{V}}, \quad \mathcal{Q} = \mathcal{Q}_h \oplus \widetilde{\mathcal{Q}}$$

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is applied to the function and test spaces

$$\mathbf{u} = \mathbf{u}_h + \widetilde{\mathbf{u}}, \quad p = p_h + \widetilde{p}$$
$$\mathbf{v} = \mathbf{v}_h + \widetilde{\mathbf{v}}, \quad q = q_h + \widetilde{q}$$

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We keep all the (eight) contributions from the splitting of the convective term

$$\mathbf{u} \cdot \nabla \mathbf{u} = \mathbf{u}_h \cdot \nabla \mathbf{u}_h + \widetilde{\mathbf{u}} \cdot \nabla \mathbf{u}_h + \mathbf{u}_h \cdot \nabla \widetilde{\mathbf{u}} + \widetilde{\mathbf{u}} \cdot \nabla \widetilde{\mathbf{u}}$$

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and all the (four) contributions from the temporal term

$$\partial_t \mathbf{u} = \partial_t \mathbf{u}_h + \partial_t \widetilde{\mathbf{u}}$$

Semidiscrete problem

FEM equations

$$B\left((\mathbf{u}_h, p_h);(\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{v}_h, q_h)\right) = L\left(\mathbf{v}_h, q_h\right)$$

SGS equations

$$B\left((\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{u}_h, p_h);(\widetilde{\mathbf{v}}, \widetilde{q})\right) = L\left(\widetilde{\mathbf{v}}, \widetilde{q}\right)$$

Semidiscrete problem

FEM equations

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$
$$+ (\mathbf{v}_h, \partial_t \widetilde{\mathbf{u}})_\Omega + (\mathcal{L}^* \mathbf{v}_h, \widetilde{\mathbf{u}})_{\Omega^h} - (\nabla \cdot \mathbf{v}_h, \widetilde{p})_{\Omega^h} = \langle \mathbf{v}_h, \mathbf{f} \rangle_\Omega$$

$$(q_h, \nabla \cdot \mathbf{u}_h)_\Omega - (\nabla q_h, \widetilde{\mathbf{u}})_{\Omega^h} = 0$$

SGS equations

$$\partial_t \widetilde{\mathbf{u}} + \tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\tau_m = \left(\frac{c_1 \nu}{h^2} + \frac{c_2 |\mathbf{a}|}{h} \right)^{-1}, \quad \tau_c = \frac{h^2}{c_1 \tau_m}$$

$$\mathbf{a} = \mathbf{u}_h + \widetilde{\mathbf{u}}$$

Semidiscrete problem

FEM equations

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$

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$$\partial_t \widetilde{\mathbf{u}} + \tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\mathbf{R}_m := \mathbf{f} - \partial_t \mathbf{u}_h - \mathcal{L} \mathbf{u}_h - \nabla p_h, \quad R_c := -\nabla \cdot \mathbf{u}_h$$

Semidiscrete problem

FEM equations

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SGS equations

$$\partial_t \widetilde{\mathbf{u}} + \tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\mathcal{P} = I \quad \text{(ASGS)}, \qquad \mathcal{P} = P_h^\perp = I - P_h \quad \text{(OSS)}$$

Semidiscrete problem

FEM equations

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$
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$$(q_h, \nabla \cdot \mathbf{u}_h)_\Omega - (\nabla q_h, \widetilde{\mathbf{u}})_{\Omega^h} = 0$$

SGS equations

$$\partial_t \widetilde{\mathbf{u}} + \tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m \quad (\textit{static/dynamic})$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\mathcal{P} = I \quad (\text{ASGS}), \qquad \mathcal{P} = \mathrm{P}_\mathrm{h}^\perp = \mathrm{I} - \mathrm{P}_\mathrm{h} \quad (\text{OSS})$$

$$\mathbf{a} = \mathbf{u}_h + \widetilde{\mathbf{u}} \quad (\textit{linear/nonlinear})$$

Numerical experiments

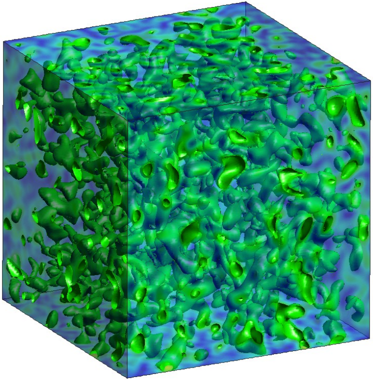
Three different turbulent benchmarks:

- Decaying of Homogeneous Isotropic Turbulence (DHIT)
- Taylor-Green Vortex (TGV) flow
- Turbulent Channel Flow (TCF)

DHIT Decay of Homogeneous Isotropic Turbulence

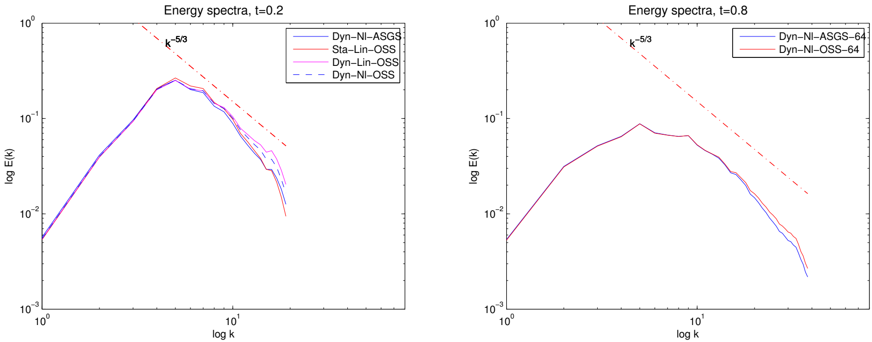
Problem setting:

- Prescribed initial energy spectra corresponding to $Re_\lambda = 952$
- Setting defined in AGARD database [Mansour & Wray, 1993]
- Different mesh discretizations (Q_1/Q_1 and Q_2/Q_2)



DHITDecay of Homogeneous Isotropic Turbulence

Energy spectra (models):



$32^3 - Q1,\ t = 0.2s$ $\quad$ $64^3 - Q1,\ t = 0.8s$

DHIT Decay of Homogeneous Isotropic Turbulence

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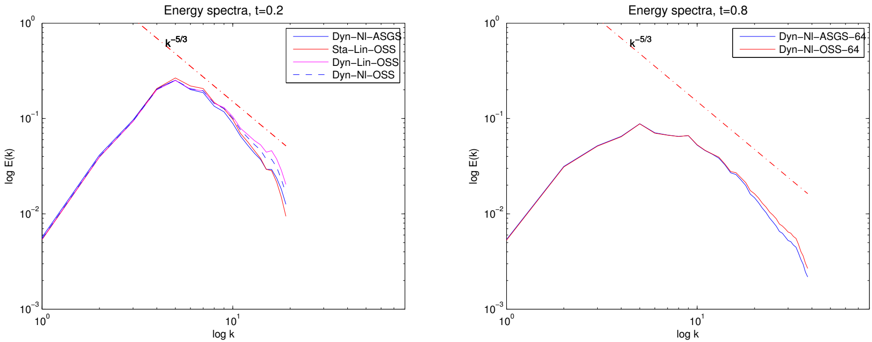
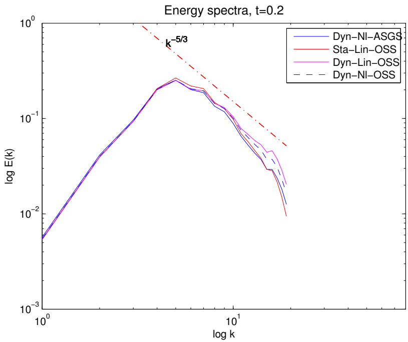


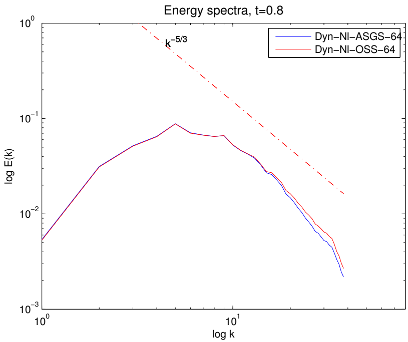
$32^3 - Q1, \ t = 0.2s$ $\qquad$ $64^3 - Q1, \ t = 0.8s$

- Small differences between methods (physical sense)

DHIT Decay of Homogeneous Isotropic Turbulence

Energy spectra (models):



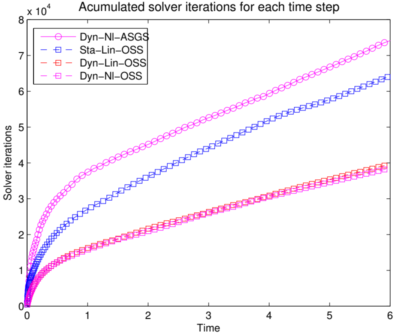


$32^3 - Q1,\ t = 0.2s$ $\qquad$ $64^3 - Q1,\ t = 0.8s$

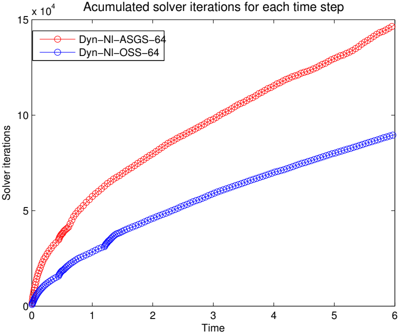
- Small differences between methods (physical sense)
- Even more similar when we refine the mesh

DHIT Decay of Homogeneous Isotropic Turbulence

Computational cost (models):



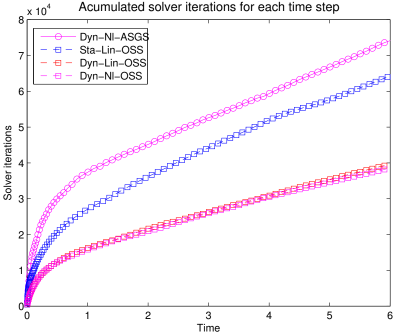
$32^3 - Q1$



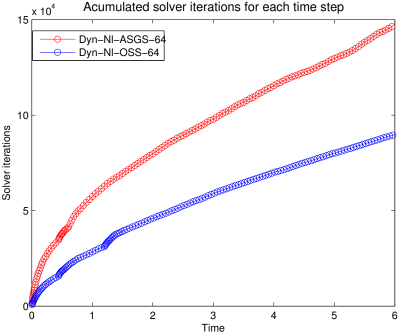
$64^3 - Q1$

DHIT Decay of Homogeneous Isotropic Turbulence

Computational cost (models):



$32^3 - Q1$

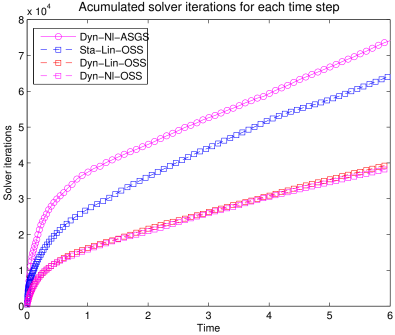


$64^3 - Q1$

- Big differences between methods (computational sense)

DHIT Decay of Homogeneous Isotropic Turbulence

Computational cost (models):



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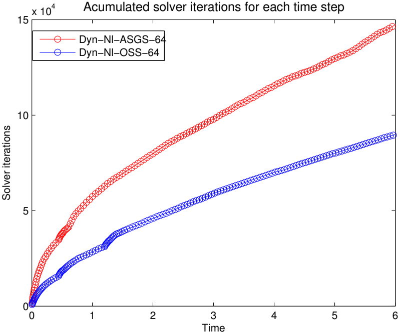
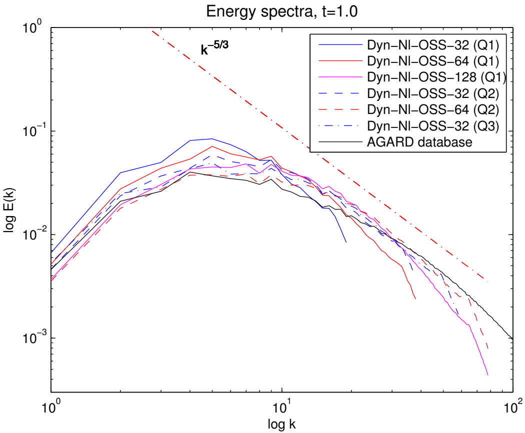


$64^3 - Q1$

- Big differences between methods (computational sense)
- Dynamic versions of OSS method are the most efficient

DHIT Decay of Homogeneous Isotropic Turbulence

Energy spectra (refinement):

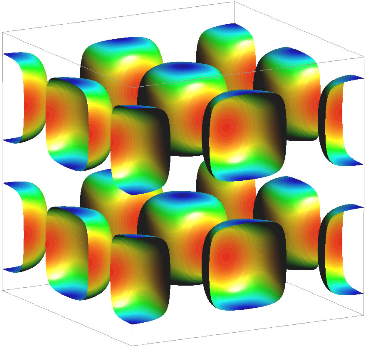


- Results become closer to the DNS when we refine the mesh

TGV Taylor-Green Vortex flow

Problem setting:

- Prescribed initial condition
- $Re = 1600$
- Different mesh discretizations (Q_1/Q_1 and Q_2/Q_2)

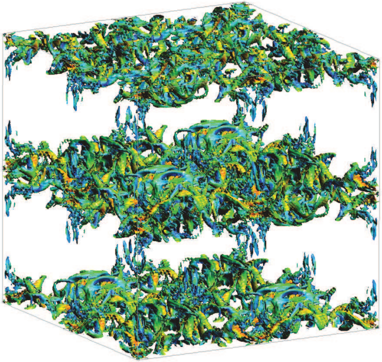


Initial vorticity isosurface $|\omega| = 1$

TGV Taylor-Green Vortex flow

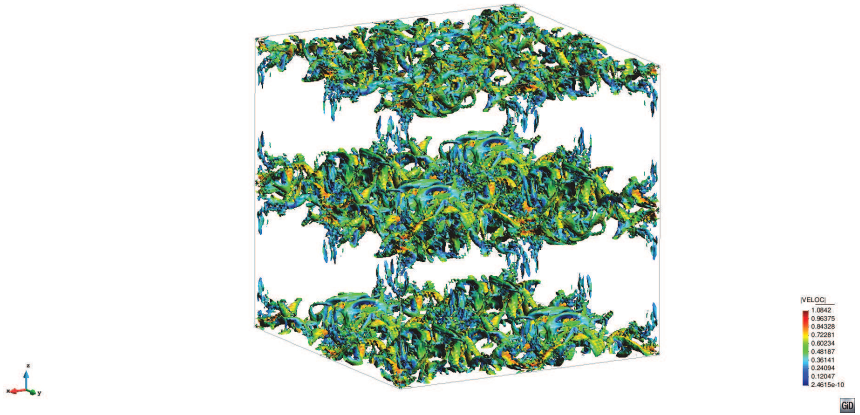
Problem setting:

