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

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Motivation

Thesis motivation

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

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1. Variational MultiScale (VMS) methods as LES models.
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 LES.

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- Scalable solvers.

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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

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

with appropriate boundary conditions on Γ.

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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

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

Incomp. Navier Stokes equations

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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

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

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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

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

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

Semidiscrete problem

FEM equations

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

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

SGS equations

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

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

Numerical experiments

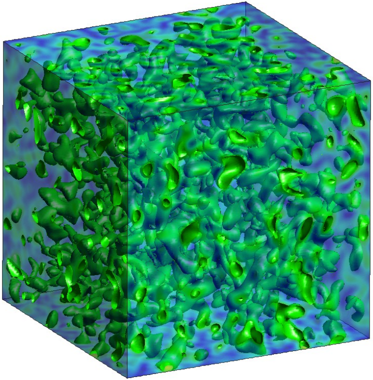
Three different turbulent benchmarks:

- 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).
- A (very simple) time step adaptation technique is used.
- Different mesh discretizations (Q_1/Q_1 and Q_2/Q_2).



DHIT Decay of Homogeneous Isotropic Turbulence

Energy espectra (models):

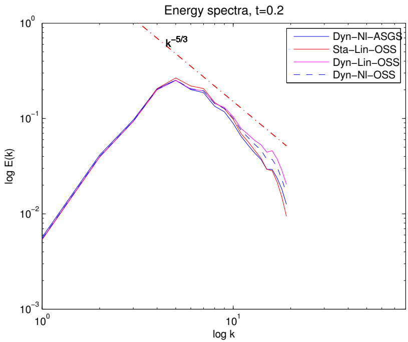


Figure : $32^3 - Q1,\ t = 0.2s$

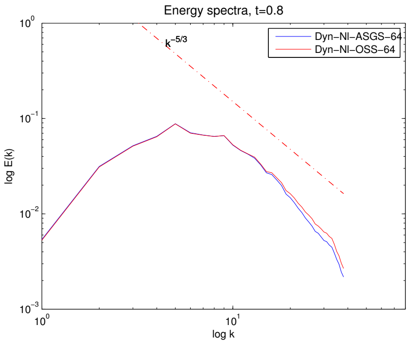


Figure : $64^3 - Q1,\ t = 0.8s$

DHIT Decay of Homogeneous Isotropic Turbulence

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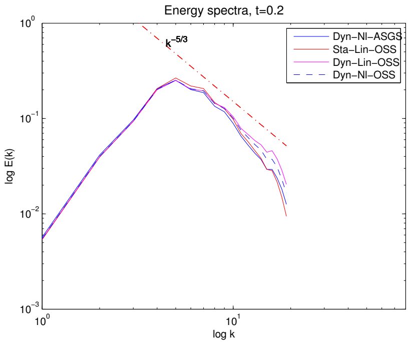

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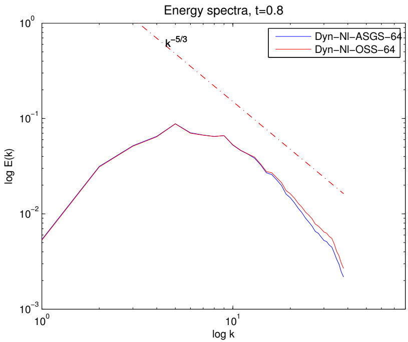

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- Small differences between methods (physical sense).

DHIT Decay of Homogeneous Isotropic Turbulence

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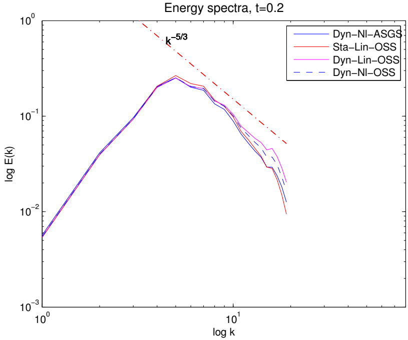

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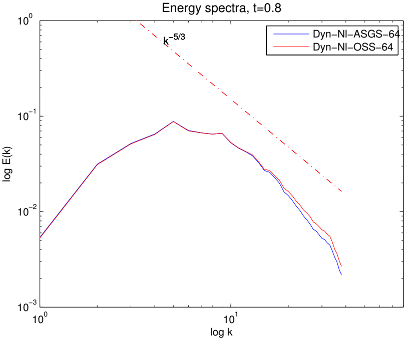
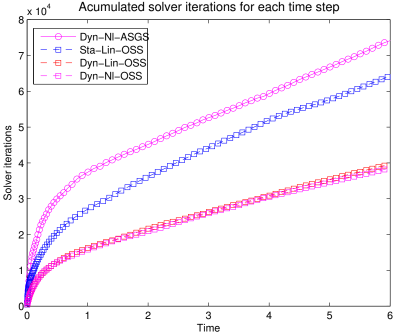


Figure : $64^3 - Q1$, $t = 0.8s$

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

DHIT Decay of Homogeneous Isotropic Turbulence

Computational cost (models):



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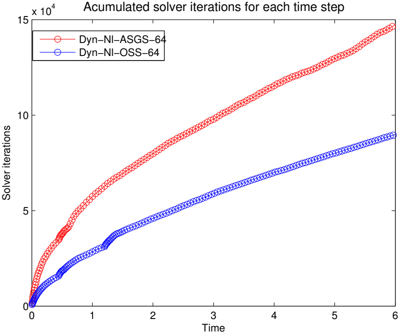

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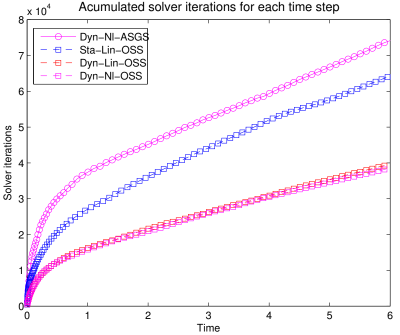

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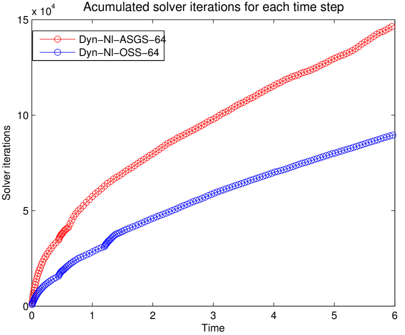

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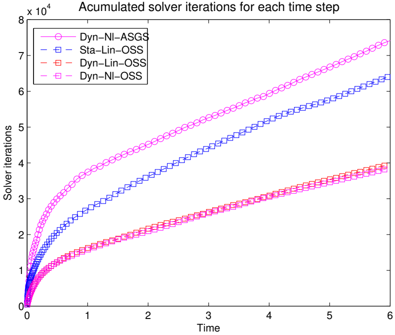

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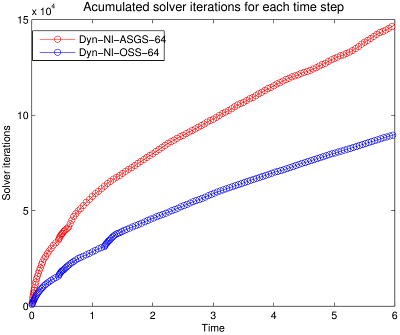
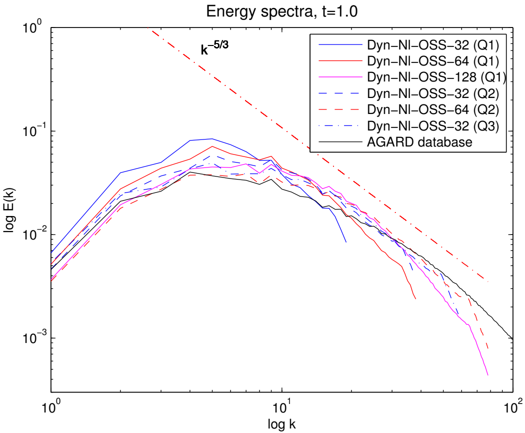


Figure : $64^3 - Q1$

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

DHIT Decay of Homogeneous Isotropic Turbulence

Energy espectra (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).

