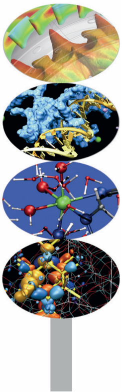
Cineca TRAINING High Performance Computing 2016

# HPC enabling of OpenFOAM® for CFD applications



## Implementation and evaluation of DES models in OpenFOAM

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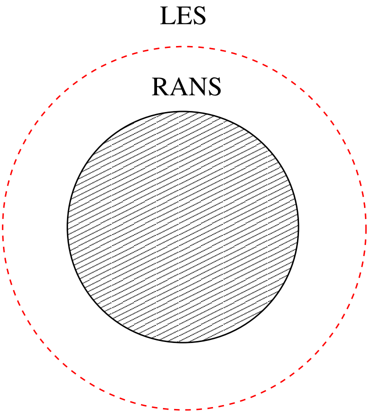
  - a quadratic constitutive relation (QCR) for Reynolds Stresses introduced in [Spalart, 2000] for RANS equations is here evaluated in SA–DES environment
- Perform an extensive DES study of the widespread analyzed flow past a circular cylinder in sub–critical regime at $\mathrm{Re} = 3900$

# DES overview






DES schematic representation

- DES technique was developed by Spalart et al., [Spalart et al., 1997] on the SA model
  - It is a non–zonal RANS/LES approach;
  - Transition from RANS to LES (for DES–97) is governed by minimum wall distance and grid size $\tilde{d} = \min(d, C_{DES}\Delta)$.
- DES–97 put in evidence some practical issues (GIS, MSD and log–layer mismatch). Fixed introducing DDES/IDDES.
- Recently DES based on other turbulence models have been introduced, *i.e.* $k$–$\omega$, ...
  - a length scale based on flow properties is used;
  - transport equation based $k$–SGS are solved (more physical than $\tilde{\nu}$);

# SA–DES/NLDES equations



$$\nabla \cdot \mathbf{u} = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\frac{1}{\rho}\nabla p + \nabla \cdot (2\nu \mathbf{D}) + \nabla \cdot \mathbf{B},$$

$$\frac{\partial \tilde{\nu}}{\partial t} + \nabla \cdot (\mathbf{u}\tilde{\nu}) = c_{b1}\tilde{S}\tilde{\nu} + \frac{c_{b2}}{\sigma}\nabla\tilde{\nu} \cdot \nabla\tilde{\nu} + \frac{1}{\sigma}\nabla \cdot ((\nu + \tilde{\nu})\nabla\tilde{\nu}) - c_{w1} f_w \left(\frac{\tilde{\nu}}{\tilde{d}}\right)^2$$

where:

$$\mathbf{B} = \mathbf{R} - c_{r1}\left(\mathbf{Q} \cdot \mathbf{R} - \mathbf{R} \cdot \mathbf{Q}\right),$$

$$\mathbf{R} = -\frac{2}{3}k\mathbf{I} + 2\nu_t \mathbf{D}, \quad \mathbf{Q} = 2\mathbf{\Omega}/\sqrt{\nabla\mathbf{u} : \nabla\mathbf{u}}\ ,$$

$$\mathbf{D} = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right), \quad \mathbf{\Omega} = \frac{1}{2}\left(\nabla\mathbf{u} - \nabla\mathbf{u}^T\right), \quad S = \sqrt{2\mathbf{\Omega} : \mathbf{\Omega}}\ ,$$

$$\tilde{S} = S + \frac{\tilde{\nu}}{k^2 d^2} f_{v2}, \quad \nu_t = f_{v1}\tilde{\nu}, \quad \tilde{d} = \min\left(d, C_{DES}\Delta\right).$$

# SA–DES/NLDES equations

- $\mathbf{B} = \mathbf{R} - c_{r1} \left( \mathbf{Q} \cdot \mathbf{R} - \mathbf{R} \cdot \mathbf{Q} \right)$
  - it was introduced in [Spalart, 2000] for RANS equations coupled with the one–equation Spalart–Allmaras turbulence model and it allows the prediction of secondary flows
  - it is related related to the proposal of [Wilcox and Rubesin, 1980]
  - this quadratic constitutive relation is considered preliminar in the sense it uses only one of the many possible combinations of strain rate and rotation tensor
  - $c_{r1} = 0.3$ was obtained in simple boundary layer flows requiring a fair level of anistropy $\overline{u'u'} > \overline{w'w'} > \overline{v'v'}$
  - it is turbulence model independent
- the closure functions and constants of the turbulence/SGS model are standard

# $\overline{v^2}$–$f$ DES equations

$$\frac{\partial k}{\partial t} + \boldsymbol{\nabla}\cdot(\mathbf{u}k) = \mathbb{P} - \epsilon_{DES} + \boldsymbol{\nabla}\cdot\left[(\nu+\nu_t)\,\boldsymbol{\nabla}k\right],$$

$$\frac{\partial \epsilon}{\partial t} + \boldsymbol{\nabla}\cdot(\mathbf{u}\epsilon) = \frac{c_{\epsilon 1}\mathbb{P} - c_{\epsilon 2}\epsilon}{T_{DES}} - \epsilon_{DES} + \boldsymbol{\nabla}\cdot\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\boldsymbol{\nabla}\epsilon\right],$$

$$\frac{\partial \overline{v^2}}{\partial t} + \boldsymbol{\nabla}\cdot\left(\mathbf{u}\overline{v^2}\right) = kf_{DES} - 6\frac{\overline{v^2}}{k}\epsilon_{DES} + \boldsymbol{\nabla}\cdot\left[(\nu+\nu_t)\,\boldsymbol{\nabla}\overline{v^2}\right],$$

$$c_L^2 L_{DES}^2 \boldsymbol{\nabla}^2 f - f = \frac{1}{T_{DES}}\left[(c_1 - 6)\frac{\overline{v^2}}{k} - \frac{2}{3}(c_1 - 1)\right] - c_2\frac{\mathbb{P}}{k}$$