- Prescribed initial condition
- $Re = 1600$
- Different mesh discretizations (Q_1/Q_1 and Q_2/Q_2)



Vorticity isosurfaces $|\omega| = 9.0$

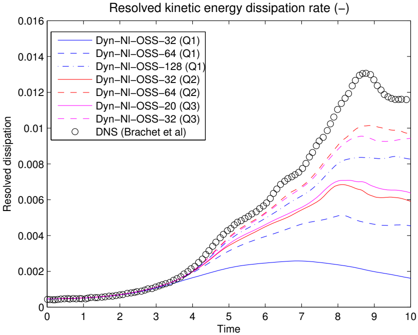
TGV Taylor-Green Vortex flow



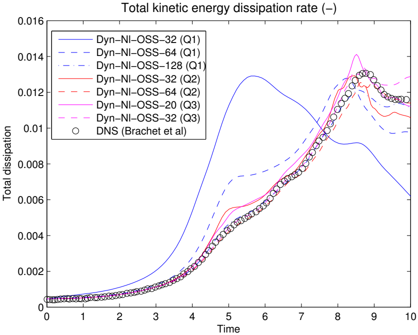
Velocity isosurface

TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement):



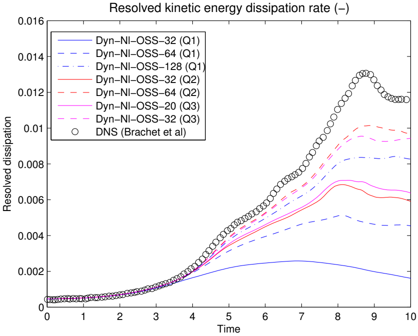
Resolved scales



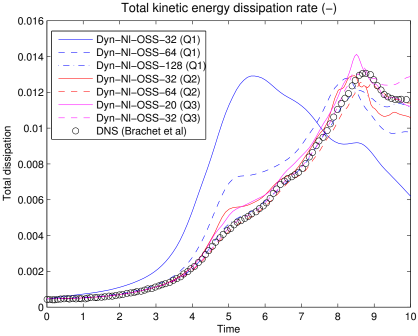
Total

TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement):



Resolved scales

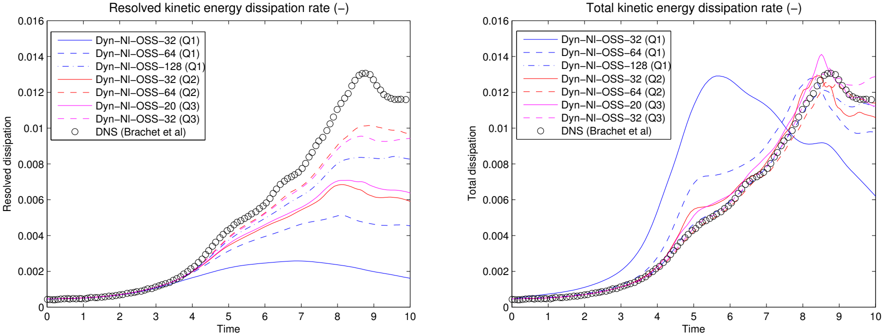


Total

- Good agreement with the DNS taking account the subscales

TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement):



Resolved scales Total

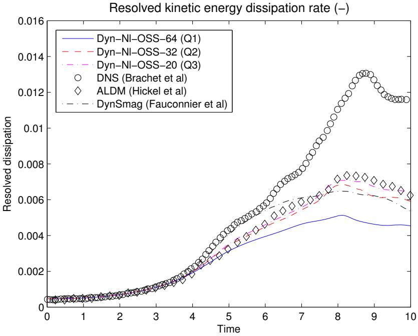
- Good agreement with the DNS taking account the subscales
- More accurate results increasing the order of approximation

TGV Taylor-Green Vortex flow

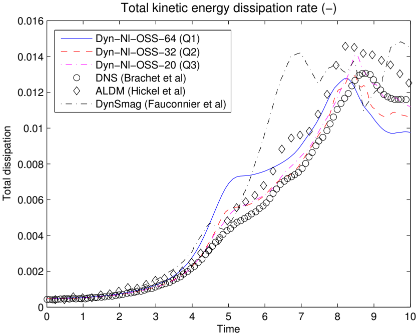
- All results until now are compared against **DNS**
- Are our methods comparable with **LES** models?

TGV Taylor-Green Vortex flow

Energy dissipation rate (against LES model):



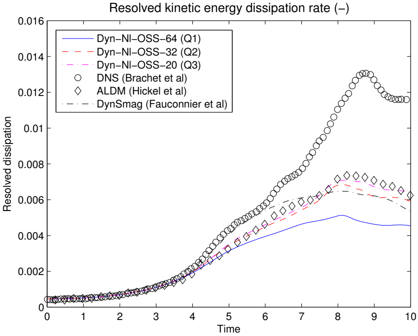
Resolved scales



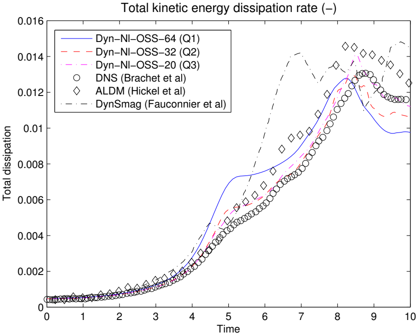
Total

TGV Taylor-Green Vortex flow

Energy dissipation rate (against LES model):



Resolved scales

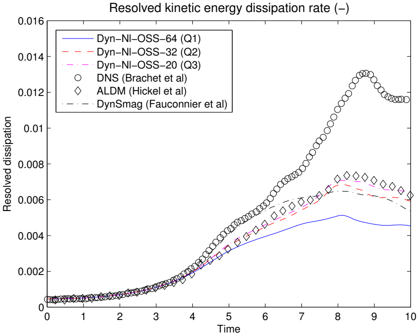


Total

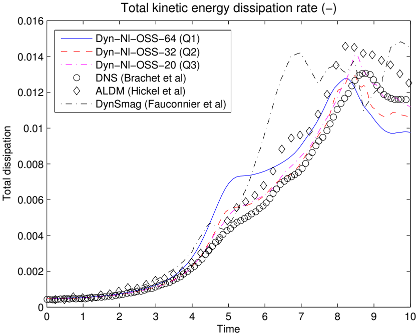
- Good agreement with the LES models on resolved scales

TGV Taylor-Green Vortex flow

Energy dissipation rate (against LES model):



Resolved scales



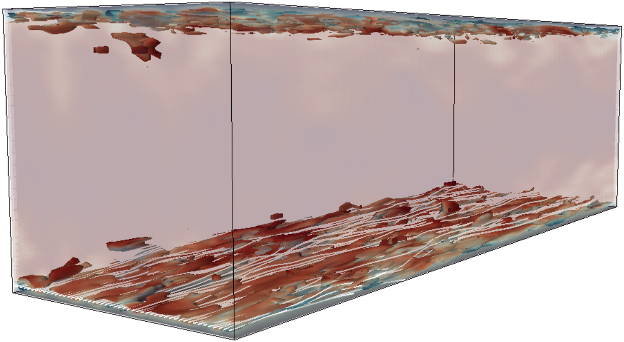
Total

- Good agreement with the LES models on resolved scales
- Better results than LES models adding subscales counterpart

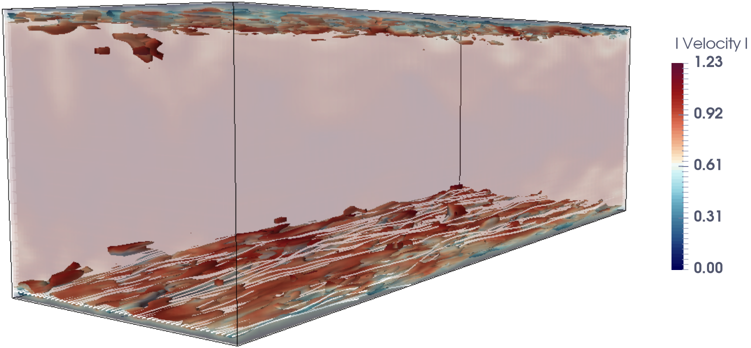
TCF Turbulent Channel Flow

Problem setting:

- Wall bounded flow
- $Re_\tau = 180$ and $Re_\tau = 395$
- Mesh resolution: $32^3 - Q1$ (stretched elements near the wall)

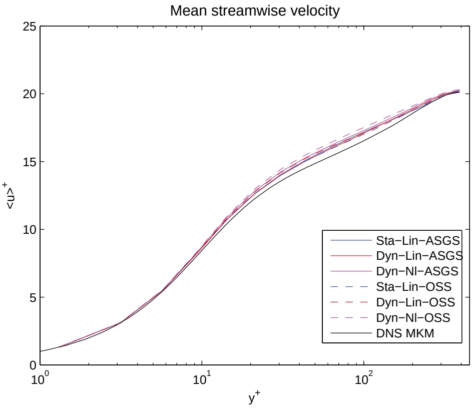


TCF Turbulent Channel Flow



TCF Turbulent Channel Flow

Mean stream-wise velocity (models):



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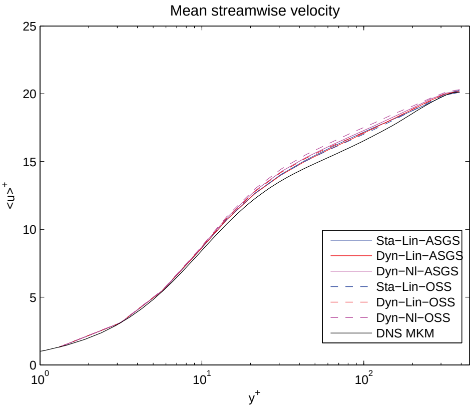

- Small differences between methods

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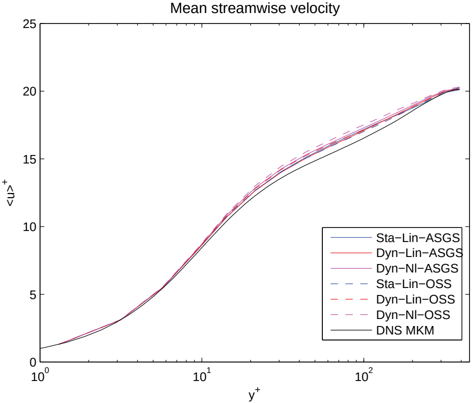

- Small differences between methods
- Very accurate results compared against the DNS

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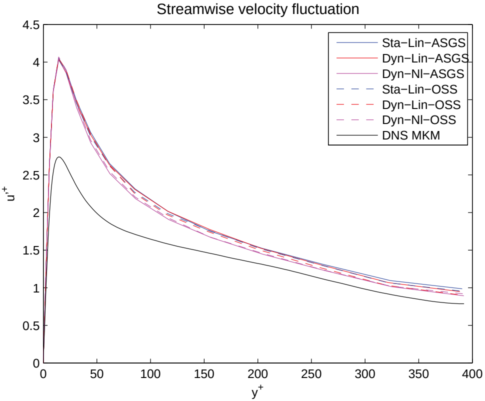

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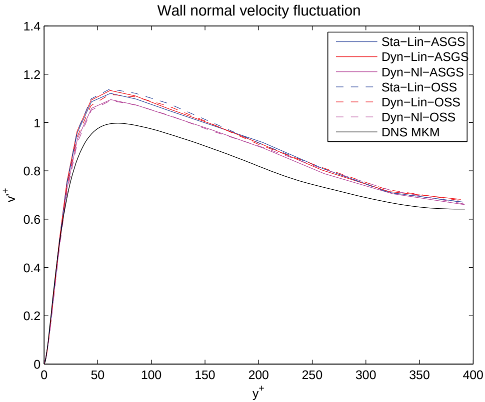

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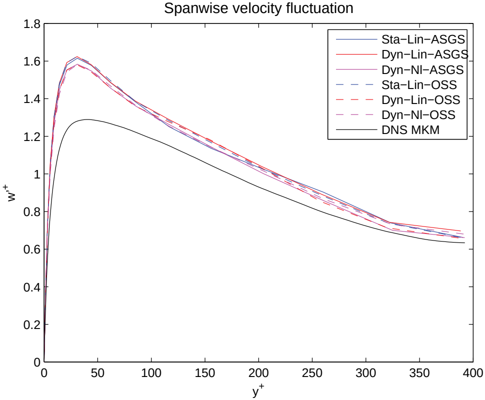

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RB-VMS Conclusions

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Contribution:

OC, Santiago Badia, Ramon Codina and Javier Principe
Assessment of variational multiscale models for the large eddy simulation of turbulent incompressible flows
Computer Methods in Applied Mechanics and Engineering, 2015

RB-VMS Limitations

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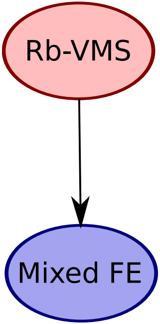
- **Desired:**
  - OSS with implicit projections


Rb-VMS
Mixed FE

Motivation

Step by step...