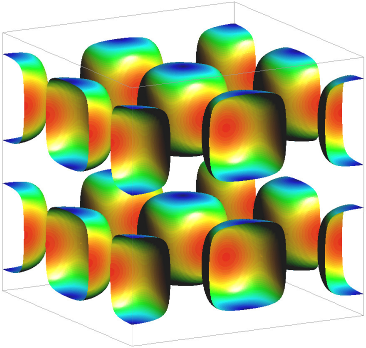


Figure : Initial vorticity isosurface $|\omega| = 1$

TGV Taylor-Green Vortex flow

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- $Re = 1600$.
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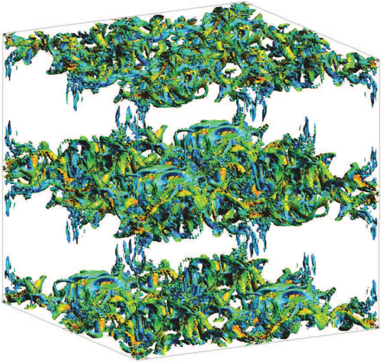


Figure : Vorticity isosurfaces $|\omega| = 9.0$

TGV Taylor-Green Vortex flow

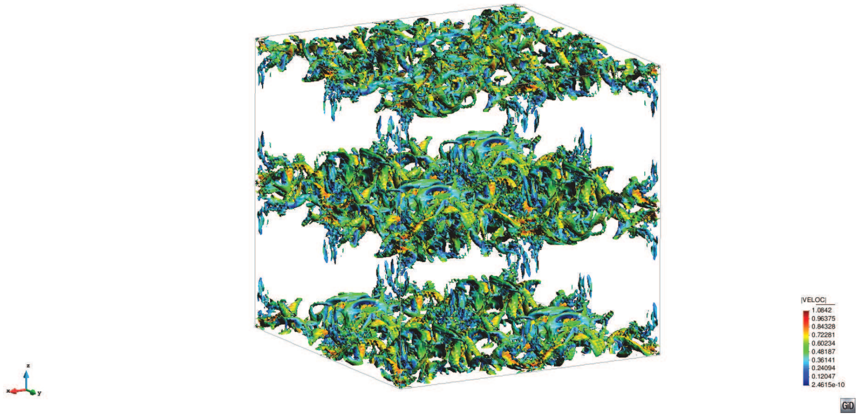


Figure : Velocity isosurface

TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement):

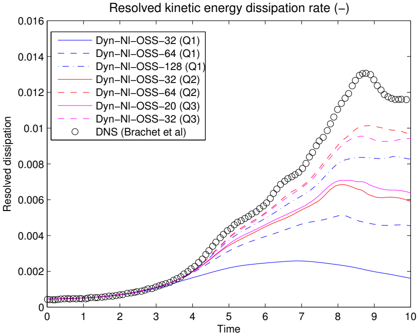


Figure : Resolved scales

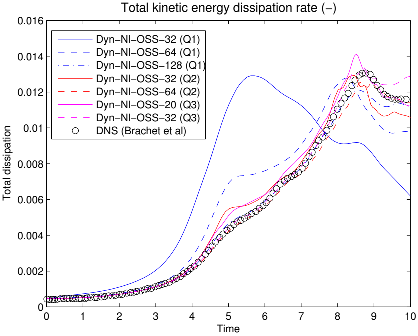
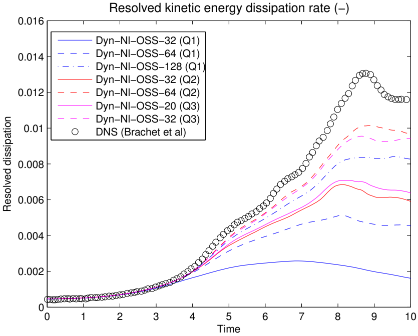


Figure : Total

TGV Taylor-Green Vortex flow

Energy dissipation rate (refinement):



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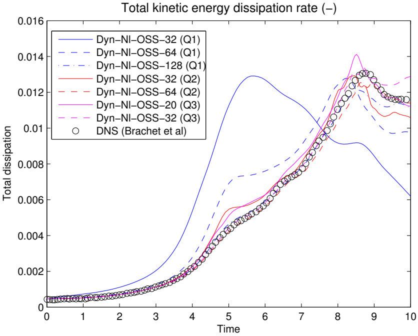

Figure : Total

- Good agreement with the DNS taking account the subscales.

TGV Taylor-Green Vortex flow

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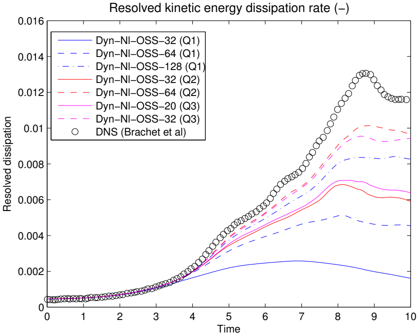

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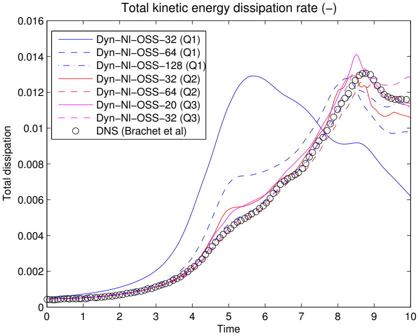

Figure : Total

- 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):

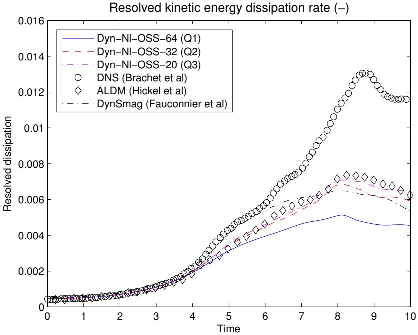

Figure : Resolved scales

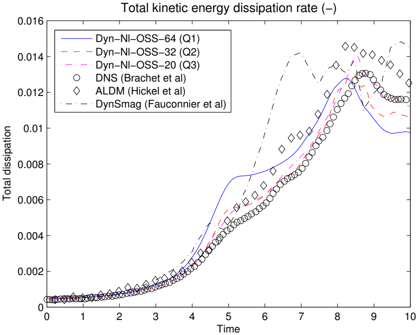

Figure : Total

TGV Taylor-Green Vortex flow

Energy dissipation rate (against LES model):

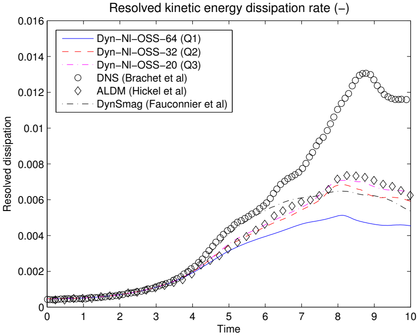

Figure : Resolved scales

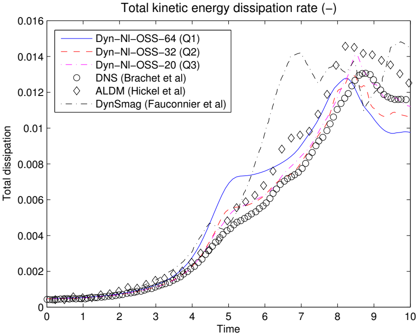

Figure : Total

- Good agreement with the LES models on resolved scales.