- Eddy–viscosity is evaluated as: $\nu_t = c_\mu \overline{v^2}\, T_{DES}$
- $\overline{v^2}$–$f$ suppresses wall normal velocity fluctuations. This element improves the prediction of separation and reattachment
- in LES mode $\overline{v^2}$–$f$ DES model give a transport equation for $k$–SGS.
- $\overline{v^2}$–$f$ computes a length scale based on flow properties ($k$, $\epsilon$ and $\nu$)

# $\overline{v^2}$–$f$ DES equations

$L_{DES}$ and $T_{DES}$ are obtained using a RANS length scale: $k^{3/2}/\epsilon$ and LES length scale: $C_{DES}\Delta$.

$$L_{DES} = \begin{cases} L_{RANS} & k^{3/2}/\epsilon < C_{DES}\Delta \\ C_{DES}\Delta & k^{3/2}/\epsilon > C_{DES}\Delta \end{cases}$$

$$T_{DES} = \begin{cases} T_{RANS} & k^{3/2}/\epsilon < C_{DES}\Delta \\ C_{DES}\Delta/\sqrt{k} & k^{3/2}/\epsilon > C_{DES}\Delta \end{cases}$$

where:

$$T_{RANS} = \min\left[\max\left[\frac{k}{\epsilon}, c_T\left(\frac{\nu}{\epsilon}\right)^{1/2}\right], \frac{0.6k}{\sqrt{6}c_\mu\overline{v^2}\,|\mathbf{D}|}\right],$$

$$L_{RANS} = \max\left[\min\left[\frac{k^{3/2}}{\epsilon}, \frac{k^{3/2}}{\sqrt{6}c_\mu\overline{v^2}\,|\mathbf{D}|}\right], c_\eta\left(\frac{\nu^3}{\epsilon}\right)^{1/4}\right].$$

# $\overline{v^2}$–$f$ DES equations

$$\frac{\partial k}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{u}k) = \mathbb{P} - \epsilon_{DES} + \boldsymbol{\nabla} \cdot [(\nu + \nu_t)\, \boldsymbol{\nabla} k]$$

where: $\mathbb{P} = 2\nu_t \left|\mathbf{D}\right|^2$ and $\epsilon_{DES} = k^{3/2}/(C_{DES}\Delta)$.

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$$\frac{\partial k}{\partial t} + \nabla \cdot (\mathbf{u} k) = \mathbb{P} - \epsilon_{DES} + \nabla \cdot \left[ (\nu + \nu_t) \nabla k \right]$$

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$$\frac{\partial \epsilon}{\partial t} + \nabla \cdot (\mathbf{u}\epsilon) = \frac{c_{\epsilon 1}\mathbb{P} - c_{\epsilon 2}\epsilon}{T_{DES}} - \epsilon_{DES} + \nabla \cdot \left[ \left( \nu + \frac{\nu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right]$$

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where: $kf_{DES} = \min\left(kf, 5\frac{\overline{v^2}}{k}\epsilon_{DES} + \frac{2}{3}\mathbb{P}\right)$

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$$c_L^2 L_{DES}^2 \nabla^2 f - f = \frac{1}{T_{DES}}\left[(c_1 - 6)\frac{\overline{v^2}}{k} - \frac{2}{3}(c_1 - 1)\right] - c_2\frac{\mathbb{P}}{k}$$

# $\overline{v^2}$–$f$ DES equations

Constants and closure functions:

$$c_\mu = 0.22, \quad \sigma_\epsilon = 1.3, \quad c_{\epsilon 1} = 1.4\left(1 + 0.045\sqrt{k/\overline{v^2}}\right),$$
$$c_{\epsilon 2} = 1.9, \quad c_1 = 1.4, \quad c_2 = 0.3,$$
$$c_T = 6, \quad c_L = 0.23, \quad c_\eta = 70, \quad C_{DES} = 0.8.$$

- the model was introduced by [Jee and Shariff, 2014];
- constants (deriving from original RANS model) were modified and
  - in the limit of isotropic turbulence $\overline{v^2}$–$f$ reduces to sgs–$k$ LES
  - $\overline{v^2}$ is statistically $2/3\ k$ in the limit of isotropic turbulence (also $kf_{DES}$ was modified for this purpose)

# $\overline{v^2}$–$f$ DES boundary conditions



Table: Turbulent variables boundary conditions

| | $k$ | $\overline{v^2}$ | $\epsilon$ | $f$ |
|---|---|---|---|---|
| Initial Conditions | $10^{-3}u_\infty^2$ | $2/3 \cdot 10^{-3}u_\infty^2$ | $10^{-3}u_\infty^3/D$ | 0 |
| Wall boundary | 0 | 0 | $\nu\partial_n^2 k$ | 0 |
| Inlet boundary | 0 | 0 | $\partial_n\epsilon = 0$ | $\partial_n f = 0$ |
| Outlet boundary | $\partial_n k = 0$ | $\partial_n \overline{v^2} = 0$ | $\partial_n\epsilon = 0$ | $\partial_n f = 0$ |