- Residual-based VMS as LES models
- Mixed FE formulations as LES models
- High-order time integration schemes
- Velocity-pressure segregation
- Scalable solvers

Semidiscrete problem

FEM equations

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$

$$+ (\mathbf{v}_h, \partial_t \widetilde{\mathbf{u}})_\Omega + (\mathcal{L}^* \mathbf{v}_h, \widetilde{\mathbf{u}})_{\Omega^h} - (\nabla \cdot \mathbf{v}_h, \widetilde{p})_{\Omega^h} = \langle \mathbf{v}_h, \mathbf{f} \rangle_\Omega$$

$$(q_h, \nabla \cdot \mathbf{u}_h)_\Omega - (\nabla q_h, \widetilde{\mathbf{u}})_{\Omega^h} = 0$$

SGS equations

$$\partial_t \widetilde{\mathbf{u}} + \tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\mathcal{P} = I \quad \text{(ASGS)}, \qquad \mathcal{P} = \mathrm{P}_\mathrm{h}^\perp = \mathrm{I} - \mathrm{P}_\mathrm{h} \quad \text{(OSS)}$$

$$\mathbf{a} = \mathbf{u}_h + \widetilde{\mathbf{u}}$$

Semidiscrete problem

FEM equations

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$$\tau_m^{-1} \widetilde{\mathbf{u}} = \mathcal{P} \mathbf{R}_m$$

$$\tau_c^{-1} \widetilde{p} = \mathcal{P} R_c$$

$$\mathcal{P} = \mathrm{P}_\mathrm{h}^\perp = \mathrm{I} - \mathrm{P}_\mathrm{h} \quad \text{(OSS)}$$

$$\mathbf{a} = \mathbf{u}_h$$

Term-by-term OSS

FEM equations

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$

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Term-by-term OSS

Term-by-term OSS (Codina 2008)

$$(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega$$

$$+ \left(\tau_m \mathbf{a} \cdot \nabla \mathbf{v}_h, \mathcal{P}_h^\perp (\mathbf{a} \cdot \nabla \mathbf{u}_h) \right)_{\Omega^h}$$

$$+ (\tau_c \nabla \cdot \mathbf{v}_h, \nabla \cdot \mathbf{u}_h)_{\Omega^h} = \langle \mathbf{v}_h, \mathbf{f} \rangle_\Omega$$

$$(q_h, \nabla \cdot \mathbf{u}_h)_\Omega + \left(\tau_m \nabla q_h, \mathcal{P}_h^\perp (\nabla p_h) \right)_{\Omega^h} = 0$$

Term-by-term OSS

Term-by-term OSS (Codina 2008)

$$
\begin{aligned}
&(\mathbf{v}_h, \partial_t \mathbf{u}_h)_\Omega + b(\mathbf{a}, \mathbf{u}_h, \mathbf{v}_h) + (\nabla \mathbf{v}_h, \nu \nabla \mathbf{u}_h)_\Omega - (\nabla \cdot \mathbf{v}_h, p_h)_\Omega \\
&+ (\tau_m \mathbf{a} \cdot \nabla \mathbf{v}_h, \mathbf{a} \cdot \nabla \mathbf{u}_h)_{\Omega^h} - (\tau_m \mathbf{a} \cdot \nabla \mathbf{v}_h, \boldsymbol{\eta}_h)_{\Omega^h} \\
&+ (\tau_c \nabla \cdot \mathbf{v}_h, \nabla \cdot \mathbf{u}_h)_{\Omega^h} = \langle \mathbf{v}_h, \mathbf{f} \rangle_\Omega
\end{aligned}
$$

$$
(q_h, \nabla \cdot \mathbf{u}_h)_\Omega + (\tau_m \nabla q_h, \nabla p_h)_{\Omega^h} - (\tau_m \nabla q_h, \boldsymbol{\xi}_h)_{\Omega^h} = 0
$$

$$
\begin{aligned}
\boldsymbol{\eta}_h &:= \mathcal{P}_h(\mathbf{a} \cdot \nabla \mathbf{u}_h) \\
\boldsymbol{\xi}_h &:= \mathcal{P}_h(\nabla p_h)
\end{aligned}
$$

Matrix form

- ASGS:

$$\begin{bmatrix} M\dot{\mathbf{U}} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} K + C + A_\tau & G + G_\tau \\ D + D_\tau & L_\tau \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{G} \end{bmatrix},$$

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- Term-by-term OSS with Inf-sup stable elements (mixed FE):

$$\begin{bmatrix} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} K + C + A_\tau & G & B_\tau \\ D & 0 & 0 \\ -B_\tau^T & 0 & M_\tau \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \\ \boldsymbol{\Upsilon} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{G} \\ \mathbf{0} \end{bmatrix},$$

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Index-2 DAE!!!

Block-recursive preconditioning

General case:

$$\begin{bmatrix} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} K+C+A_\tau & G & B_{\eta,\tau} & 0 \\ D & L_\tau & 0 & B_{\xi,\tau} \\ -B_{\eta,\tau}^T & 0 & M_{\eta,\tau} & 0 \\ 0 & -B_{\xi,\tau}^T & 0 & M_{\xi,\tau} \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \\ \boldsymbol{\Upsilon} \\ \boldsymbol{\Xi} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{G} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix},$$

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- Outer block matrix:

$$\widetilde{A} = \left[\begin{array}{cc|cc} M_{\eta,\tau} & 0 & -B_{\eta,\tau}^T & 0 \\ 0 & M_{\xi,\tau} & 0 & -B_{\xi,\tau}^T \\ \hline B_{\eta,\tau} & 0 & K+C+A_\tau & G \\ 0 & B_{\xi,\tau} & D & L_\tau \end{array}\right]$$

Block-recursive preconditioning

General case:

$$\begin{bmatrix} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \hline \mathbf{0} \\ \mathbf{0} \end{bmatrix} + \left[\begin{array}{cc|cc} K + C + A_\tau & G & B_{\eta,\tau} & 0 \\ D & L_\tau & 0 & B_{\xi,\tau} \\ \hline -B^T_{\eta,\tau} & 0 & M_{\eta,\tau} & 0 \\ 0 & -B^T_{\xi,\tau} & 0 & M_{\xi,\tau} \end{array}\right] \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \\ \hline \boldsymbol{\Upsilon} \\ \boldsymbol{\Xi} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{G} \\ \hline \mathbf{0} \\ \mathbf{0} \end{bmatrix},$$

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$$\widetilde{A} = \left[\begin{array}{cc} \widetilde{M}_\tau & -\widetilde{B}_\tau^T \\ \widetilde{B}_\tau & \widetilde{K}_\tau \end{array}\right] = \left[\begin{array}{cc} I & 0 \\ \widetilde{B}_\tau \widetilde{M}_\tau^{-1} & I \end{array}\right] \left[\begin{array}{cc} \widetilde{M}_\tau & -\widetilde{B}_\tau^T \\ 0 & \widetilde{S} \end{array}\right],$$

Block-recursive preconditioning

General case:

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$$\widetilde{S} = \widetilde{K}_\tau + \widetilde{B}_\tau \widetilde{M}_\tau^{-1} \widetilde{B}_\tau^T,$$

Block-recursive preconditioning

General case:

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$$\widetilde{S} = \widetilde{K}_\tau + \widetilde{B}_\tau \widetilde{M}_\tau^{-1} \widetilde{B}_\tau^T,$$

$$P_U(\widetilde{A}) = \begin{bmatrix} \widetilde{M}_\tau & -\widetilde{B}_\tau^T \\ 0 & \widetilde{S} \end{bmatrix}^{-1} = \begin{bmatrix} \widetilde{M}_\tau^{-1} & \widetilde{M}_\tau^{-1} \widetilde{B}_\tau^T \widetilde{S}^{-1} \\ 0 & \widetilde{S}^{-1} \end{bmatrix},$$

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$$P_U(\widetilde{A}) = \begin{bmatrix} \widetilde{M}_\tau & -\widetilde{B}_\tau^T \\ 0 & \widetilde{S} \end{bmatrix}^{-1} = \begin{bmatrix} \widetilde{M}_\tau^{-1} & \widetilde{M}_\tau^{-1} \widetilde{B}_\tau^T \widetilde{S}^{-1} \\ 0 & \widetilde{S}^{-1} \end{bmatrix},$$

$$\widetilde{S}^{-1} \approx \widetilde{K}_\tau^{-1}.$$

Block-recursive preconditioning

General case:

$$\left[\begin{array}{c} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \hdashline \mathbf{0} \\ \mathbf{0} \end{array}\right] + \left[\begin{array}{cc:cc} K+C+A_\tau & G & B_{\eta,\tau} & 0 \\ D & L_\tau & 0 & B_{\xi,\tau} \\ \hdashline -B_{\eta,\tau}^T & 0 & M_{\eta,\tau} & 0 \\ 0 & -B_{\xi,\tau}^T & 0 & M_{\xi,\tau} \end{array}\right] \left[\begin{array}{c} \mathbf{U} \\ \mathbf{P} \\ \hdashline \boldsymbol{\Upsilon} \\ \boldsymbol{\Xi} \end{array}\right] = \left[\begin{array}{c} \mathbf{F}_u \\ \mathbf{G} \\ \hdashline \mathbf{0} \\ \mathbf{0} \end{array}\right],$$

- Inner block matrix:

$$\widetilde{K}_\tau = \left[\begin{array}{cc} K_\tau & G \\ D & L_\tau \end{array}\right] = \left[\begin{array}{cc} I & 0 \\ DK_\tau^{-1} & I \end{array}\right] \left[\begin{array}{cc} K_\tau & G \\ 0 & S \end{array}\right],$$

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$$S = L_\tau - DK_\tau^{-1}G,$$

Block-recursive preconditioning

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$$P_U(\widetilde{K}_\tau) = \begin{bmatrix} K_\tau & G \\ 0 & S \end{bmatrix}^{-1} = \begin{bmatrix} K_\tau^{-1} & -K_\tau^{-1}GS^{-1} \\ 0 & S^{-1} \end{bmatrix},$$

Block-recursive preconditioning

General case:

$$\left[\begin{array}{c} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \hline \mathbf{0} \\ \mathbf{0} \end{array}\right] + \left[\begin{array}{cc:cc} K+C+A_\tau & G & B_{\eta,\tau} & 0 \\ D & L_\tau & 0 & B_{\xi,\tau} \\ \hdashline -B_{\eta,\tau}^T & 0 & M_{\eta,\tau} & 0 \\ 0 & -B_{\xi,\tau}^T & 0 & M_{\xi,\tau} \end{array}\right] \left[\begin{array}{c} \mathbf{U} \\ \mathbf{P} \\ \hline \boldsymbol{\Upsilon} \\ \boldsymbol{\Xi} \end{array}\right] = \left[\begin{array}{c} \mathbf{F}_u \\ \mathbf{G} \\ \hline \mathbf{0} \\ \mathbf{0} \end{array}\right],$$

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$$S = L_\tau - DK_\tau^{-1}G,$$

$$P_U(\widetilde{K}_\tau) = \begin{bmatrix} K_\tau & G \\ 0 & S \end{bmatrix}^{-1} = \begin{bmatrix} K_\tau^{-1} & -K_\tau^{-1}GS^{-1} \\ 0 & S^{-1} \end{bmatrix},$$

$$\widetilde{S}^{-1} \approx L_p^{-1}.$$

Numerical experiments

Manufactured analytical solution:

- Colliding flow

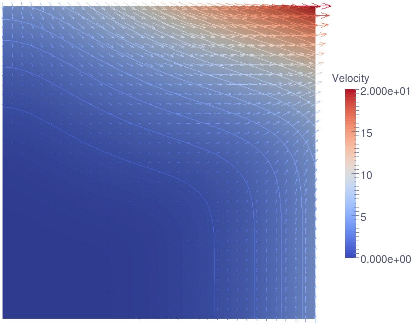
Two different turbulent benchmarks:

- Taylor-Green Vortex (TGV) flow
- Turbulent Channel Flow (TCF)

Colliding flow

Problem setting:

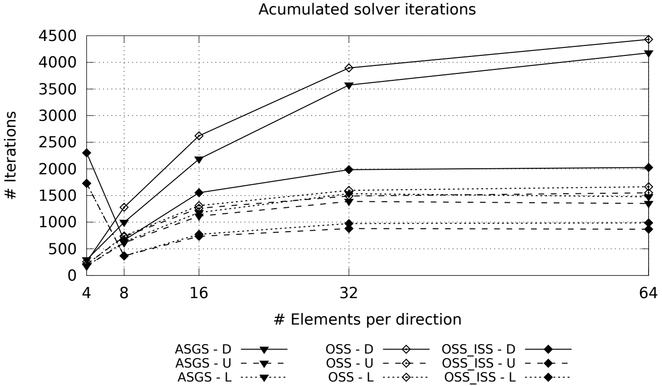
- Analytical solution
- $Re = 25$
- Mesh refinement: 4^3 to 64^3 $Q1/Q1$ elements (ASGS and OSS) or 2^3 to $32^3 Q2/Q1$ elements (OSS-ISS)



Velocity field

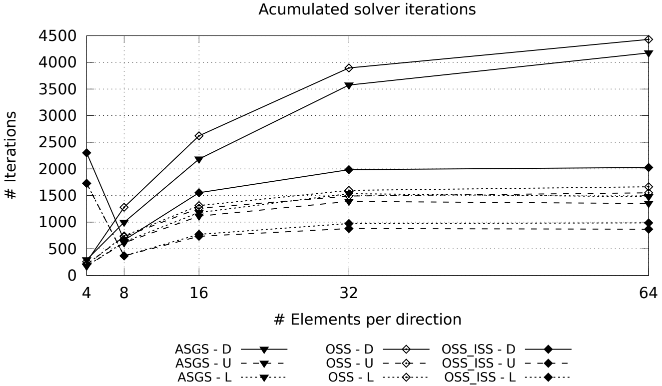
Colliding flow

Accumulated solver iterations: (using $P_U(\widetilde{A})$)



Colliding flow

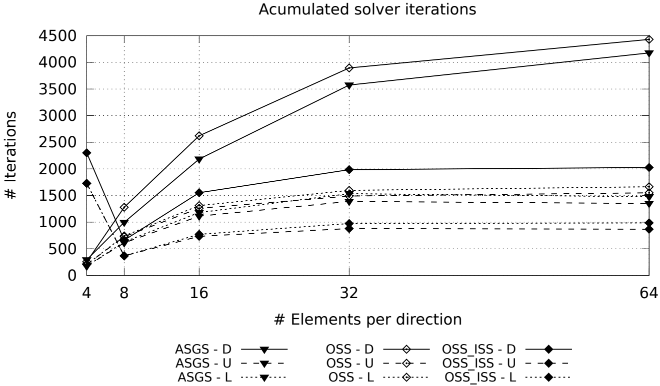
Accumulated solver iterations: (using $P_U(\widetilde{A})$)