TGV Taylor-Green Vortex flow

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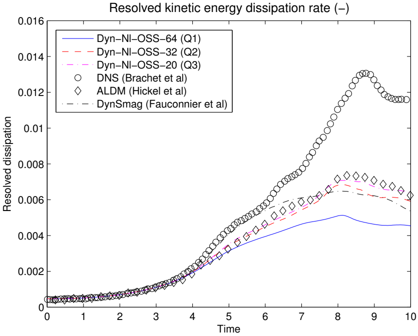

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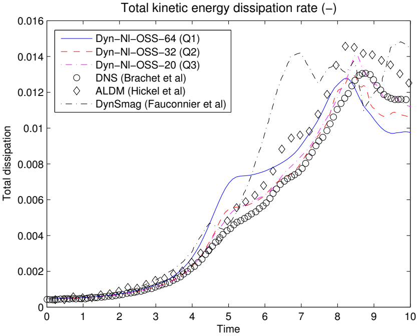


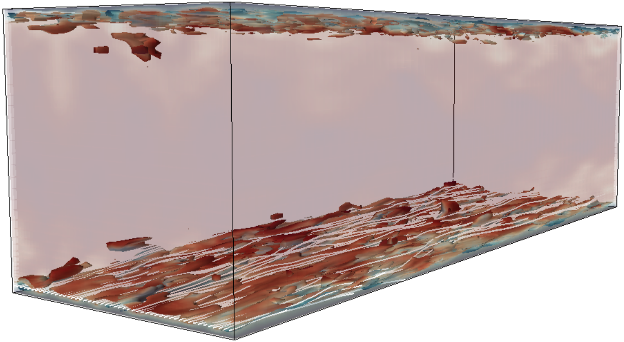
Figure : Total

- 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: $32^3 - Q1$.



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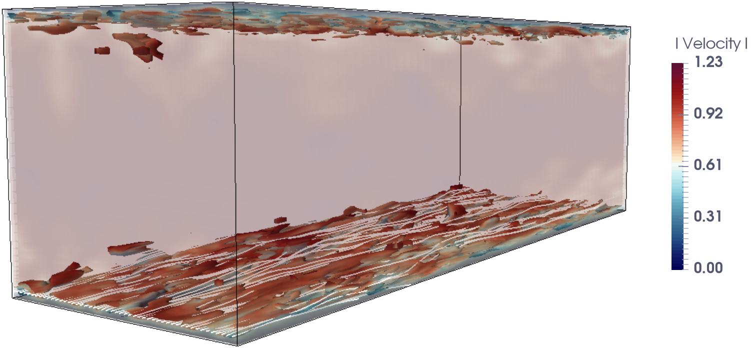
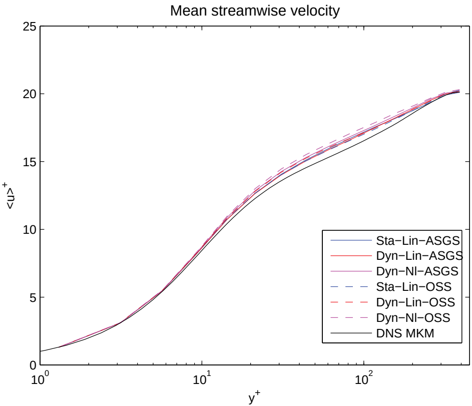


TCF Turbulent Channel Flow

Mean streamwise velocity (models):



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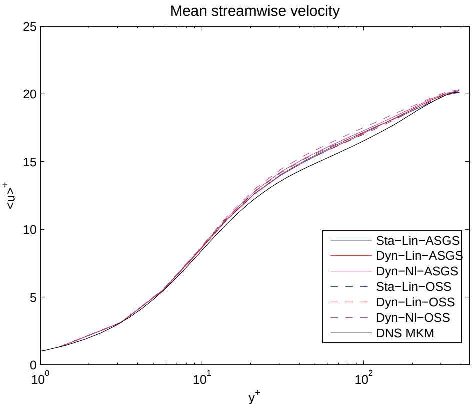

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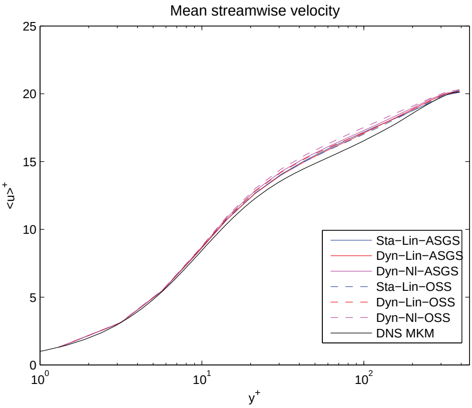

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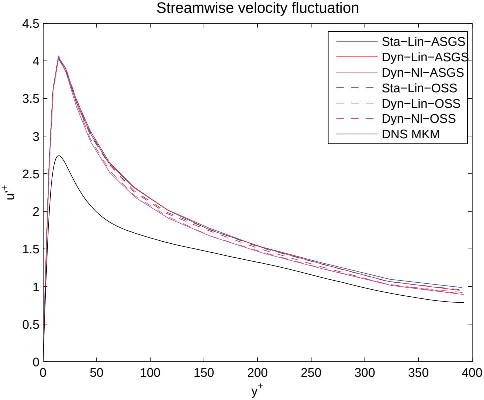

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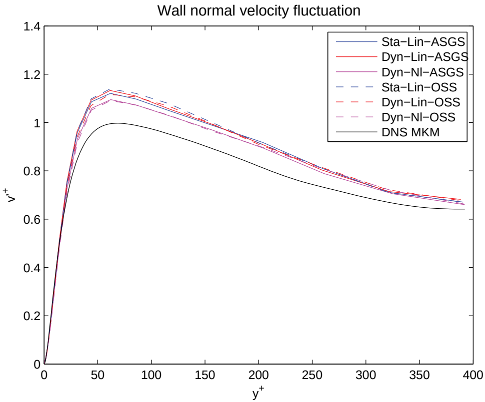

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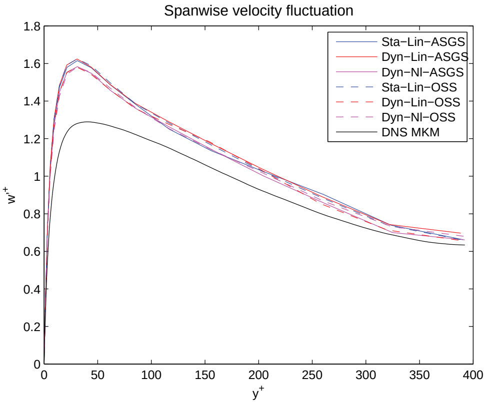

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RB-VMS Conclusions

- VMS formulations of NS equations can be used for the numerical simulation of turbulent flows.

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  seem to be important to simulate turbulent flows.
- Among them dynamic and orthogonal subscales (linear or nonlinear) are the most effective.
- The skewsymmetric formulation is important to keep stability.

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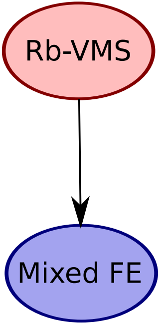
- **Desired:**
  - OSS with implicit projections.

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



Motivation

Step by step...

- Residual-based VMS as LES models.
- Mixed FE formulations LES.
- High-order FE methods.
- High-order time integration schemes.
- Adaptive time stepping techniques.
- Velocity-pressure segregation.
- Scalable solvers.
- Application.

