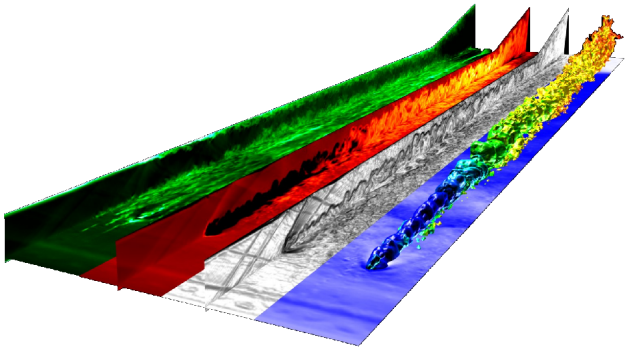
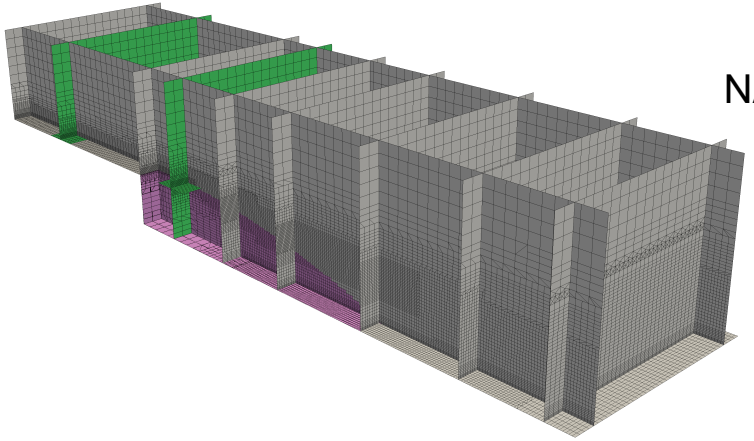
Grid-adaptation for large eddy simulations: a sequence of ideas over five years

Johan Larsson
Department of Mechanical Engineering
University of Maryland





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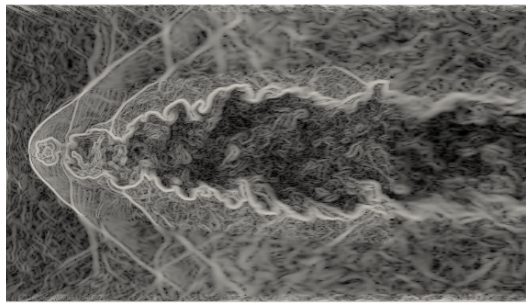

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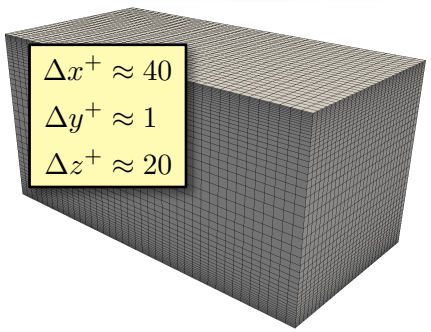
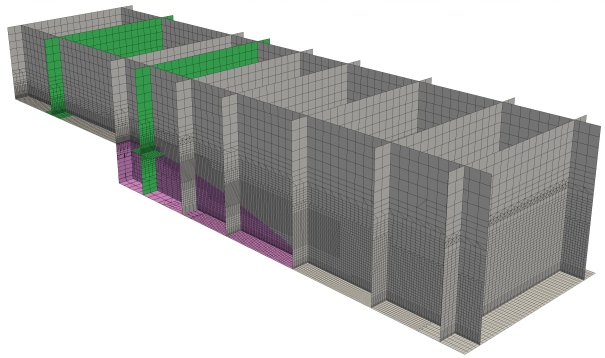
The grid is the single most important factor in LES!