- $P_U(\widetilde{K}_\tau)$ and $P_L(\widetilde{K}_\tau)$ optimal block-preconditioners for all methods

Colliding flow

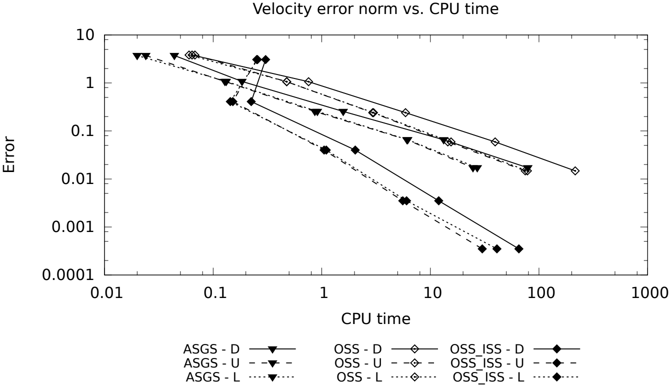
Accumulated solver iterations: (using $P_U(\widetilde{A})$)



- $P_U(\widetilde{K}_\tau)$ and $P_L(\widetilde{K}_\tau)$ optimal block-preconditioners for all methods
- Less solver iterations for the OSS-ISS method with the same velocity DOFs

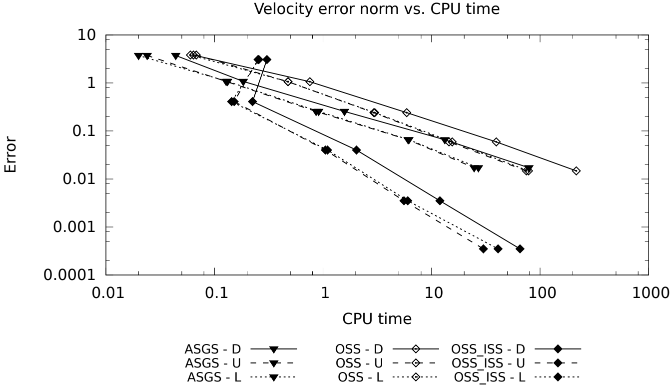
Colliding flow

Efficiency: Velocity



Colliding flow

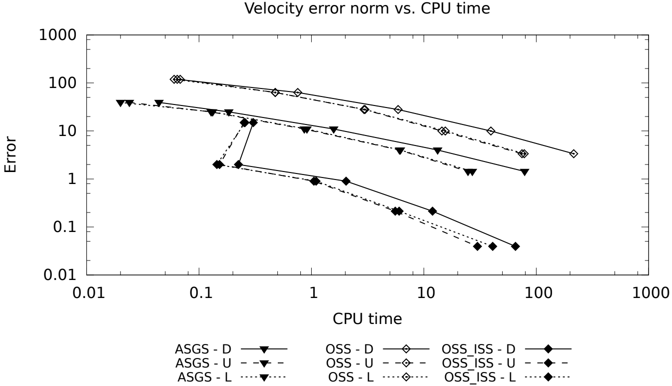
Efficiency: Velocity



- OSS-ISS the most efficient method

Colliding flow

Efficiency: Pressure

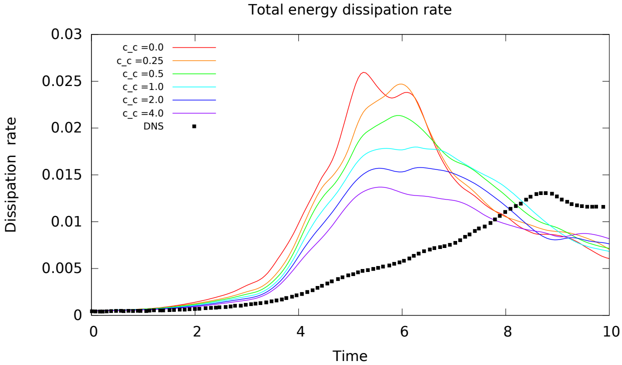


- Also for pressures

The method works properly for the laminar case, but what happens for turbulent problems?

TGV Taylor-Green Vortex flow

Effect of the grad-div term $(\tau_c \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$: (coarse mesh)



Total energy dissipation rate

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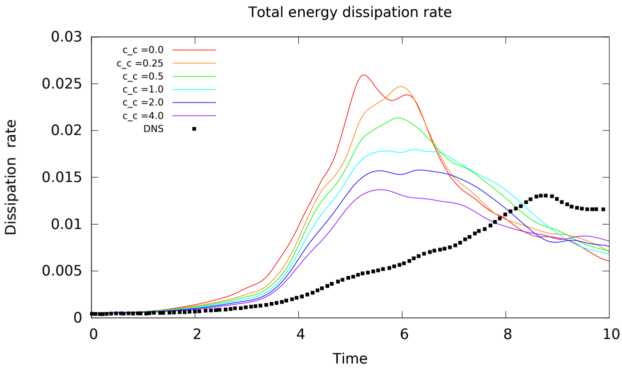

Total energy dissipation rate

- Bad results when $c_c \to 0$

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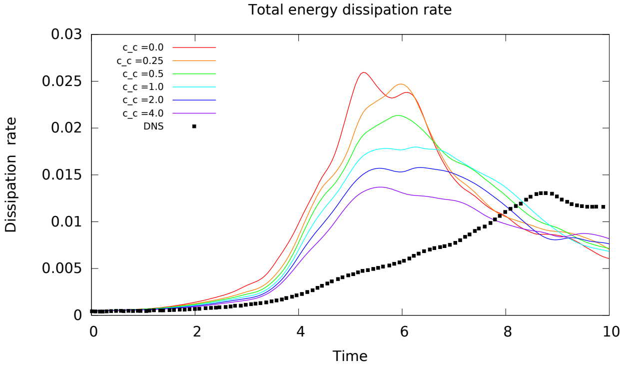
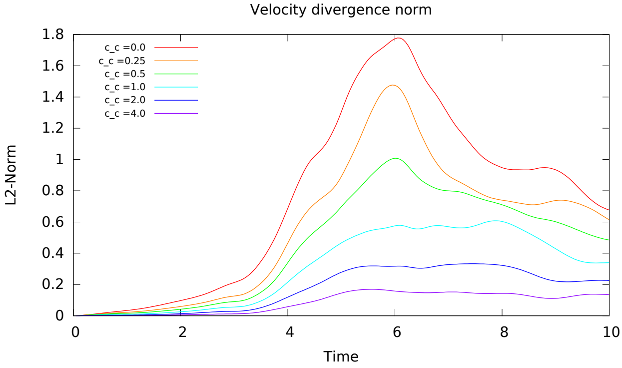


Total energy dissipation rate

- Bad results when $c_c \to 0$
- Best option $c_c = 4.0$

TGV Taylor-Green Vortex flow

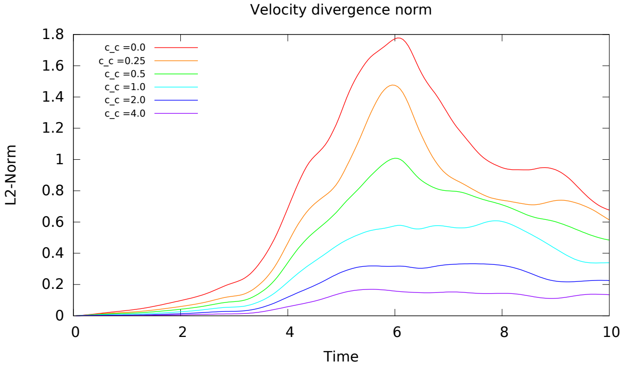
Effect of the grad-div term $(\tau_c \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$: (coarse mesh)



$$\|\nabla \cdot \mathbf{u}\|$$

TGV Taylor-Green Vortex flow

Effect of the grad-div term $(\tau_c \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$: (coarse mesh)



$$\|\nabla \cdot \mathbf{u}\|$$

- Incompressibility constraint not satisfied

TGV Taylor-Green Vortex flow

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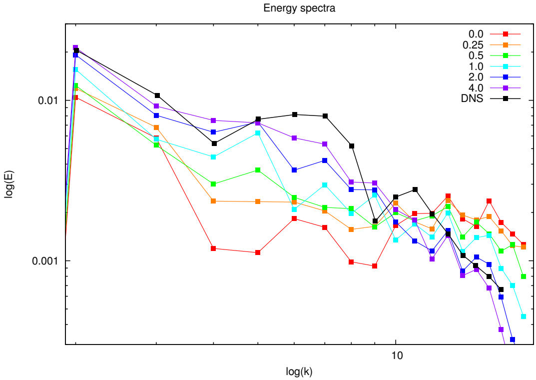
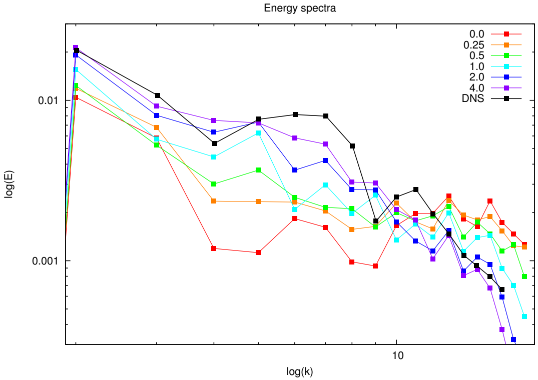


Energy spectra

TGV Taylor-Green Vortex flow

Effect of the grad-div term $(\tau_c \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$: (coarse mesh)

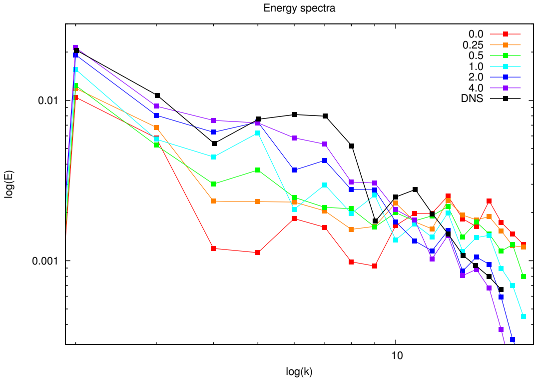


Energy spectra

- Over-dissipation on the large scales when $c_c \to 0$

TGV Taylor-Green Vortex flow

Effect of the grad-div term $(\tau_c \nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$**:** (coarse mesh)

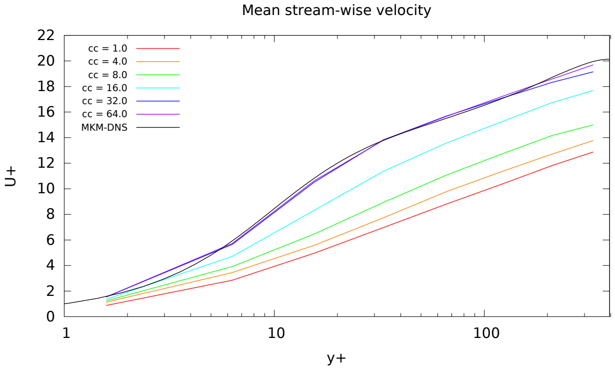


Energy spectra

- Over-dissipation on the large scales when $c_c \to 0$
- Infra-dissipation on the small scales when $c_c \to 0$

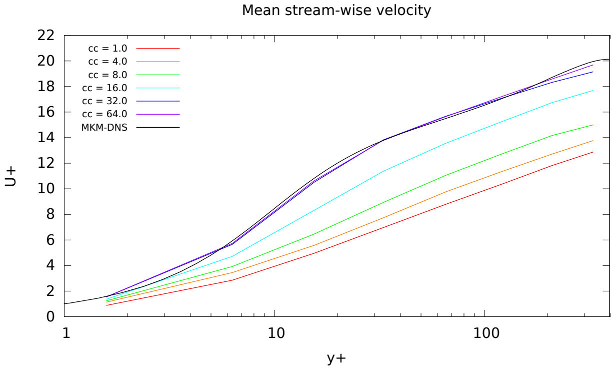
TCF Turbulent Channel Flow at $Re_\tau = 395$

Mean stream-wise velocity (models):



TCF Turbulent Channel Flow at $Re_\tau = 395$

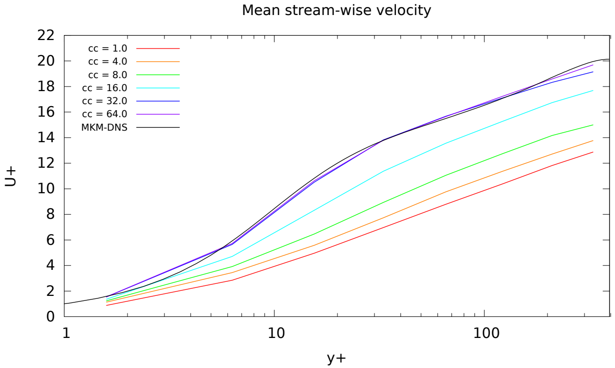
Mean stream-wise velocity (models):



- Same behaviour observed for TCF test

TCF Turbulent Channel Flow at $Re_\tau = 395$

Mean stream-wise velocity (models):



- Same behaviour observed for TCF test
- Best option $c_c = 32.0$

Mixed FE VMS Conclusions

- Optimal recursive block-preconditioners

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Contribution:

OC, Santiago Badia and Javier Principe
Mixed finite element methods with convection stabilization for the large eddy simulation of incompressible turbulent flows
Computer Methods in Applied Mechanics and Engineering, 2016

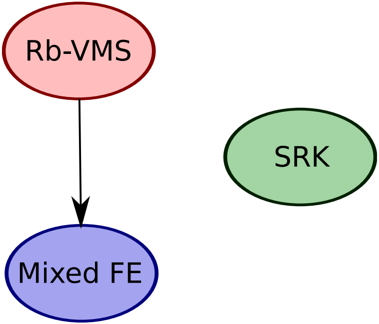
Mixed FE VMS Limitations

- Strong dependency on the grad-div stabilization term

Mixed FE VMS Limitations

- Strong dependency on the grad-div stabilization term
- Optimal choice of c_c is problem dependent

1. Motivation
2. Residual-based VMS
3. Mixed FE VMS
4. Segregated Runge-Kutta
   - Formulation
   - Numerical experiments
   - Conclusions
5. Segregated VMS
6. Conclusions



Motivation

Step by step...