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

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

Term-by-term OSS

FEM equations

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

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Term-by-term OSS

Term-by-term OSS (Codina 2008)

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

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

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

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

Term-by-term OSS

Term-by-term OSS (Codina 2008)

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

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

$$
\begin{aligned}
\boldsymbol{\eta}_h &:= \mathcal{P}_h(\mathbf{a} \cdot \nabla \mathbf{u}_h) \\
\boldsymbol{\xi}_h &:= \mathcal{P}_h(\nabla p_h) \\
\mathcal{P}_h(\nabla \cdot \mathbf{u}_h) &\approx 0
\end{aligned}
$$

Matricial form

- ASGS:

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

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

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Index-2 DAE!!!

Block-recursive preconditioning

General case:

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

Block-recursive preconditioning

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

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Block-recursive preconditioning

General case:

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

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

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

Block-recursive preconditioning

General case:

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

- Outer block matrix:

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

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

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

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

Block-recursive preconditioning

General case:

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

- Inner block matrix:

$$\widetilde{K}_\tau = \begin{bmatrix} K_\tau & G \\ D & L_\tau \end{bmatrix} = \begin{bmatrix} I & 0 \\ DK_\tau{}^{-1} & I \end{bmatrix} \begin{bmatrix} K_\tau & G \\ 0 & S \end{bmatrix},$$

Block-recursive preconditioning

General case:

$$
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$$

$$
S = L_\tau - DK_\tau G,
$$

Block-recursive preconditioning

General case:

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

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

$$S = L_\tau - DK_\tau G,$$

$$P_U(\widetilde{K}_\tau) = \left[\begin{array}{cc} K_\tau & G \\ 0 & S \end{array}\right]^{-1} = \left[\begin{array}{cc} K_\tau^{-1} & -K_\tau^{-1}GS^{-1} \\ 0 & S^{-1} \end{array}\right],$$

Block-recursive preconditioning

General case:

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

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$$S = L_\tau - DK_\tau G,$$

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

$$\widetilde{S}^{-1} \approx L_p^{-1} \quad (\delta t L_p^{-1}).$$

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)

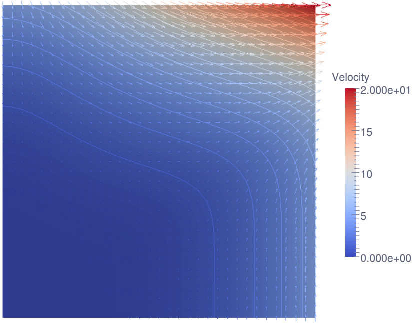
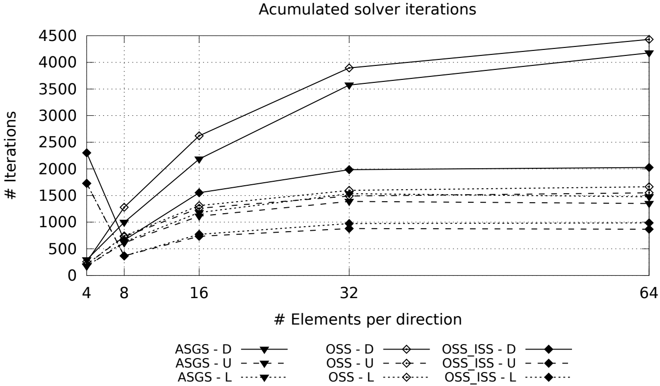


Figure : Velocity field

Colliding flow

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



Colliding flow

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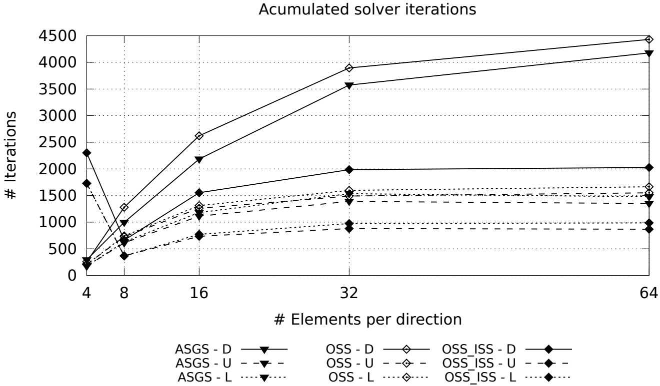
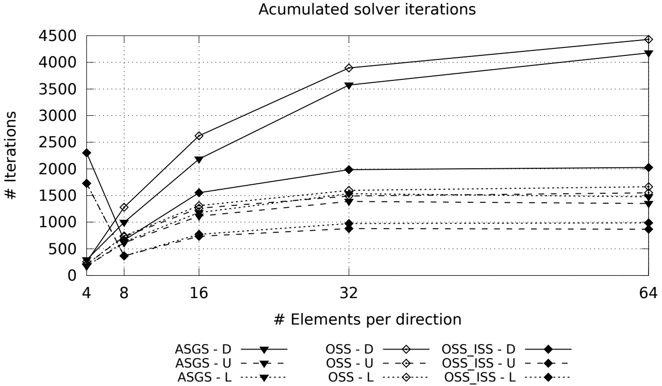


- $P_U(\widetilde{K}_\tau)$ and $P_L(\widetilde{K}_\tau)$ scalable block-preconditioners for all methods.

Colliding flow

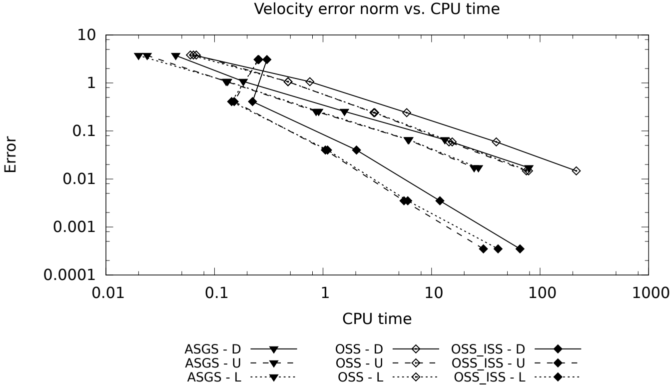
Acumulated solver iterations: (using $P_U(\widetilde{A})$)



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

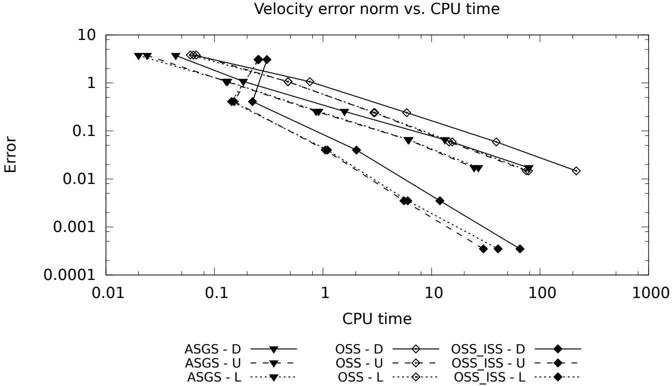
Colliding flow

Efficiency: Velocity



Colliding flow

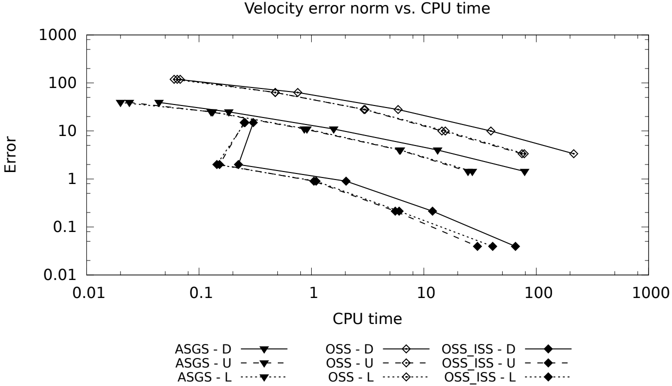
Efficiency: Velocity



- OSS-ISS the most efficient method.