[Jee and Shariff, 2014] proposed a Neumann type BC for $\epsilon$. In this work a Dirichlet BC for $\epsilon$ is used:

$$\epsilon_w = \nu\left(\frac{\partial^2 k}{\partial n^2}\right)_w \rightarrow \quad \epsilon_w = 2\nu k/y^2$$

# $\overline{v^2}$–$f$ DES boundary conditions

The wall boundary condition for $\epsilon$ was introduced by [Chien, 1982] starting from $\epsilon = \nu\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}}$. In particular close to the wall we have:

$$\begin{aligned} u &= a_0 + a_1 y + a_2 y^2 + \dots \\ v &= b_0 + b_1 y + b_2 y^2 + \dots \\ w &= c_0 + c_1 y + c_2 y^2 + \dots \end{aligned} \quad \Longrightarrow \left\{ \begin{array}{l} \partial/\partial y >> \partial/\partial x \simeq \partial/\partial z \\ u \simeq w >> v \\ \epsilon = \nu \overline{\left(\frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial y}\right)^2} \end{array} \right.$$

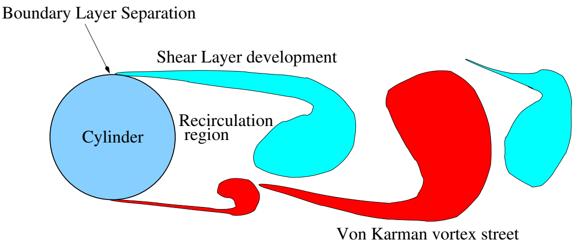
Thus is possible to estimate $k$ and $\epsilon$ in the wall region:

$$k = \frac{1}{2}\left(\overline{a_1^2} + \overline{c_1^2}\right) y^2 + \dots \quad \epsilon = \nu\left(\overline{a_1^2} + \overline{c_1^2}\right) + \dots$$

fixing $a_1 = c_1$, we obtain: $\epsilon_w = 2\nu k / y^2$.

- This Dirichlet wall condition for $\epsilon$ is equivalent to $\epsilon = \nu \partial_n^2 k|_w$.
- The condition is easy to be coded (second order space accuracy is guaranteed)

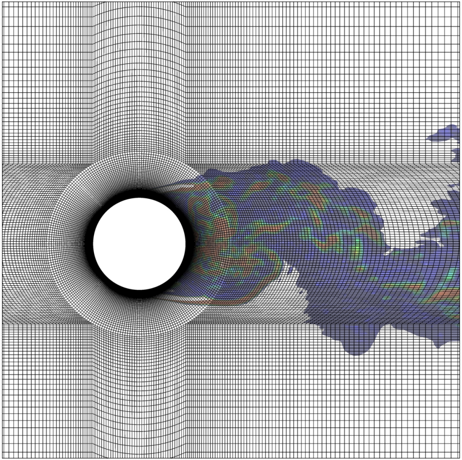
# Flow past a cylinder at $\mathrm{Re} = 3900$




- Laminar boundary layer
- Kelvin–Helmoltz instabilities before the turbulent region
- Von Karman vortex street in the wake region

We have computed with: SA–DES (97), SA–IDDES, NLDES, $\overline{v^2}$–$f$ DES

# Computational Grid (finest)



- Structured non–orthogonal grid
- Rectangular domain:
  - 40 D in the wake region
  - 20 D in transverse direction
  - $\pi$ D in span–wise direction
- First cell height: $2 \cdot 10^{-4} D$
- $N_z = 48$ cells (span–wise direction)
- No wall functions
- No perturbations added at the inlet
- $n_c = 3955200$ cells ($< 4 \cdot 10^6$)

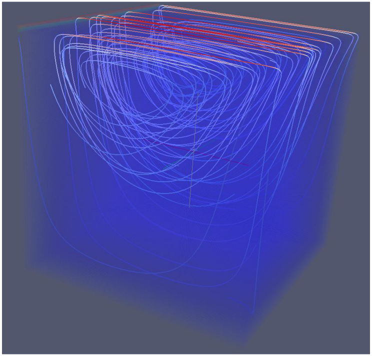
# Computational Grid

Table: Computational grids parameters

| | $n_c$ | $L_z$ | $N_z$ | $n_{c_{x,y}}$ | $\Delta z$ |
|---|---|---|---|---|---|
| G1 | 3955200 | $\pi D$ | 48 | 82400 | $6.54 \cdot 10^{-2}$ |
| G2 | 494400 | $\pi D$ | 24 | 20600 | $1.308 \cdot 10^{-1}$ |
| G3 | 659200 | $\pi D$ | 8 | 82400 | $3.92 \cdot 10^{-1}$ |
| G4 | $2.06 \cdot 10^6$ | $0.5D$ | 25 | 82400 | $2 \cdot 10^{-2}$ |
| G5 | 659200 | $0.5D$ | 8 | 82400 | $6.25 \cdot 10^{-2}$ |