- Residual-based VMS as LES models
- Mixed FE formulations as LES models
- High-order time integration schemes
- Velocity-pressure segregation
- Scalable solvers

Incomp. Navier Stokes equations

Find $\mathbf{u}$ and p defined in Ω

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nu \nabla^2 \mathbf{u} = \mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

with appropriate boundary conditions on Γ

Incomp. Navier Stokes equations

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with appropriate boundary conditions on Γ

- Laminar case (no convection stabilization required)

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- Saddle-point structure (stability via mixed FE)

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- Saddle-point structure (stability via mixed FE)
- Index-2 DAE system (time integration with care)

Incomp. Navier Stokes equations

Find $\mathbf{U}$ and $\mathbf{P}$

$$
\begin{aligned}
M\dot{\mathbf{U}} + (K + C(\mathbf{U}))\mathbf{U} + G\mathbf{P} &= \mathbf{F}, \\
D\mathbf{U} &= \mathbf{G}
\end{aligned}
$$

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We want to integrate in time with:

Incomp. Navier Stokes equations

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We want to integrate in time with:

- High-order schemes

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We want to integrate in time with:

- High-order schemes
- Velocity-pressure segregation

Velocity-pressure splitting

Existing methods: Fractional step / pressure segregation methods

$$\dot{\mathbf{U}} + M^{-1}(K + C(\mathbf{U}))\mathbf{U} + M^{-1}G\mathbf{P}^{*} = \mathbf{F}, \qquad \text{in } (t^{n}, t^{n+1}],$$
$$-DM^{-1}G\mathbf{P} = DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbf{G}}, \qquad \text{in } t^{n+1},$$

with P^{*} extrapolation from previous time steps

Velocity-pressure splitting

Existing methods: Fractional step / pressure segregation methods

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with P^* extrapolation from previous time steps
High-order time integration:

- Fractional step techniques + (e.g.) Runge-Kutta for momentum equation: [Nikitin'06; Knikker'09; Kampanis et al'06...]
- Fractional step techniques + (e.g.) BDF3 for momentum equation: [Castillo & Codina '15]
- Introduce segregation error (2nd order)

Velocity-pressure splitting

Existing methods: Fractional step / pressure segregation methods

$$\begin{aligned} \dot{\mathbf{U}} + M^{-1}(K + C(\mathbf{U}))\mathbf{U} + M^{-1}G\mathbf{P}^{*} &= \mathbf{F}, && \text{in } (t^{n}, t^{n+1}], \\ -DM^{-1}G\mathbf{P} &= DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbf{G}}, && \text{in } t^{n+1}, \end{aligned}$$

with P^{*} extrapolation from previous time steps

Drawbacks:

- Segregation error can jeopardize high order time integrators
- Effect of segregation on pressure error unclear (not reported in literature)

Velocity-pressure splitting

Existing methods: Half-explicit RK methods (HERK)

$$\frac{1}{\delta t}\mathbf{U}_i = \frac{1}{\delta t}\mathbf{U}_n + \sum_{j=1}^{i-1} \hat{a}_{ij} M^{-1}(KU_j + C(U_j)U_j + GP_j),$$

$$D\mathbf{U}_i = \mathbf{G}(t_i),$$

Velocity-pressure splitting

Existing methods: Half-explicit RK methods (HERK)

$$\frac{1}{\delta t}\mathbf{U}_i = \frac{1}{\delta t}\mathbf{U}_n - \sum_{j=1}^{i-1} \hat{a}_{ij} M^{-1}(KU_j + C(U_j)U_j + GP_j),$$

$$D\mathbf{U}_n - \delta t \sum_{j=1}^{i-1} \hat{a}_{ij} DM^{-1}(KU_j + C(U_j)U_j + GP_j) = \mathbf{G}(t_i).$$

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High-order time integration:

- Recently applied to the Navier-Stokes equations [Sanderse & Koren'12]
- Velocity-pressure segregation by the time integrator
- No additional splitting needed (high-order feasible, not spoiled)

Velocity-pressure splitting

Existing methods: Half-explicit RK methods (HERK)

$$\frac{1}{\delta t}\mathbf{U}_i = \frac{1}{\delta t}\mathbf{U}_n - \sum_{j=1}^{i-1} \hat{a}_{ij} M^{-1}(KU_j + C(U_j)U_j + GP_j),$$

$$D\mathbf{U}_n - \delta t \sum_{j=1}^{i-1} \hat{a}_{ij} DM^{-1}(KU_j + C(U_j)U_j + GP_j) = \mathbf{G}(t_i).$$

Drawbacks:

- All terms must be treated explicitly (viscous + convective terms)
- A straightforward application with implicit/IMEX integrators leads to, e..g, $D(M + \delta t K_V)^{-1} G$ matrix for the pressure (not affordable)

Segregated RK methods

- **Observation:** No implicit / IMEX high-order integrators with implicit velocity-pressure segregation

Segregated RK methods

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- **Target:** Develop such algorithms (of RK type)

Segregated RK methods

- **Observation:** No implicit / IMEX high-order integrators with implicit velocity-pressure segregation
- **Target:** Develop such algorithms (of RK type)
- **Result:** Segregated RK methods [OC & Badia, 2015]

Segregated RK methods

The idea:

1. Consider the projected momentum eq'on on the discretely divergence free space

$$
\begin{aligned}
M\dot{\mathbf{U}} + (K + C(\mathbf{U}))\mathbf{U} + G\mathbf{P} &= \mathbf{F}, \\
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\end{aligned}
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Segregated RK methods

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1. Consider the projected momentum eq'on on the discretely divergence free space

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\begin{aligned}
M\dot{\mathbf{U}} + (K + C(\mathbf{U}))\mathbf{U} + G\mathbf{P} &= \mathbf{F}, \\
-DM^{-1}G\mathbf{P} &= DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbf{G}}
\end{aligned}
$$

Segregated RK methods

The idea:

1. Consider the projected momentum eq'on on the discretely divergence free space

$$M\dot{\mathbf{U}} + P(K + C(\mathbf{U}))\mathbf{U} = P\mathbf{F} + G(DM^{-1}G)^{-1}\dot{\mathbf{G}},$$
$$\text{with} \quad P := (I - G(DM^{-1}G)^{-1}DM^{-1})$$

Segregated RK methods

The idea:

1. Consider the projected momentum eq'on on the discretely divergence free space
2. Integrate the resulting ODE system w/ preferred IMEX RK method (diagonally implicit)...

$$M\dot{\mathbf{U}} = \mathcal{F}(\mathbf{U}) + \mathcal{G}(\mathbf{U}), \qquad \mathcal{F}: \text{ implicit terms}, \quad \mathcal{G}: \text{ explicit ones}$$

Segregated RK methods

The idea:

1. Consider the projected momentum eq'on on the discretely divergence free space
2. Integrate the resulting ODE system w/ preferred IMEX RK method (diagonally implicit)...
3. $\mathcal{G}$ must include $G(DM^{-1}G)^{-1}\left(DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbf{G}}\right)$ for velocity-pressure segregation

$$M\dot{\mathbf{U}} = \mathcal{F}(\mathbf{U}) + \mathcal{G}(\mathbf{U}), \qquad \mathcal{F}: \text{ implicit terms}, \quad \mathcal{G}: \text{ explicit ones}$$

Segregated RK methods

The idea:

1. Consider the projected momentum eq'on on the discretely divergence free space
2. Integrate the resulting ODE system w/ preferred IMEX RK method (diagonally implicit)...
3. $\mathcal{G}$ must include $G(DM^{-1}G)^{-1}\left(DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbf{G}}\right)$ for velocity-pressure segregation
4. The rest of terms can be treated implicitly / explicitly

$$M\dot{\mathbf{U}} = \mathcal{F}(\mathbf{U}) + \mathcal{G}(\mathbf{U}), \qquad \mathcal{F}: \text{ implicit terms}, \quad \mathcal{G}: \text{ explicit ones}$$

Segregated RK methods

At each stage i, the time-discrete algorithm reads:

$$\frac{1}{\delta t} M\mathbf{U}_i = \frac{1}{\delta t} M\mathbf{U}_n + \sum_{j=1}^{i} a_{ij}\mathcal{F}(\mathbf{U}_j) + \sum_{j=1}^{i-1} \hat{a}_{ij}\mathcal{G}(\mathbf{U}_j)$$

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- Viscous / convective can be treated implicitly / explicitly

$\mathcal{F}(\mathbf{U}) := -K\mathbf{U} + \mathbf{F} - C(\mathbf{U})\mathbf{U}$, $\quad \tilde{\mathcal{G}}(\mathbf{U}, P) = -GP \quad$ or

$\mathcal{F}(\mathbf{U}) := -K\mathbf{U} + \mathbf{F}$, $\quad \tilde{\mathcal{G}}(\mathbf{U}, P) = -C(\mathbf{U})\mathbf{U} - GP$

SRK Some properties

- Segregation at the time integration level (no additional splitting)
- High order achievable (the one of the ODE RK integration)
- Implicit LES turbulent model (stabilization terms)
- Equal-order & optimal velocity-pressure methods (of interest in FSI, etc.)
- HERK and SRK methods are *equivalent* for full explicit treatment

Numerical experiments

Manufactured analytical solutions:

- Simple $sin(t) \cdot \exp(t)$ function

Laminar benchmark:

- 2D Laminar flow around a cylinder

Manufactured analytical solution

Problem setting:

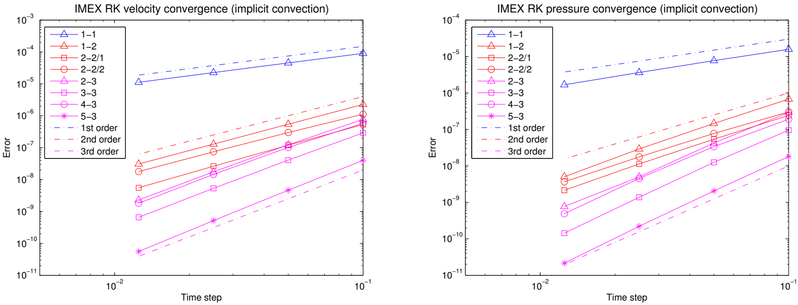
- Analytical solution:

$$\mathbf{u}(x,y,t) = \begin{bmatrix} x \\ -y \end{bmatrix} \sin(\frac{\pi}{10}t)\exp(\frac{t}{25}),$$
$$p(x,y) = x + y$$

- $Re = 1/10/100$
- Different IMEX Butcher tableaus with 1st, 2nd and 3rd order

Manufactured analytical solution

Implicit convection:

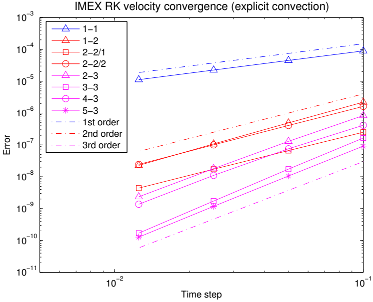


(a) Velocity convergence, $\nu = 0.01$ (b) Pressure convergence, $\nu = 0.01$

Fully implicit SRK

Manufactured analytical solution

Explicit convection:



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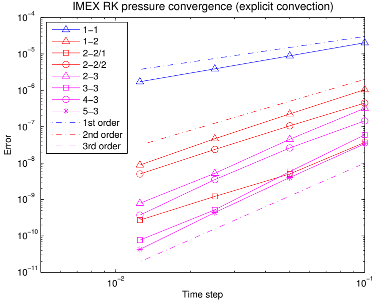


(b) Pressure convergence, $\nu = 0.01$

SRK convergence with convection integrated explicitly and diffusion integrated implicitly

2D Laminar flow around a cylinder

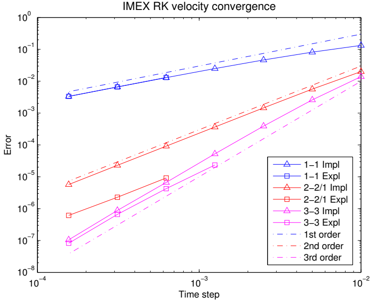
Problem setting:

- Widely used benchmark.
- $Re = 100$.
- Time convergence.
- Drag and Lift coefficients.

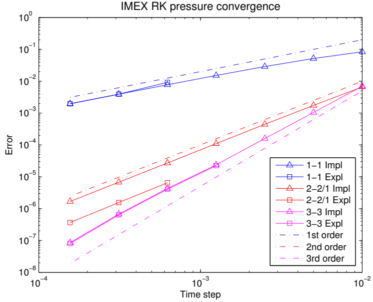
Vorticity field at $t = 8.0$.

2D Laminar flow around a cylinder

Implicit & explicit convection:



(a) Velocity convergence



(b) Pressure convergence

Fully implicit and IMEX-SRK convergence rate comparison.

Segregated Runge-Kutta Conclusions

- Velocity-pressure segregated by the time integrator (IMEX RK)

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Contribution:

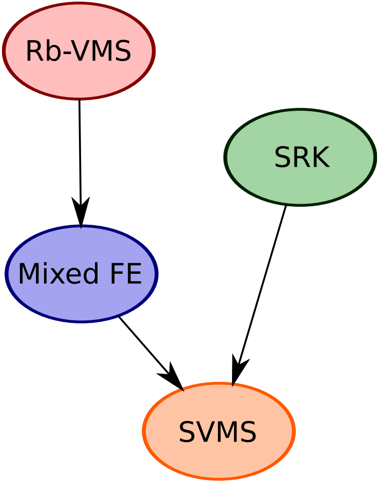
OC and Santiago Badia
Segregated Runge-Kutta schemes for the incompressible Navier-Stokes equations
International Journal for Numerical Methods in Engineering, 2016

Segregated Runge-Kutta Limitations

- Only for index-2 DAE

Segregated Runge-Kutta Limitations

- Only for index-2 DAE
- Not applicable for equal-order stabilization methods


Rb-VMS
SRK
Mixed FE
SVMS

Motivation

Step by step...