Colliding flow

Efficiency: Pressure



- Also for pressures.

TGV Taylor-Green Vortex flow

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

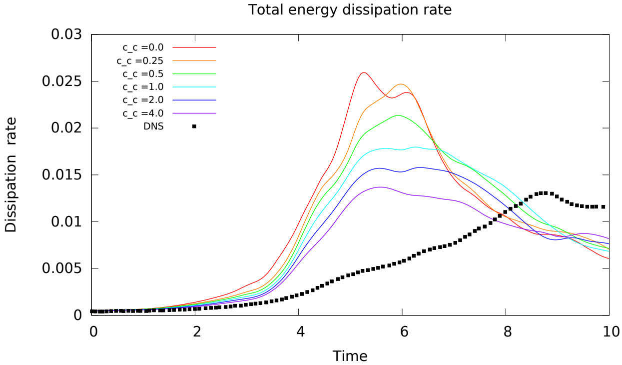


Figure : Total energy dissipation rate.

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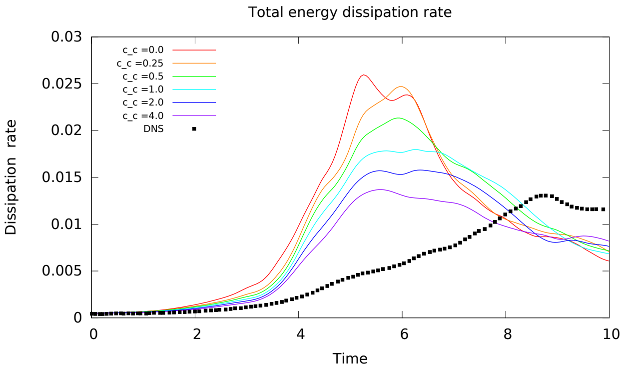

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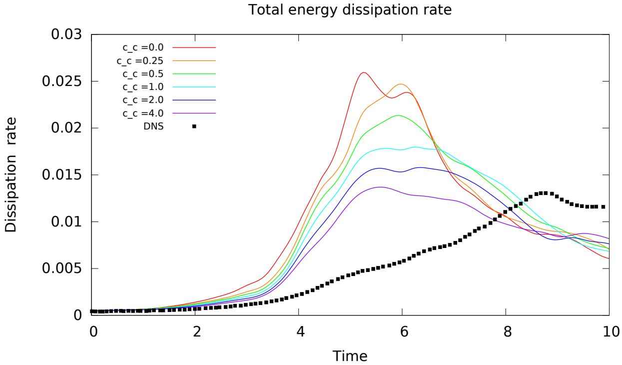


Figure : Total energy dissipation rate.

- 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)

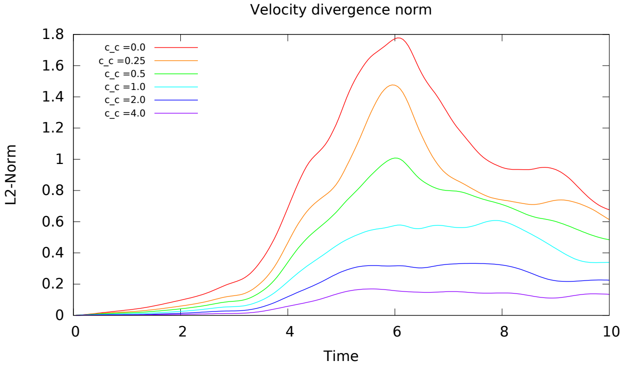


Figure : $\|\nabla \cdot \mathbf{u}\|$.

TGV Taylor-Green Vortex flow

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

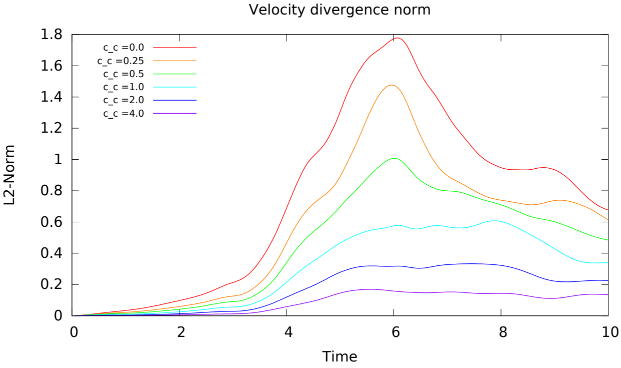


Figure : $\|\nabla \cdot \mathbf{u}\|$.

- Incompressibility constraint not satisfied.

TGV Taylor-Green Vortex flow

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

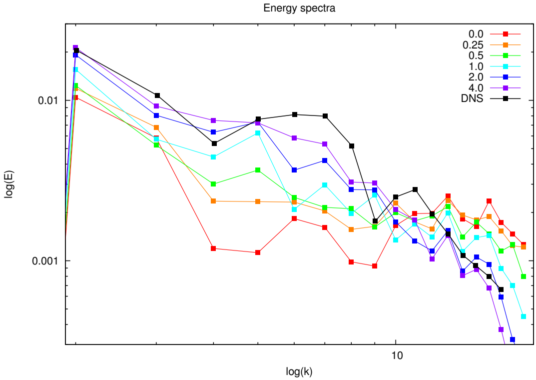


Figure : Energy spectra.

TGV Taylor-Green Vortex flow

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

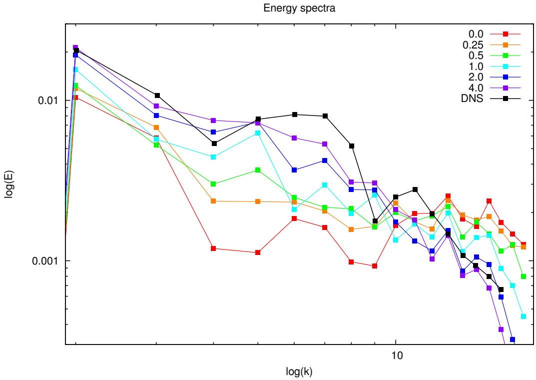


Figure : Energy spectra.

- Overdissipation 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)

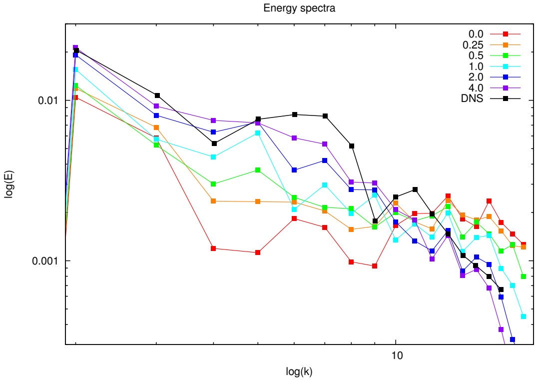
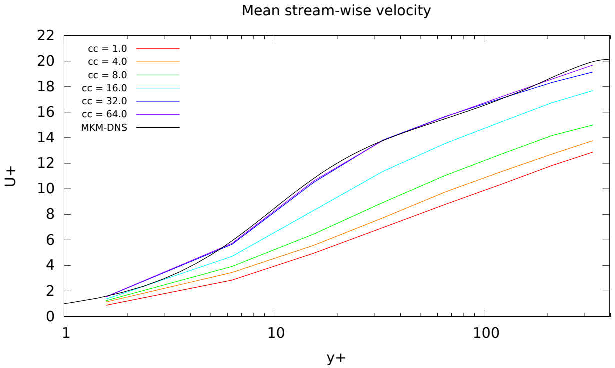


Figure : Energy spectra.