- G1 is our finest grid
- G2 is the coarse version of G1 ($n_{c,G1}/n_{c,G2} = 8$)
- G3 is used to study the influence resolution in $z$–direction
- G4 and G5 are used to used the influence of domain size in span–wise direction
- G5 and G1 have very similar span–wise resolution

# Scalability

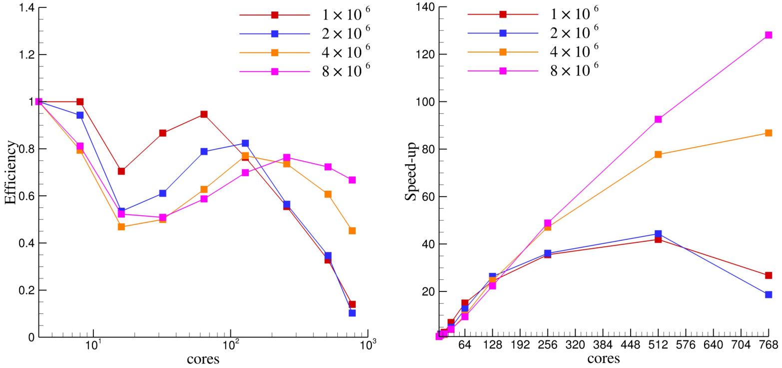


Streamlines, [Vratis Ltd, 2015]

- Cubic domain, $H = 1$, $\mathrm{Re} = 10$;
- `icoFoam` solver/Lid–driven cavity;
- Structured uniformly spaced grid;
- 40 time–steps without I/O as in [Culpo, 2011];
- $\Delta t = 10^{-4}$;
- Default linear–solvers:
  - PCG for $p$ with DIC preconditioner;
  - smoothSolver for $\mathbf{u}$ (`symGaussSeidel`);
  - PISO correctors: 2;
- Default tolerances: $p$: $10^{-6}$, $\mathbf{u}$: $10^{-5}$.

# Scalability (GALILEO)






(a) Efficiency (b) Speed-up

Figure: Effect of different total number of grid cells

# Scalability (GALILEO)


- 10 kCells/core are suitable for about $n_c = 4 \cdot 10^6$
- 384 CPU–cores on GALILEO@CINECA for G1 (about $2 \cdot 10^6$, finest)
- 192 CPU–cores on GALILEO@CINECA for G5 (about $2 \cdot 10^6$)
- small grids computations have been run on a small Linux–Cluster (AMD Opteron)

# Numerics

- `pisoFOAM` solver (2 PISO correctors)
- second order implicit time integration ($\Delta t = 10^{-3} D/u_\infty$)
- some div–terms:

```
div(phi,U)              Gauss linear;
div(phi,nuTilda)        Gauss limitedLinear 0.333;
div(nonlinearStress)    Gauss linear corrected;
```

```
div(phi,U)          Gauss Gamma 0.15;
div(phi,k)          Gauss Gamma 0.15;
div(phi,epsilon)    Gauss Gamma 0.15;
div(phi,v2)         Gauss Gamma 0.15;
```

- For all laplacians `Gauss linear corrected`
- Linear solvers:
  - PBiCG with DILU for $\mathbf{u}$, $\tilde{\nu}$, $\overline{v^2}$, $k$, $\epsilon$
  - PCG with DIC for $\mathrm{p}$ and $f$
- Tolerances: $10^{-5}$ for $\mathrm{p}$, $10^{-9}$ for $\mathbf{u}$, $\tilde{\nu}$, $\overline{v^2}$, $k$, $f$, $\epsilon$

# What is the correct solution ?

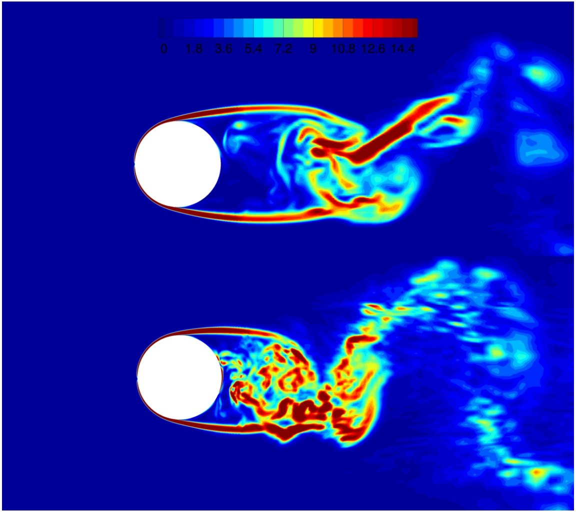



Figure: Instantaneous vorticity magnitude at $t = 10^3\ D/u_\infty$

# Flow past a cylinder at $\mathrm{Re} = 3900$



Critical issues (for CFD and experiments)

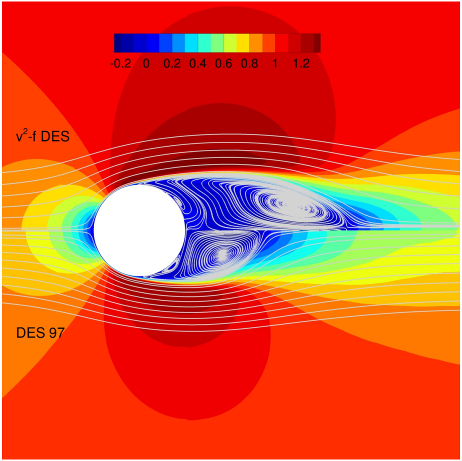



Figure: Mean streamwise velocity

- Shape recirculation region
- Size recirculation region
- Mean separation angle

| Exp. PIV | $\langle L_r/D \rangle$ |
|---|---|
| [Lourenco, 1993] | 1.18 |
| [Parnaudeau et al., 2008a] | 1.51 |