- Residual-based VMS as LES models
- Mixed FE formulations as LES models
- High-order time integration schemes
- Velocity-pressure segregation
- Scalable solvers

Looking backward...

VMS as LES models: Residual-based VMS methods

- Velocity + pressure stabilization, applied to equal-order FEs
- Intensively tested methods (several works in the literature)
- Nature of the problem changes, not DAE-2 type (!)
- It prevents us to use segregated RK methods

Looking backward...

VMS as LES models: Mixed FE VMS methods

- Only the term that we need, i.e., convection stabilization
- To keep accuracy, we use orthogonal projections ($\mathcal{P}_h^\perp$)
- Many choices for the $\mathcal{P}_h$ projector: local, global (OSS)
- Discrete problem still index-2 DAE
- Segregated RK schemes can be used

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- Only the term that we need, i.e., convection stabilization
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Now, we can use Segregated RK methods for ILES of turbulent flows

Formulation

OSS-ISS: Semi-discrete form

$$\begin{bmatrix} M\dot{\mathbf{U}} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} K + C(\mathbf{U}) + A_\tau & G & B_\tau \\ D & 0 & 0 \\ -B_\tau^T & 0 & M_\tau \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \\ \boldsymbol{\Upsilon} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_u \\ \mathbf{G} \\ \mathbf{0} \end{bmatrix},$$

Formulation

OSS-ISS: Semi-discrete form

$$
\begin{aligned}
M\dot{\mathbf{U}} + (K + C(\mathbf{U}) + A_\tau)\mathbf{U} + G\mathbf{P} + B_\tau \boldsymbol{\Upsilon} &= \mathbf{F}_u, \\
M_\tau \boldsymbol{\Upsilon} - B_\tau^T \mathbf{U} &= \mathbf{0}, \\
D\mathbf{U} &= \mathbf{G}.
\end{aligned}
$$

Formulation

OSS-ISS:

1. Consider the projected momentum eq'on on the discretely divergence free space

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Final discrete problem

At each stage of the Runge-Kutta scheme: (explicit convective term and projection version)

$$\frac{1}{\delta t} M \mathbf{U}_i = \frac{1}{\delta t} M \mathbf{U}_n + \sum_{j=1}^{i} a_{ij} \mathcal{F}(\mathbf{U}_j) + \sum_{j=1}^{i-1} \hat{a}_{ij} \mathcal{G}(\mathbf{U}_j, \boldsymbol{\Upsilon}_j, \mathbf{P}_j),$$

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- Elasticity-type matrix for the momentum equation
- Mass-type matrix for the projection equation

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- Elasticity-type matrix for the momentum equation
- Mass-type matrix for the projection equation
- Darcy-type system for the pressure equation

Large scale simulations

Momentum system matrix: $\frac{1}{\delta t}M + a_{ii}K$

- Multilevel/overlapped Balancing domain decomposition (BDDC) for $M + \delta t K$
- Excellent weak scalability results (up to $\sim 460,000$ IBM BG/Q cores) [Badia *et al* '15]

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Pressure system matrix: $DM^{-1}G$

- Spectrally equivalent to standard Laplacian L_p
- Written as

$$\begin{bmatrix} M & G \\ D & 0 \end{bmatrix} \quad \text{preconditioned w/} \quad \begin{bmatrix} M & 0 \\ 0 & L_p \end{bmatrix}$$

- Multilevel/overlapped Balancing domain decomposition (BDDC) for L_p
- Excellent weak scalability results (up to $\sim 460,000$ IBM BG/Q cores) [Badia *et al* '15]

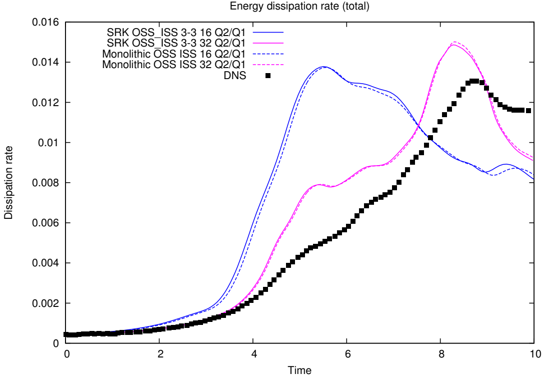
Numerical experiments

Three different turbulent benchmarks:

- Taylor-Green Vortex (TGV) flow
- Turbulent Channel Flow (TCF)
- Flow around a NACA profile

TGV Taylor-Green Vortex flow

Monolithic vs Segregated Runge-Kutta:



Total energy dissipation rate

TGV Taylor-Green Vortex flow

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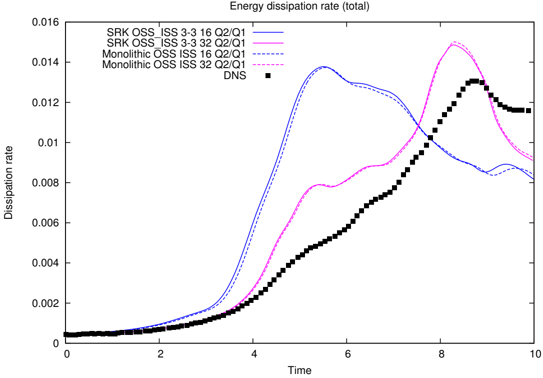

Total energy dissipation rate

- Almost Identical results obtained with Crank-Nicolson

TGV Taylor-Green Vortex flow

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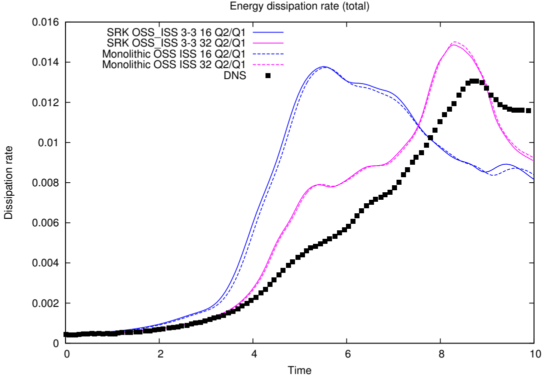
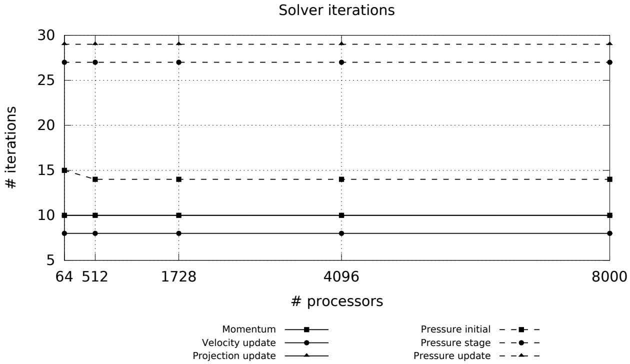


Total energy dissipation rate

- Almost Identical results obtained with Crank-Nicolson
- Velocity-pressure segregation and adaptive time stepping

TGV Taylor-Green Vortex flow

Weak scalability: HLRN-III Cray XC40 with Intel Xeon Haswell



Solver iterations

TGV Taylor-Green Vortex flow

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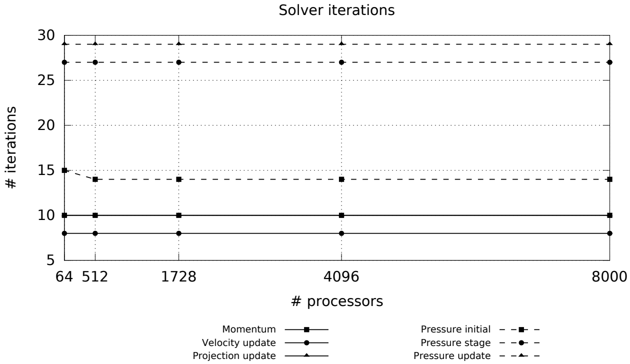

Solver iterations

- Perfect scalability in terms of solver iterations

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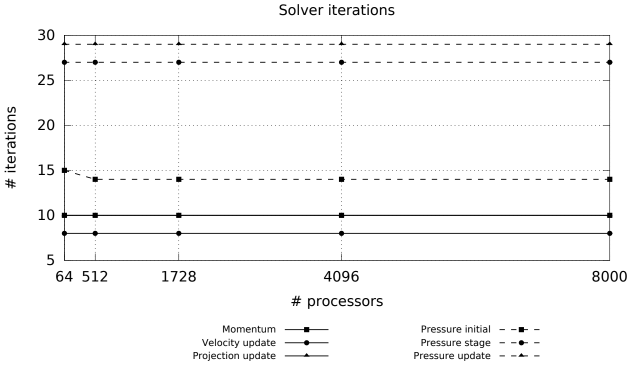

Solver iterations

- Perfect scalability in terms of solver iterations
- Darcy-type problem requires more iterations

TGV Taylor-Green Vortex flow

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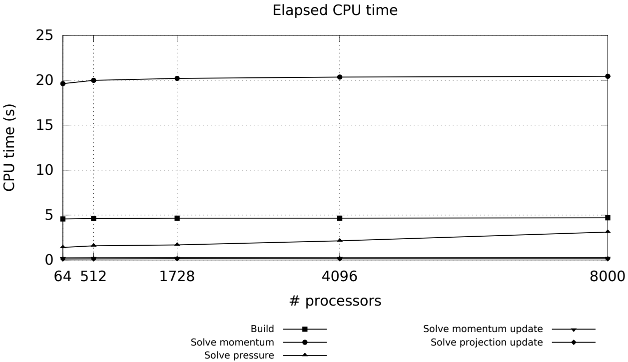
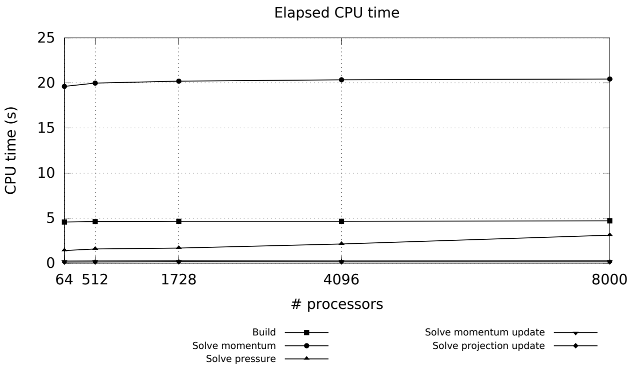


CPU time

TGV Taylor-Green Vortex flow

Weak scalability: HLRN-III Cray XC40 with Intel Xeon Haswell



CPU time

- Perfect scalability in CPU time consumed

TGV Taylor-Green Vortex flow

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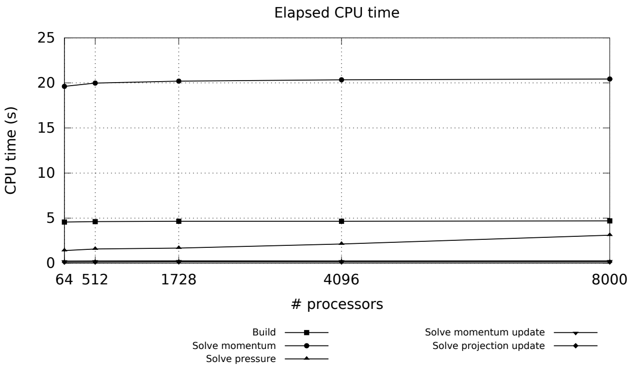


CPU time

- Perfect scalability in CPU time consumed
- Momentum problem requires more time

TCF Turbulent Channel Flow at $Re_\tau = 395$

LES for wall bounded flows?

Problem:

- LES models cannot accurately simulate boundary layers without stretched meshes

TCF Turbulent Channel Flow at $Re_\tau = 395$

LES for wall bounded flows?

Problem:

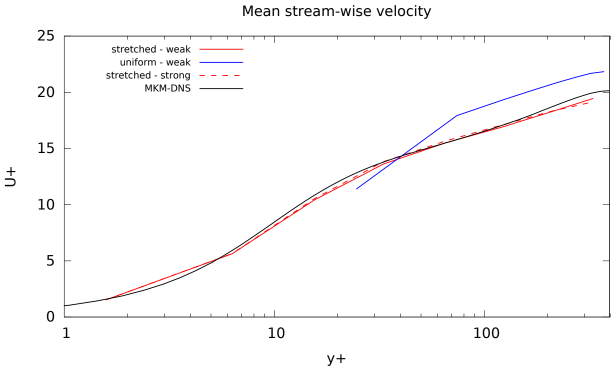
- LES models cannot accurately simulate boundary layers without stretched meshes

Solution:

- Use of weak boundary conditions (Nitche's method)
- Impose the tangential traction on the wall from a wall law model [Bazilevs *et al* '07]
- We also impose weakly the wall-normal component

TCF Turbulent Channel Flow at $Re_\tau = 395$

Weak boundary conditions:



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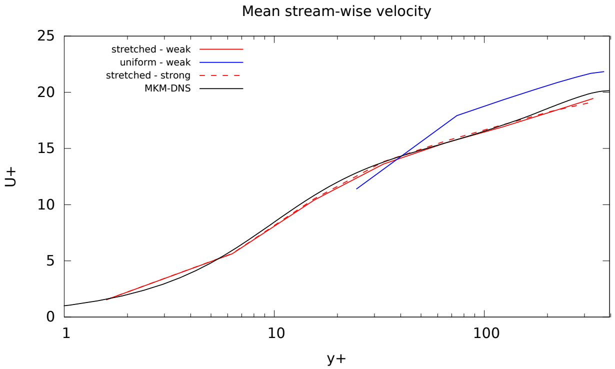