- Overdissipation on the large scales when $c_c \to 0$.
- Infradissipation on the small scales when $c_c \to 0$.

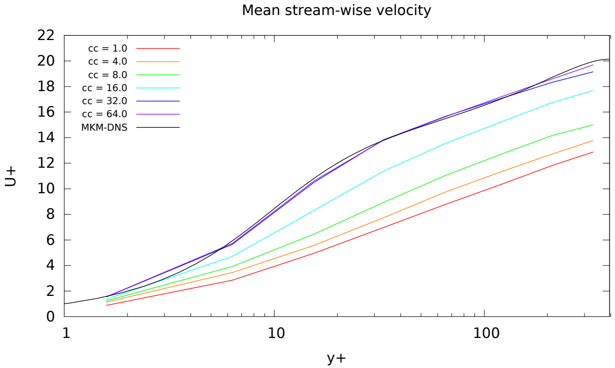
TCF Turbulent Channel Flow at $Re_\tau = 395$

Mean streamwise velocity (models):



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

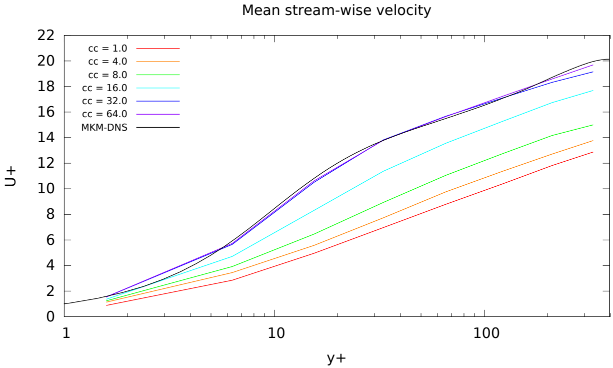
Mean streamwise velocity (models):



- Same behaviour observed for TCF test.

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

Mean streamwise velocity (models):



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

Mixed FE VMS Conclusions

- Scalable recursive block-preconditioners.

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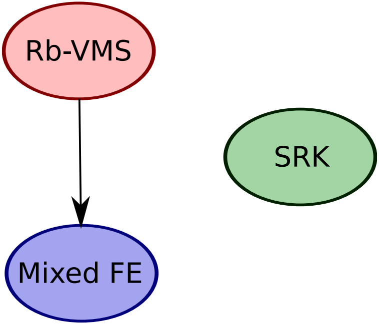
Mixed FE VMS Conclusions

- Scalable recursive block-preconditioners.
- Sligthly better results for equal-order interpolations.
- Mixed FE OSS the most efficient method.
- Mixed FE OSS keeps the index-2 DAE nature in time of the problem.

Mixed FE VMS Limitations

- Strong dependency on the grad-div stabilization term.

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 LES.
- High-order FE methods.
- High-order time integration schemes.
- Adaptive time stepping techniques.
- Velocity-pressure segregation.
- Scalable solvers.
- Application.

Incomp. Navier Stokes equations

Find $\mathbf{u}$ and p defined in Ω

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

with appropriate boundary conditions on Γ.

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- Laminar case (no convection stabilization required).

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- Saddle-point structure (stability via mixed FE).

Incomp. Navier Stokes equations

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\end{aligned}
$$

with appropriate boundary conditions on Γ.

- Laminar case (no convection stabilization required).
- Saddle-point structure (stability via mixed FE).
- Index-2 DAE system (time integration with care)

Incomp. Navier Stokes equations

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

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

with appropriate boundary conditions on Γ.

- Laminar case (no convection stabilization required).
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Segregated RK methods

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

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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 [Colomés & SB'15]

Segregated RK methods

The idea:

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

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

Segregated RK methods

The idea:

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

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

Segregated RK methods

The idea:

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

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

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)...

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

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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 $G(DM^{-1}G)^{-1}\left(DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbb{G}}\right)$ 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 $G(DM^{-1}G)^{-1}\left(DM^{-1}(K + C(\mathbf{U})\mathbf{U} - \mathbf{F}) + \dot{\mathbb{G}}\right)$ 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

It leads to the time-discrete algorithm:

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

After re-ordering (pressure again):

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

$$-DM^{-1} G(\mathbf{P}_i) = DM^{-1}((K + C(\mathbf{U}_i))\mathbf{U}_i - \mathbf{F}(t_i)) + \dot{\mathbb{G}}(t_i)$$

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$$-DM^{-1}G(\mathbf{P}_i) = DM^{-1}((K + C(\mathbf{U}_i))\mathbf{U}_i - \mathbf{F}(t_i)) + \dot{\mathbb{G}}(t_i)$$

- Viscous / convective can be treated implicitly / explicitly

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

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

Segregated RK methods

It leads to the time-discrete algorithm:

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

After re-ordering (pressure again):

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

$$-DM^{-1}G(\mathbf{P}_i) = DM^{-1}((K + C(\mathbf{U}_i))\mathbf{U}_i - \mathbf{F}(t_i)) + \dot{\mathbb{G}}(t_i)$$

Features:

1. Segregation at the time integration level (no additional splitting)
2. High order achievable (the one of the ODE RK integration)
3. Implicit LES turbulent model (stabilization terms)

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:

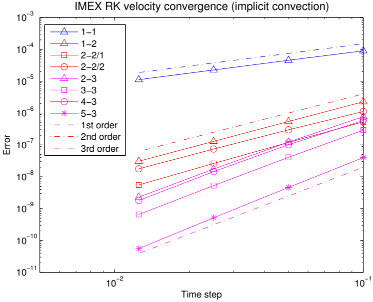
- Analytical solution:

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

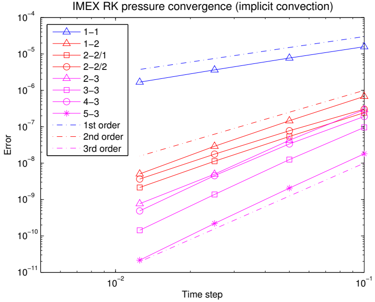
- $Re = 1/10/100$.
- Different IMEX Butcher tableaus with 1st, 2nd and 3rd order.

Manufactured analytical solution

Implicit convection:



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



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

Figure : Fully implicit SRK.

Manufactured analytical solution

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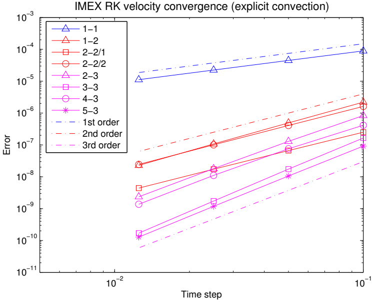

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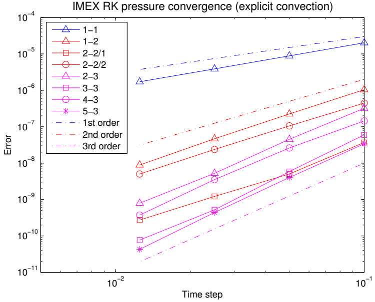


(b) Pressure convergence, $\nu = 0.01$

Figure : SRK convergence with convection integrated explicitly and diffusion integrated implicitly.

2D Laminar flow around a cylinder

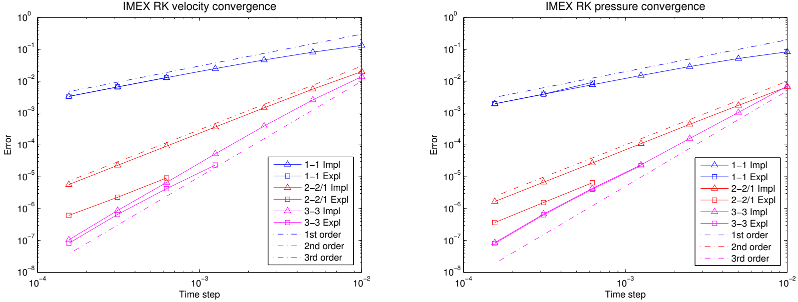
Problem setting:

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

Figure : Vorticity field at $t = 8.0$.