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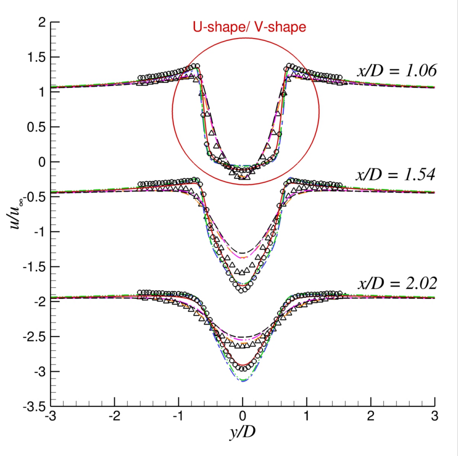


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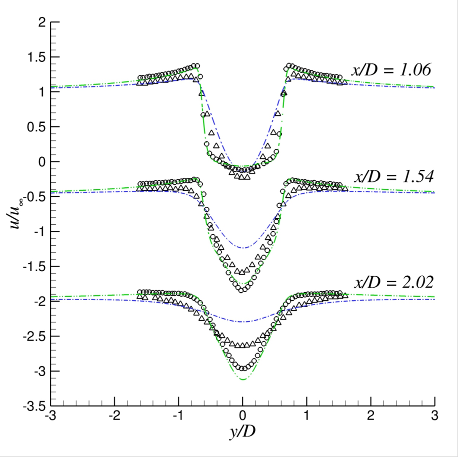


- - - $\overline{v^2}$–$f$ DES (G1)
-·-· $\overline{v^2}$–$f$ DES (G2)
△ Exp. [Lourenco, 1993]
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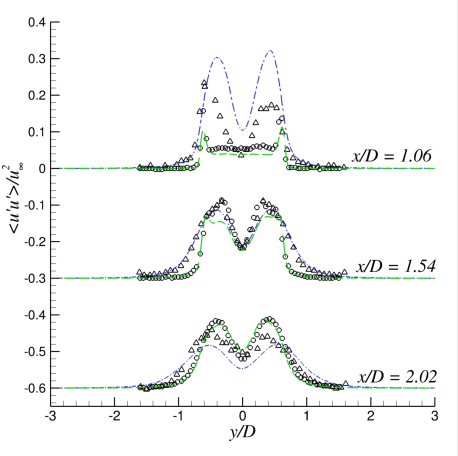


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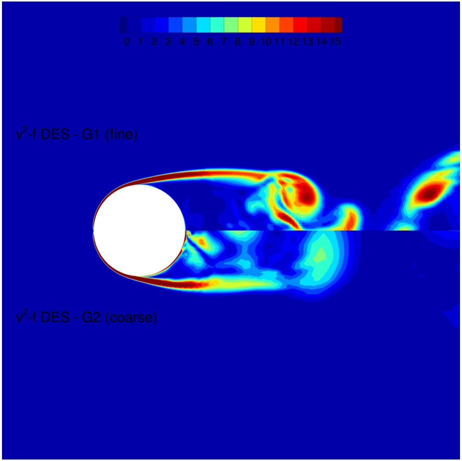
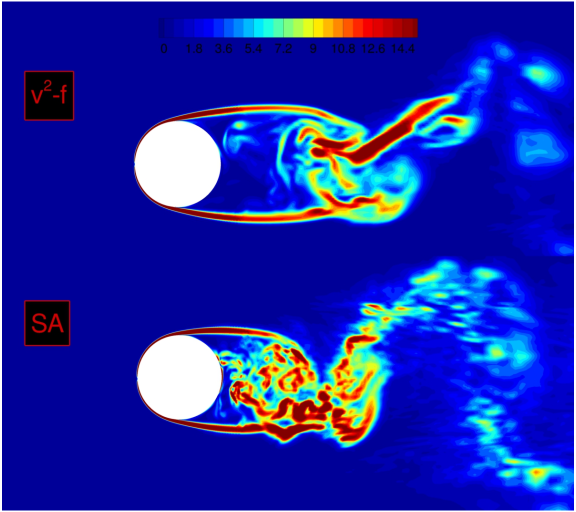



Figure: Instantaneous vorticity magnitude

- Profile shape is strictly to shear layer transition
  - early transition: V–shape
  - delay transition: U–shape
- Shear layer is longer in simulations with finer grid
- Coarse grid (G2) is inadequate to resolve shear layer hence we have early transition.
- Lourenco and Shih probably had early transition (agreeement with under–resolved simulations)