- We recover the strong BC results when stretched mesh is used

TCF Turbulent Channel Flow at $Re_\tau = 395$

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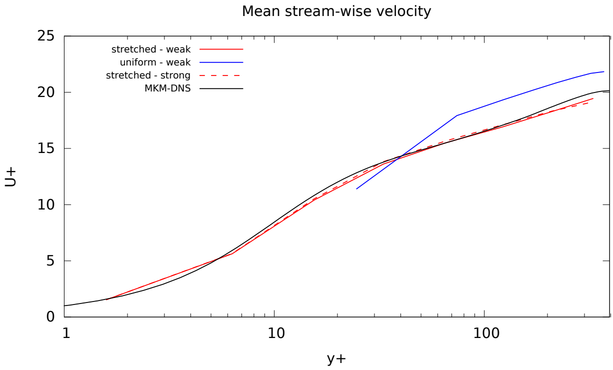

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- Acceptable results for uniform meshes

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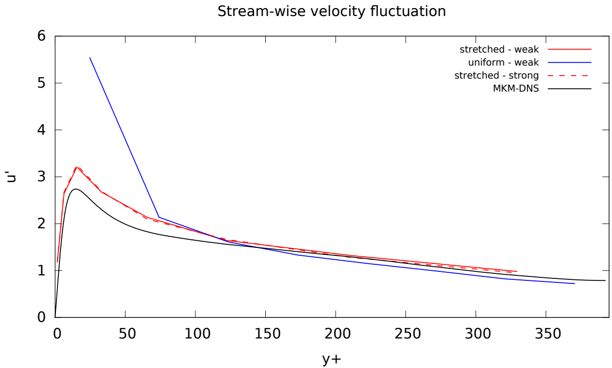
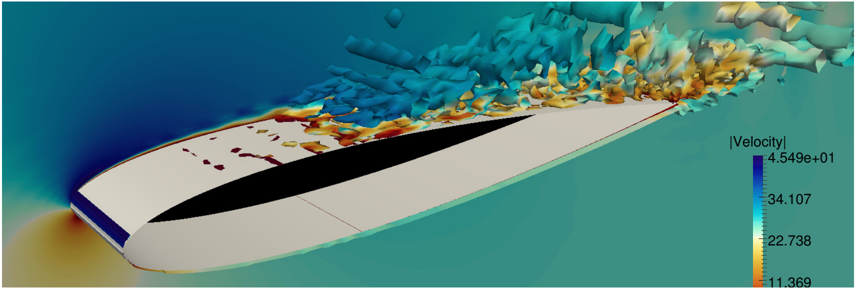


- We recover the strong BC results when stretched mesh is used
- Acceptable results for uniform meshes

Turbulent flow around a NACA profile

- Low Reynolds number, $Re = 23000$
- Weak boundary conditions also on the wall-normal component
- Coarse mesh



Q-criterion isosurfaces for a fully developed flow

Segregated VMS Conclusions

- Implicit LES for mixed FEs + convection stabilization
  - Similar behavior as VMS-type solvers
  - Not affecting nature of the system (index-2 DAE)
- Large scale computations
  - Segregation leads to coercive blocks to be solved
  - Highly scalable multilevel/overlapped implementation of BDDC
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Segregated VMS Conclusions

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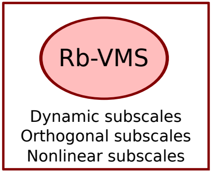
Contribution:

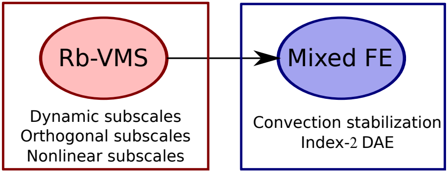
OC and Santiago Badia
Segregated Runge-Kutta time integration of convection-stabilized mixed finite element schemes for wall-unresolved LES of incompressible flows
Submitted, 2016

Final Conclusions



- Demonstrated suitability of Residual-based VMS methods as LES models

Final Conclusions



- Demonstrated suitability of Residual-based VMS methods as LES models
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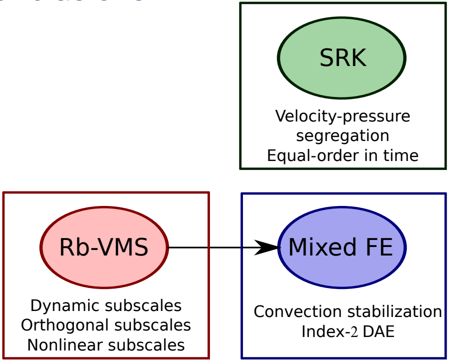
Final Conclusions



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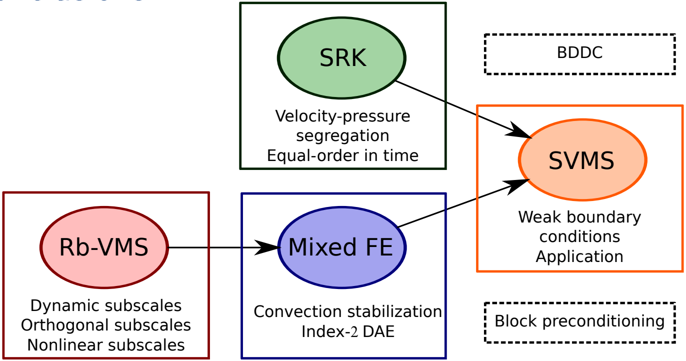
Final Conclusions



- Demonstrated suitability of Residual-based VMS methods as LES models
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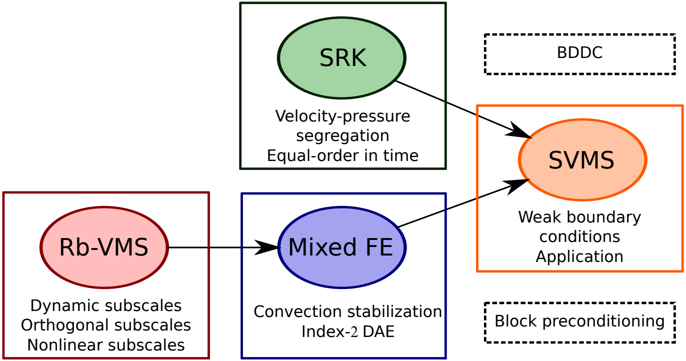
- Highly-scalable FE solvers for the simulation of turbulent incompressible flows

Final Conclusions



Thesis goal

Highly scalable Finite Element (FE) framework for Large Eddy Simulations (LES) of incompressible turbulent flows

Acknowledgements

I would like to thank

- my advisor, Santiago Badia
- all LSSC team
- my family

Thank you!

OC, Santiago Badia, Ramon Codina and Javier Principe
Assessment of variational multiscale models for the large eddy simulation of turbulent incompressible flows
Computer Methods in Applied Mechanics and Engineering, 2015

OC and Santiago Badia
Segregated Runge-Kutta schemes for the incompressible Navier-Stokes equations
International Journal for Numerical Methods in Engineering, 2016

OC, Santiago Badia and Javier Principe
Mixed finite element methods with convection stabilization for the large eddy simulation of incompressible turbulent flows
Computer Methods in Applied Mechanics and Engineering, 2016

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Segregated Runge-Kutta time integration of convection-stabilized mixed finite element schemes for wall-unresolved LES of incompressible flows
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Rb-VMS Summary

	Sgs space	Sgs dynamics	Advection
1	ASGS	Static	Linear
2	ASGS	Dynamic	Linear
3	ASGS	Dynamic	Nonlinear
4	OSS	Static	Linear
5	OSS	Dynamic	Linear
6	OSS	Dynamic	Nonlinear

1 It is the most standard method (SUPG for linear elements) up to the choice of the stabilization parameters. Unknown stability properties.

4 Strictly point-wise positive for linear elements (no backscatter).

5 Convergent to weak solutions of NS equations (Badia & Gutierrez 2012).

Energy statements

FE counterpart:

$$B\left((\mathbf{u}_h, p_h);(\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{u}_h, p_h)\right) = L\left(\mathbf{u}_h, p_h\right)$$

SGS counterpart:

$$B\left((\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{u}_h, p_h);(\widetilde{\mathbf{u}}, \widetilde{p})\right) = L\left(\widetilde{\mathbf{u}}, \widetilde{p}\right)$$

TOTAL:

$$\begin{aligned} &B\left((\mathbf{u}_h, p_h);(\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{u}_h, p_h)\right) \\ +&B\left((\widetilde{\mathbf{u}}, \widetilde{p});(\mathbf{u}_h, p_h);(\widetilde{\mathbf{u}}, \widetilde{p})\right) = L\left(\mathbf{u}_h, p_h\right) + L\left(\widetilde{\mathbf{u}}, \widetilde{p}\right) \end{aligned}$$

Energy statements

FE counterpart:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + b(\mathbf{a},\mathbf{u}_h,\mathbf{u}_h)$$
$$+ (\partial_t\widetilde{\mathbf{u}},\mathbf{u}_h) + (\mathcal{L}_a^*(\mathbf{u}_h,p_h),\widetilde{\mathbf{u}}) - (\nabla\cdot\mathbf{u}_h,\widetilde{p}) = \langle\mathbf{f},\mathbf{u}_h\rangle$$

SGS counterpart:

$$\frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2$$
$$+ (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p}) = \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

TOTAL:

Energy statements

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TOTAL:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2$$

Energy statements

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TOTAL:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \nu\|\nabla\mathbf{u}_h\|^2$$

Energy statements

FE counterpart:

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TOTAL:

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Energy statements

FE counterpart:

$$\frac{1}{2} d_t \|\mathbf{u}_h\|^2 + \nu \|\nabla \mathbf{u}_h\|^2 + b(\mathbf{a}, \mathbf{u}_h, \mathbf{u}_h) + (\partial_t \widetilde{\mathbf{u}}, \mathbf{u}_h) + (\mathcal{L}_a^*(\mathbf{u}_h, p_h), \widetilde{\mathbf{u}}) - (\nabla \cdot \mathbf{u}_h, \widetilde{p}) = \langle \mathbf{f}, \mathbf{u}_h \rangle$$

SGS counterpart:

$$\frac{1}{2} d_t \|\widetilde{\mathbf{u}}\|^2 + \tau_m^{-1} \|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1} \|\widetilde{p}\|^2 + (\mathcal{P}(\partial_t \mathbf{u}_h), \widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h, p_h)), \widetilde{\mathbf{u}}) - (\mathcal{P}(\nabla \cdot \mathbf{u}_h), \widetilde{p}) = \langle \mathcal{P}(\mathbf{f}), \widetilde{\mathbf{u}} \rangle$$

TOTAL:

$$\frac{1}{2} d_t \|\mathbf{u}_h\|^2 + \frac{1}{2} d_t \|\widetilde{\mathbf{u}}\|^2 + \nu \|\nabla \mathbf{u}_h\|^2 + \tau_m^{-1} \|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1} \|\widetilde{p}\|^2$$

Energy statements

FE counterpart:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + b(\mathbf{a},\mathbf{u}_h,\mathbf{u}_h)$$
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TOTAL:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2$$
$$+ (\partial_t\widetilde{\mathbf{u}},\mathbf{u}_h) + (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{L}_a^*(\mathbf{u}_h,p_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}})$$
$$- (\nabla\cdot\mathbf{u}_h,\widetilde{p}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p})$$

Energy statements

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$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + b(\mathbf{a},\mathbf{u}_h,\mathbf{u}_h) + (\partial_t\widetilde{\mathbf{u}},\mathbf{u}_h) + (\mathcal{L}_a^*(\mathbf{u}_h,p_h),\widetilde{\mathbf{u}}) - (\nabla\cdot\mathbf{u}_h,\widetilde{p}) = \langle\mathbf{f},\mathbf{u}_h\rangle$$

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Energy statements

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SGS counterpart:

$$\frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2 + (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p}) = \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

TOTAL: **Static subscales**

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2 + (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{L}_a^*(\mathbf{u}_h,p_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}}) - (\nabla\cdot\mathbf{u}_h,\widetilde{p}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p}) = \langle\mathbf{f},\mathbf{u}_h\rangle + \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

Energy statements

FE counterpart:

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SGS counterpart:

$$\frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2 + (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p}) = \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

TOTAL: **Dynamic subscales - ASGS**

$$\frac{1}{2}d_t\|\mathbf{u}_h+\widetilde{\mathbf{u}}\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2 - 2\,(\nu\Delta\mathbf{u}_h,\widetilde{\mathbf{u}}) = \langle\mathbf{f},\mathbf{u}_h\rangle + \langle\mathbf{f},\widetilde{\mathbf{u}}\rangle$$

Energy statements

FE counterpart:

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + b(\mathbf{a},\mathbf{u}_h,\mathbf{u}_h)$$
$$+ (\partial_t\widetilde{\mathbf{u}},\mathbf{u}_h) + (\mathcal{L}_a^*(\mathbf{u}_h,p_h),\widetilde{\mathbf{u}}) - (\nabla\cdot\mathbf{u}_h,\widetilde{p}) = \langle\mathbf{f},\mathbf{u}_h\rangle$$

SGS counterpart:

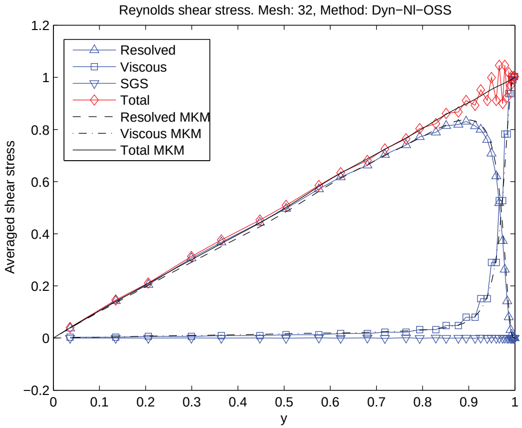
$$\frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2$$
$$+ (\mathcal{P}(\partial_t\mathbf{u}_h),\widetilde{\mathbf{u}}) + (\mathcal{P}(\mathcal{L}_a^*(\mathbf{u}_h,p_h)),\widetilde{\mathbf{u}}) - (\mathcal{P}(\nabla\cdot\mathbf{u}_h),\widetilde{p}) = \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

TOTAL: Dynamic subscales - OSS

$$\frac{1}{2}d_t\|\mathbf{u}_h\|^2 + \frac{1}{2}d_t\|\widetilde{\mathbf{u}}\|^2 + \nu\|\nabla\mathbf{u}_h\|^2 + \tau_m^{-1}\|\widetilde{\mathbf{u}}\|^2 + \tau_c^{-1}\|\widetilde{p}\|^2$$
$$- 2(\nu\Delta\mathbf{u}_h,\widetilde{\mathbf{u}})$$
$$= \langle\mathbf{f},\mathbf{u}_h\rangle + \langle\mathcal{P}(\mathbf{f}),\widetilde{\mathbf{u}}\rangle$$

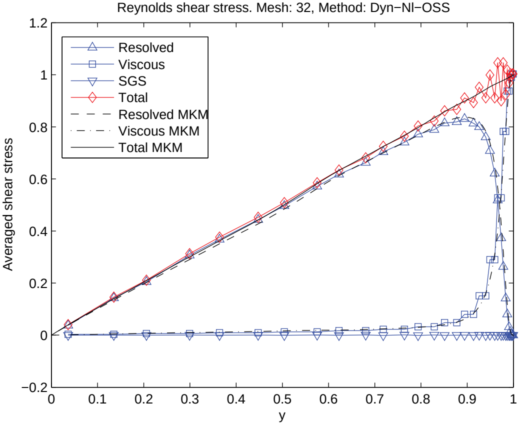
Rb-VMS TCF Turbulent Channel Flow

Reynolds shear stress (models):



Rb-VMS TCF Turbulent Channel Flow

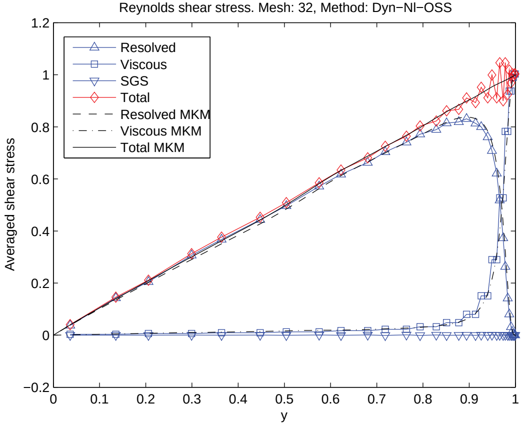
Reynolds shear stress (models):



- Almost identical to the DNS.