2D Laminar flow around a cylinder

Implicit convection:



(a) Velocity convergence

(b) Pressure convergence

Figure : 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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- No additional splitting needed
- Equal order in time (pressure error not spoiled)

Segregated Runge-Kutta Limitations

- Only for index-2 DAE.

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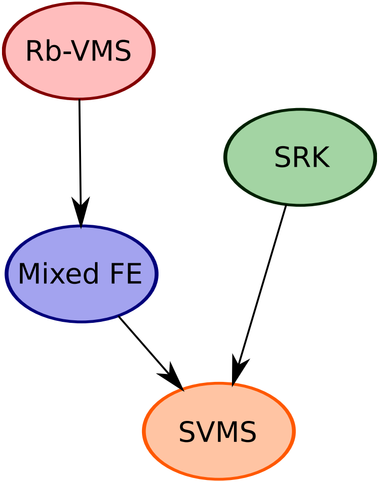
- Only for index-2 DAE.
- Not applicable for equal-order stabilization methods.


Rb-VMS
SRK
Mixed FE
SVMS

Motivation

Step by step...

- Residual-based VMS as LES models.
- Mixed FE formulations LES.
- High-order FE methods.
- High-order time integration schemes.
- Adaptive time stepping techniques.
- Velocity-pressure segregation.
- Scalable solvers.
- Application.

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.

Looking backward...

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

Now, we can use Segregated RK methods for ILES of turbulent flows

Formulation

OSS-ISS: Semi-discrete form

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

Formulation

OSS-ISS: Semi-discrete form

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

Formulation

OSS-ISS:

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

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&-DM^{-1}G\mathbf{P} = DM^{-1}(K + C(\mathbf{U})\mathbf{U} + B_\tau \boldsymbol{\Upsilon} - \mathbf{F}_u).
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$$

Formulation

OSS-ISS:

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)...

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

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Final discrete problem

At each stage of the Runge-Kutta scheme: (explicit convection version)

$$
\begin{aligned}
&\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), \\
&M_\tau \boldsymbol{\Upsilon}_i - B_\tau^T \mathbf{U}_i = \mathbf{0}, \\
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\end{aligned}
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At each stage of the Runge-Kutta scheme: (explicit convection version)

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

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- Mass-type matrix for the projection equation.

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At each stage of the Runge-Kutta scheme: (explicit convection version)

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

- Implicit viscous: Balancing domain decomposition (BDDC) for $M + \delta t K$
- Coercive operator, algorithmically scalable algorithm, freezed as mesh fixed

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- Coercive operator, algorithmically scalable algorithm, freezed as mesh fixed

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

- Spectrally equivalent to standard Laplacian L
- Written as

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

- Optimal + scalable method (BDDC)

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

Monolithc vs Segregated Runge-Kutta:

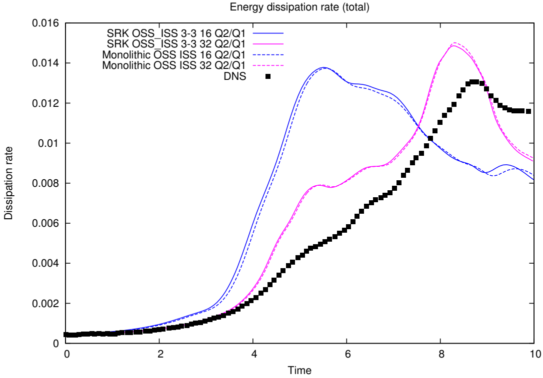

Figure : Total energy dissipation rate

TGV Taylor-Green Vortex flow

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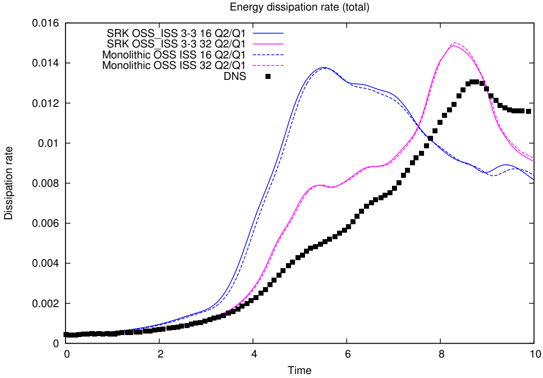

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- Almost Identical results obtained with Crank-Nicolson.

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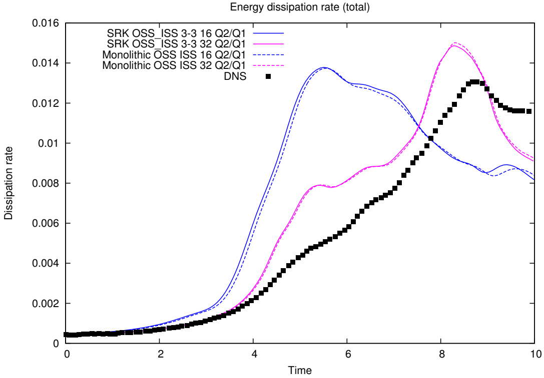

Figure : Total energy dissipation rate

- Almost Identical results obtained with Crank-Nicolson.
- IMEX and adaptive time stepping.

TGV Taylor-Green Vortex flow

Weak scalability:

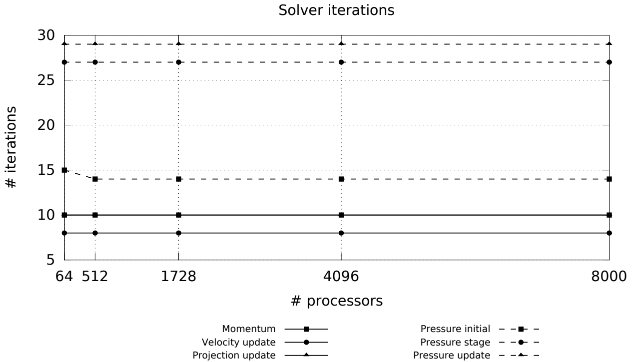

Figure : Solver iterations

TGV Taylor-Green Vortex flow

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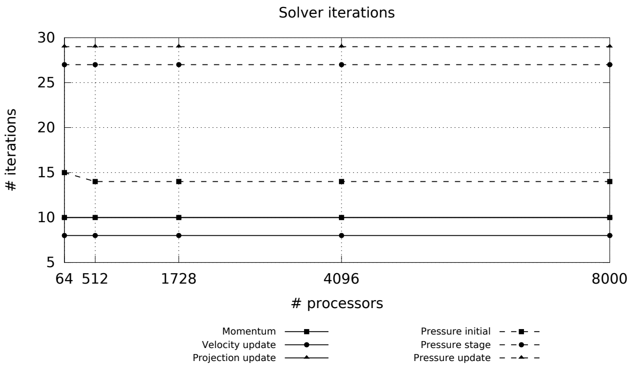

Figure : Solver iterations

- Perfect scalability in terms of solver iterations.