# What is the correct solution ?

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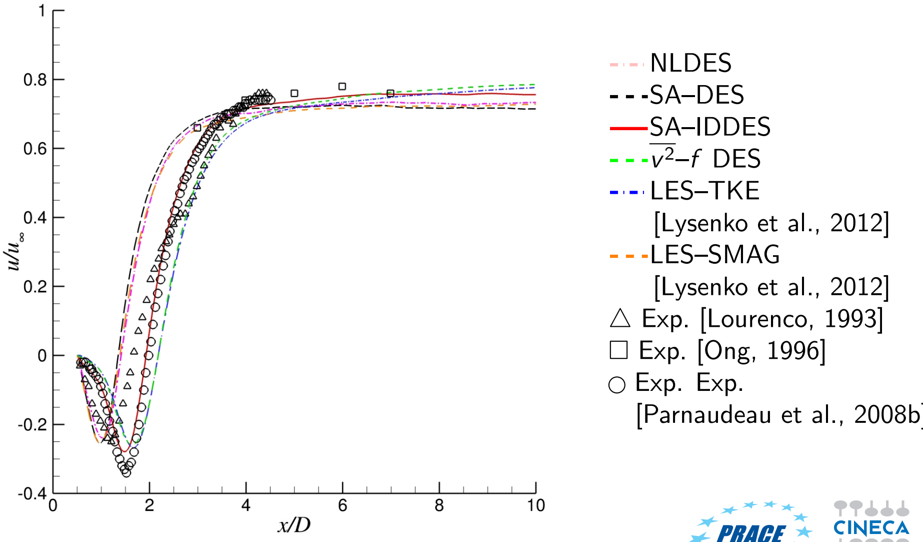
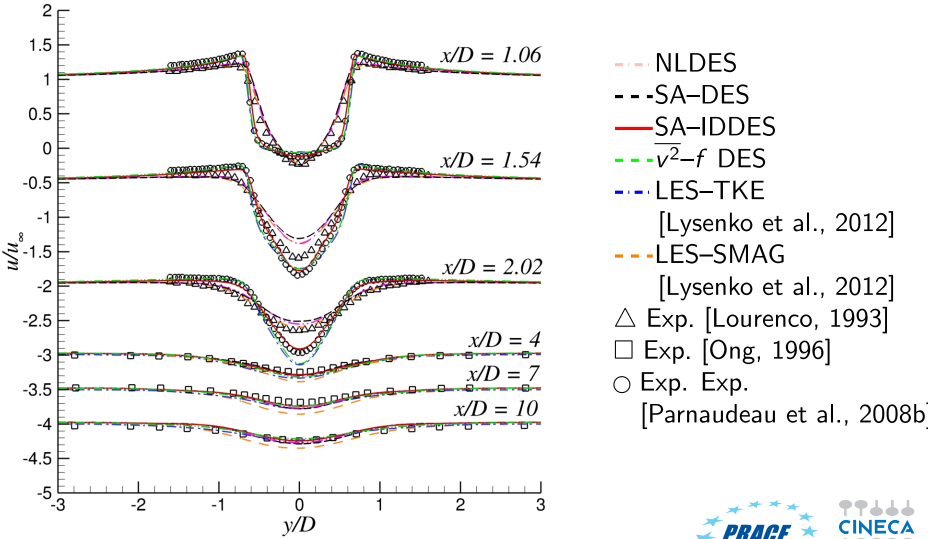
# Centerline streamwise velocity profile