Rb-VMS TCF Turbulent Channel Flow

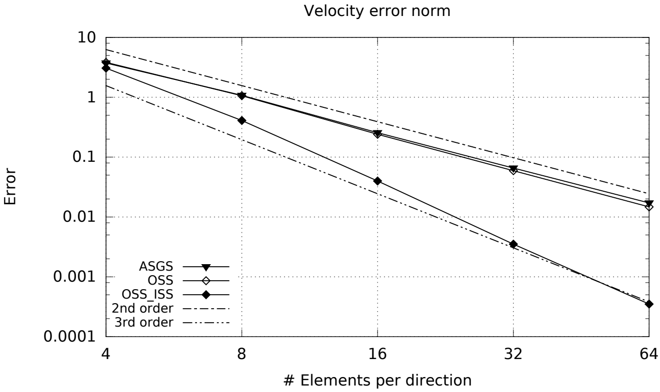
Reynolds shear stress (models):



- Almost identical to the DNS.
- SGS counterpart does not contribute to the Reynolds shear stress.

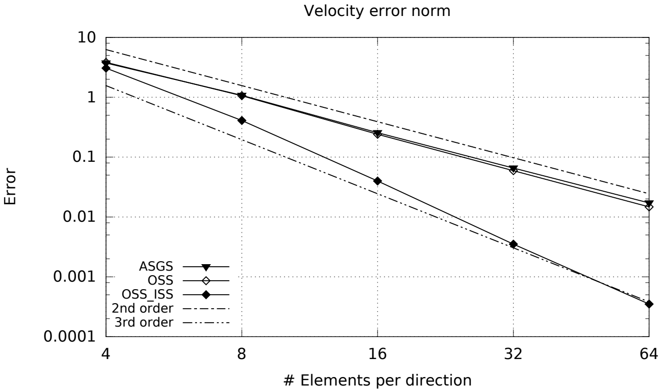
Mixed FE Colliding flow

Accuracy: Velocity error



Mixed FE Colliding flow

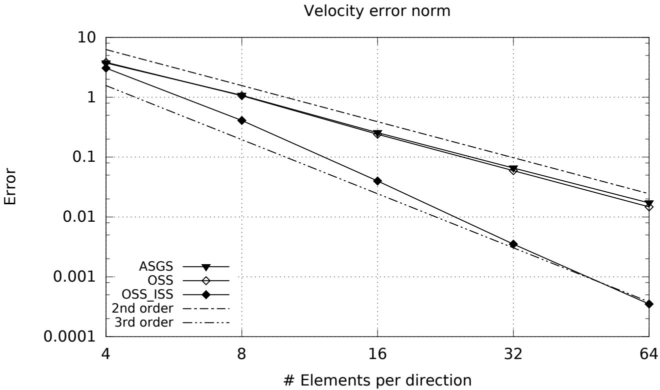
Accuracy: Velocity error



- 2nd order convergence rate for ASGS and OSS methods.

Mixed FE Colliding flow

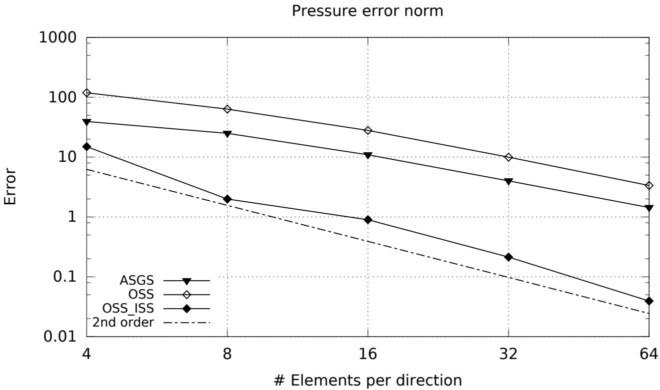
Accuracy: Pressure error



- 2nd order convergence rate for ASGS and OSS methods.
- 3rd order convergence rate for OSS-ISS method.

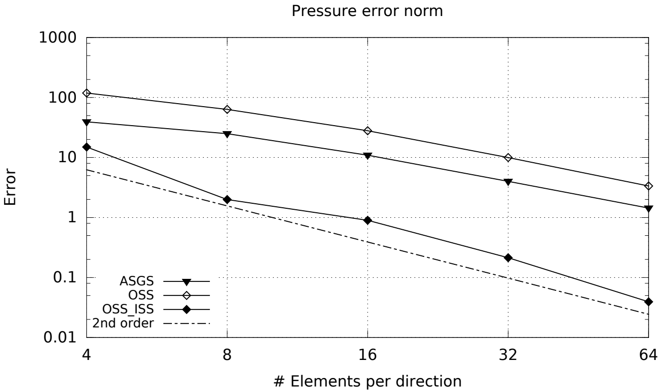
Mixed FE Colliding flow

Accuracy: Pressure error



Mixed FE Colliding flow

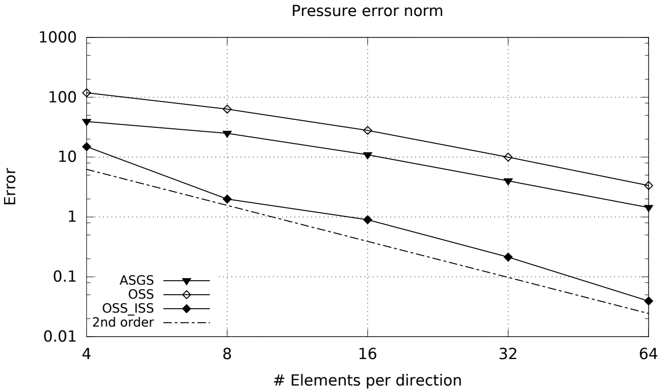
Accuracy:



- 2nd order convergence rate for all methods.

Mixed FE Colliding flow

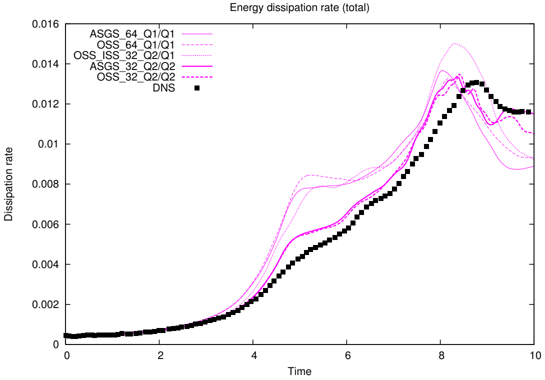
Accuracy:



- 2nd order convergence rate for all methods.
- Best accuracy for OSS-ISS method.

Mixed FE TGV Taylor-Green Vortex flow

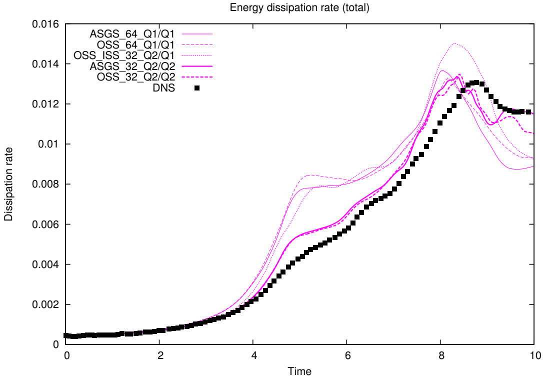
Energy dissipation rate (different methods):



Total energy dissipation rate

Mixed FE TGV Taylor-Green Vortex flow

Energy dissipation rate (different methods):

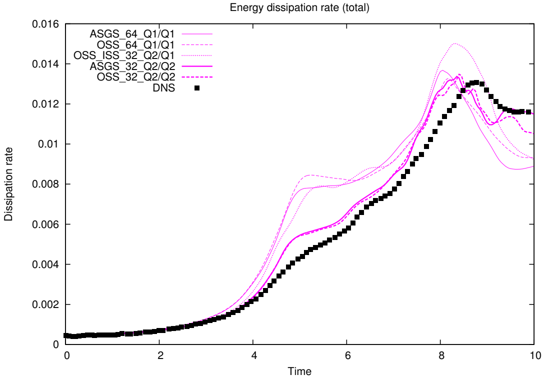


Total energy dissipation rate

- Good agreement with the DNS (coarse mesh).

Mixed FE TGV Taylor-Green Vortex flow

Energy dissipation rate (different methods):

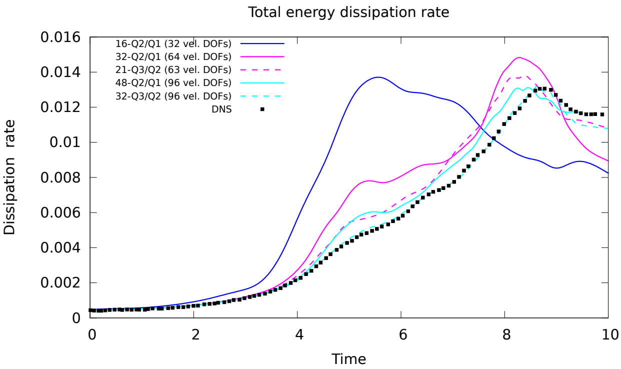


Total energy dissipation rate

- Good agreement with the DNS (coarse mesh).
- More accurate results with equal-order elements.

Mixed FE TGV Taylor-Green Vortex flow

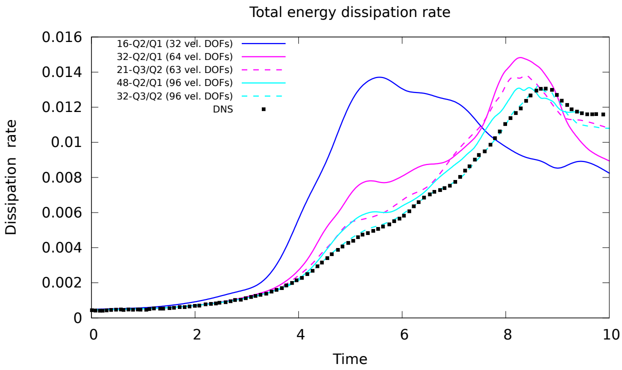
Energy dissipation rate (refinement OSS-ISS):



Total energy dissipation rate

Mixed FE TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement OSS-ISS):

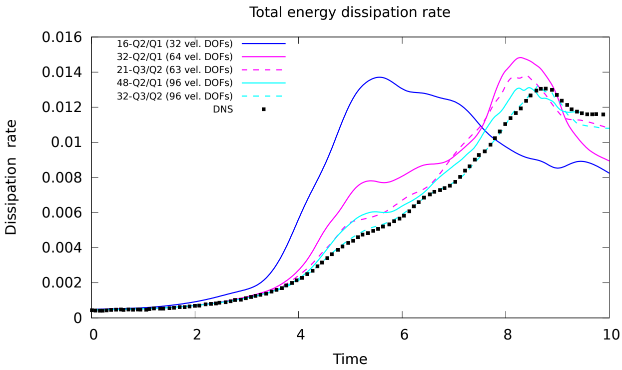


Total energy dissipation rate

- Good agreement with the DNS.

Mixed FE TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement OSS-ISS):

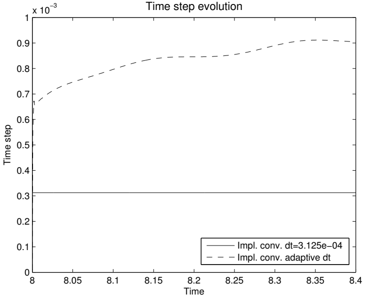


Total energy dissipation rate

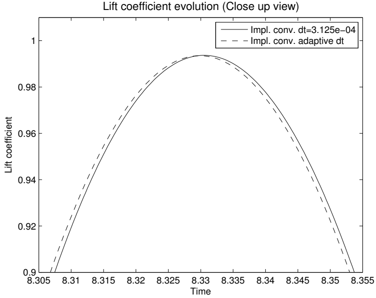
- Good agreement with the DNS.
- 32^3 $Q3/Q2$ elements mesh on top of DNS.

SRK 2D Laminar flow around a cylinder

Adaptive time stepping:



(a) Time step evolution



(b) Lift coefficient (zoom)

Adaptive time stepping.