TGV Taylor-Green Vortex flow

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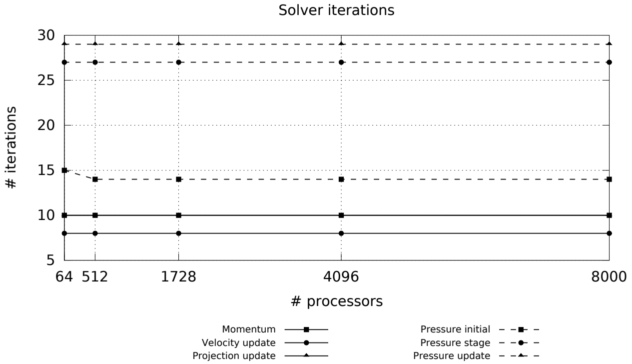

Figure : Solver iterations

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

TGV Taylor-Green Vortex flow

Weak scalability:

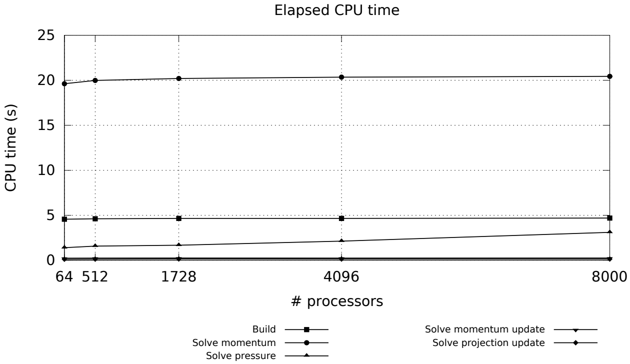

Figure : CPU time

TGV Taylor-Green Vortex flow

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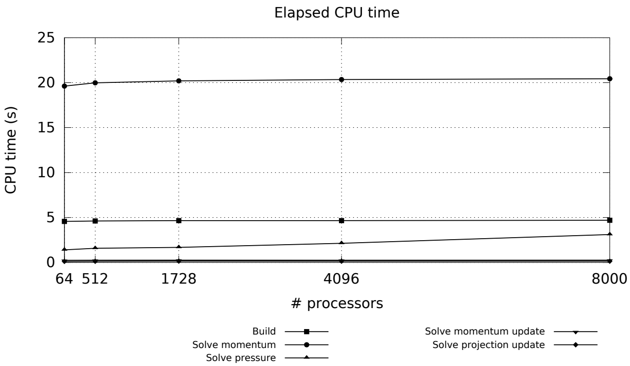

Figure : CPU time

- Perfect scalability in CPU time consumed.

TGV Taylor-Green Vortex flow

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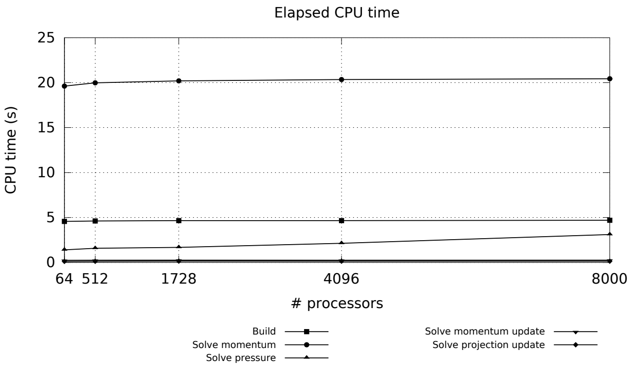
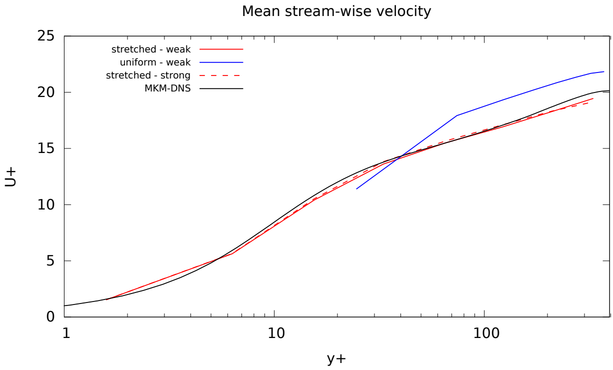


Figure : CPU time

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

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

Weak boundary conditions:



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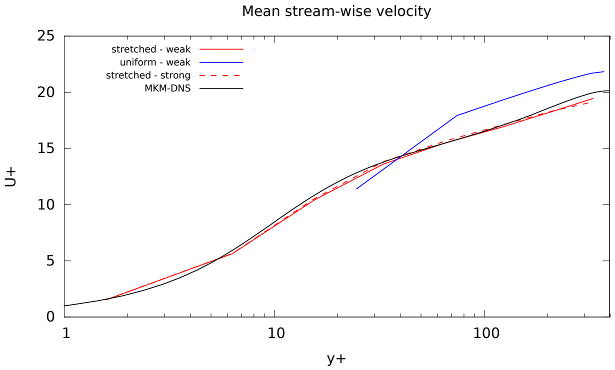

- We recover the strong BC results when stretched mesh is used.

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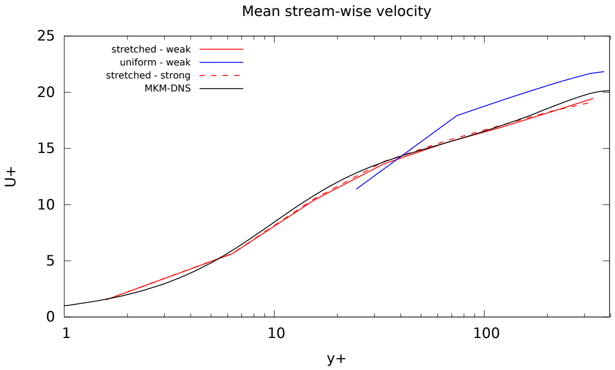

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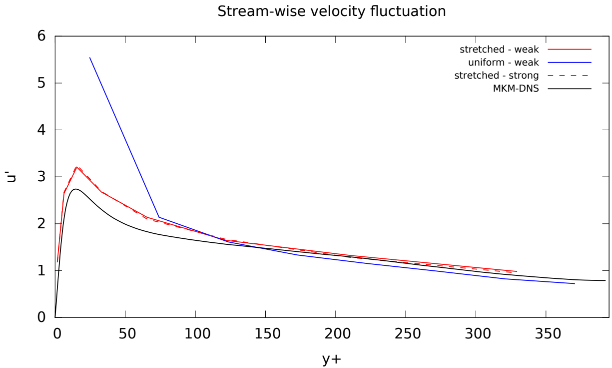

- We recover the strong BC results when stretched mesh is used.
- Acceptable results for uniform meshes.

Turbulent flow around a NACA profile

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

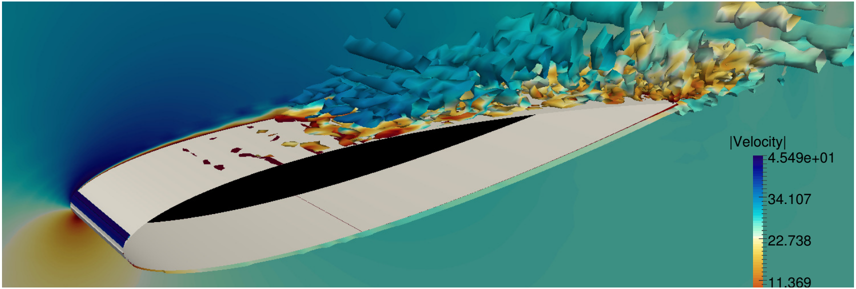

Figure : Q-criterion isosurfaces for a fully developed flow

Segregated VMS Conclusions

- Implicit LES for mixed FEs + SPS 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
- Weak boundary conditions on all components

Final Conclusions

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

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Final Conclusions

- Demonstrated suitability of Residual-based VMS methods as LES models.
- Defined Mixed FE methods with convection stabilization.
- Developed novel Segregated Runge-Kutta methods.
- Highly-scalable FE solvers for the simulation of turbulent incompressible flows .

Thank you!