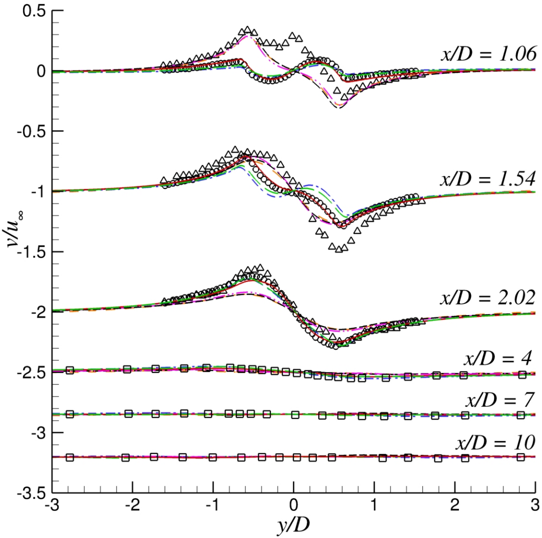


# Mean streamwise velocity profiles





# Mean transverse velocity profiles




- NLDES
- SA–DES
- SA–IDDES
- $\overline{v^2}$–$f$ DES
- LES–TKE [Lysenko et al., 2012]
- LES–SMAG [Lysenko et al., 2012]
- △ Exp. [Lourenco, 1993]
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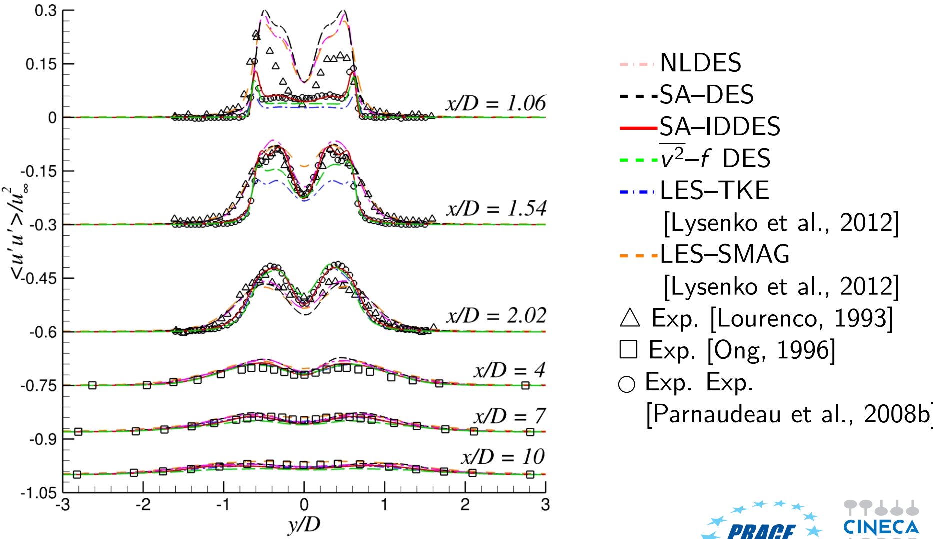
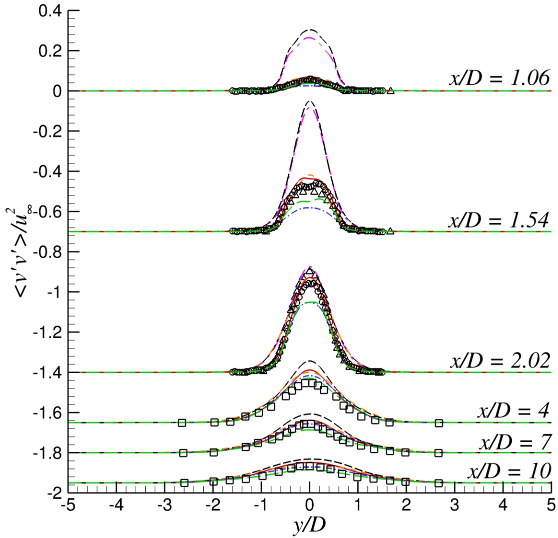
- ○ Exp. Exp. [Parnaudeau et al., 2008b]

# $\overline{u'u'}$ profiles





# $\overline{v'v'}$ profiles




- NLDES
- SA–DES
- SA–IDDES
- $\overline{v^2}$–$f$ DES
- LES–TKE [Lysenko et al., 2012]
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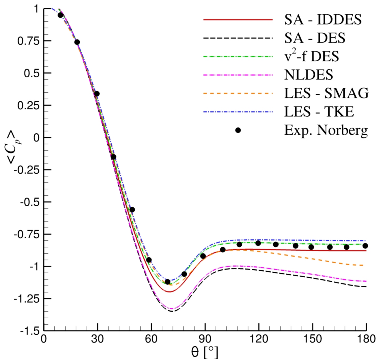
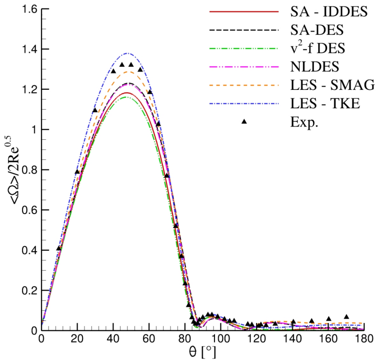
- ○ Exp. Exp. [Parnaudeau et al., 2008b]

# Wall data




(a) Pressure coefficient




(b) Wall vorticity magnitude

Figure: Mean wall data (G1 grid).

# Wall data

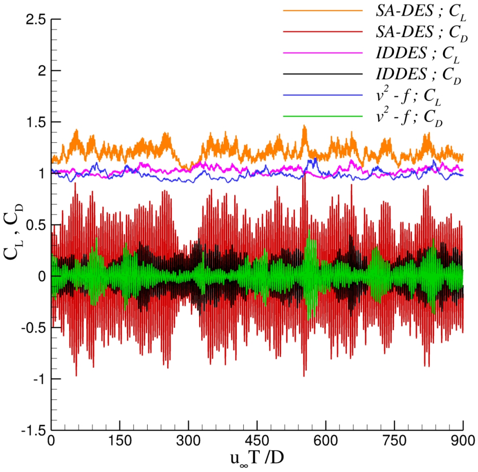



Figure: Force coefficients (G1 grid)

# Vortical structures

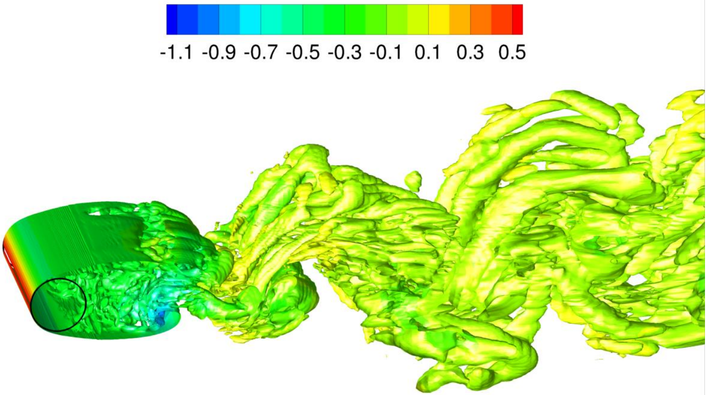



Figure: $Q = 0.5u_\infty^2/D^2$ at $T = 500D/u_\infty$. $\overline{v^2}$–$f$ DES

# Vortical structures

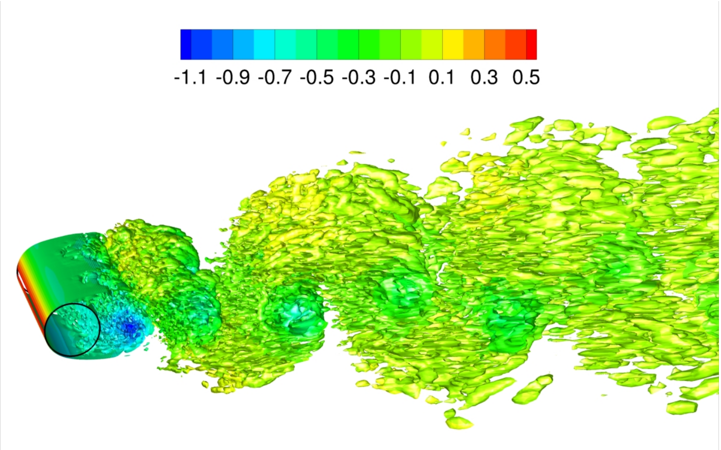



Figure: $Q = 0.5u_\infty^2/D^2$ at $T = 500D/u_\infty$. SA–DES

# Integrated flow quantities

| | $C_{L,rms}$ | $\langle C_D \rangle$ | St |
|---|---|---|---|
| [Lourenco, 1993] (Exp.) | – | 0.99 | – |
| [Parnaudeau et al., 2008a] (Exp.) | – | – | 0.21 |
| [Norberg, 1994] (Exp.) | – | 0.98 | – |
| Present SA–IDDES | 0.1458 | 1.0235 | 0.222 |
| Present NLDES | 0.3832 | 1.1751 | 0.217 |
| Present SA–DES | 0.4248 | 1.2025 | 0.215 |
| Present $\overline{v^2}$–$f$ DES | 0.1088 | 0.9857 | 0.214 |
| [Lysenko et al., 2012] (SMAG) | 0.444 | 1.18 | 0.19 |
| [Lysenko et al., 2012] (TKE) | 0.09 | 0.97 | 0.209 |
| [Jee and Shariff, 2014] ($\overline{v^2}$–$f$) | – | 1.0 | 0.214 |
| [Jee and Shariff, 2014] (SA–DDES) | – | 0.965 | 0.221 |
| [Parnaudeau et al., 2008a] (LES) | – | – | 0.21 |
| [Mittal and Moin, 1997] (LES) | – | 1.00 | 0.22 |
| [Kravchenko and Moin, 2000] (LES) | – | 1.04 | 0.21 |

# Integrated flow quantities



| | $-\langle C_{p,b} \rangle$ | $\langle L_r/D \rangle$ | $\langle \theta_{sep} \rangle$ |
|---|---|---|---|
| [Lourenco, 1993] (Exp.) | – | 1.18 | – |
| [Parnaudeau et al., 2008a] (Exp.) | – | 1.51 | – |
| [Norberg, 1994] (Exp.) | 0.84 | – | – |
| Present SA–IDDES | 0.878 | 1.427 | 87.0° |
| Present NLDES | 1.037 | 0.911 | 88.99° |
| Present SA–DES | 1.077 | 0.850 | 89.28° |
| Present $\overline{v^2}$–$f$ DES | 0.829 | 1.678 | 86.40° |
| [Lysenko et al., 2012] (SMAG) | 0.8 | 0.9 | 89° |
| [Lysenko et al., 2012] (TKE) | 0.91 | 1.67 | 88° |
| [Jee and Shariff, 2014] ($\overline{v^2}$–$f$) | 0.928 | 1.44 | 86.1° |
| [Jee and Shariff, 2014] (SA–DDES) | 0.969 | 1.37 | 88.3° |
| [Parnaudeau et al., 2008a] (LES) | – | 1.56 | – |
| [Mittal and Moin, 1997] (LES) | – | 1.588 | 87° |
| [Kravchenko and Moin, 2000] (LES) | 0.94 | 1.35 | 88° |

# 1D energy spectra



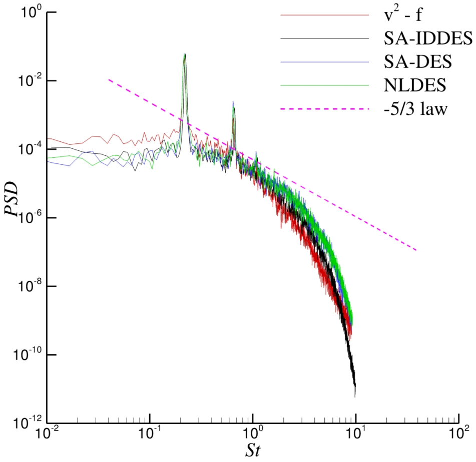



Figure: $x/D = 3.0$

# Conclusions

- Flow past a circular cylinder at $\mathrm{Re} = 3900$ has been carefully computed
- The DES capabilities of OpenFOAM were investigated
- $\overline{v^2}$–$f$ (with a Dirichlet condition for $\epsilon$) and NLDES have implemented and tested
  - $\overline{v^2}$–$f$ DES was able to obtain reliable and accurate results on this flow benchmark
  - limited benefits have been obtained from NLDES
- Future work will be devoted to test $k$–$\omega$–$\overline{v^2}$–$f$ (already implemented)

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