Current practice in grid-generation: manual, based on user experience

- requires a lot of human time
- grids may be far from "optimal" – unnecessarily many cells in some regions
- not systematic – different users end up with different grids and possibly different results

A better approach – a grid-adaptation process:

1. easy-to-generate (coarse/uniform/isotropic) initial grid
2. obtain solution on this grid
3. using this solution, determine the "optimal" grid-spacing for the next grid
   a) where to refine in space?
   b) how to refine (isotropically or not)?
4. create the adapted grid
5. goto 2 (repeat until convergence)

the sole focus of this work

Why is adaptation for LES different from adaptation for RANS?

1. No affordable adjoint (at least not yet)

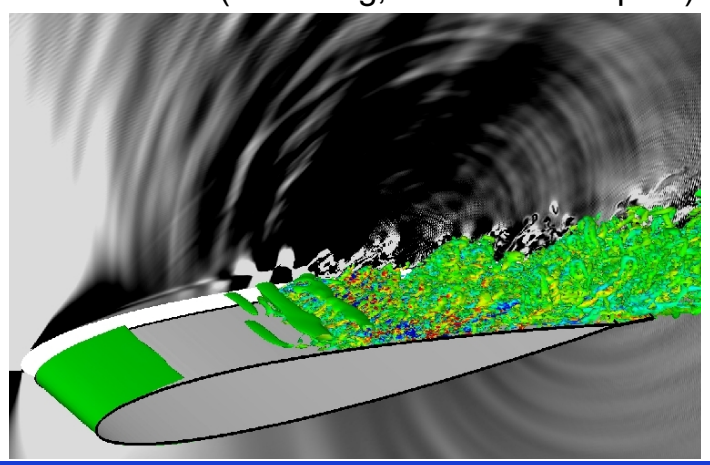
2. The grid controls both numerical and modeling error – and the latter can't be estimated by math alone

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \approx -2\nu_{\text{sgs}} S_{ij} + \tau_{kk}\,\delta_{ij}/3$$

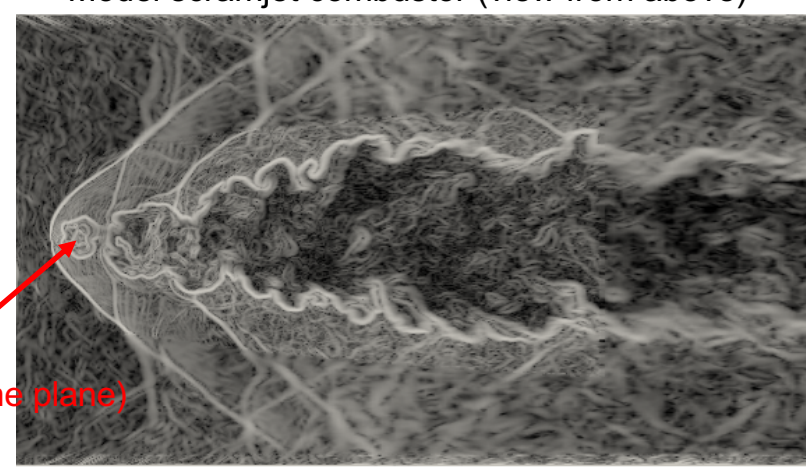
$$\nu_{\text{sgs}} = \begin{cases} C\Delta^2 |S| & \text{(Smagorinsky)} \\ C\Delta^2 \dfrac{\left(\mathcal{S}^d_{ij}\mathcal{S}^d_{ij}\right)^{3/2}}{\left(S_{ij}S_{ij}\right)^{5/2} + \left(\mathcal{S}^d_{ij}\mathcal{S}^d_{ij}\right)^{5/4}} & \text{(WALE)} \end{cases}$$

3. Stationary vs non-stationary grid?

Airfoil noise (Sandberg, Univ. Southampton)



Model scramjet combustor (view from above)



The different approaches to grid-adaptation that we have tried…

1. Estimating error sources from the energy in the smallest scales
   $\mathcal{A}(\mathbf{x}, \mathbf{n})$
2. Estimating error sources from the test-filtered evolution equation
   $\mathcal{G}(\mathbf{x}, \mathbf{n})$
3. Estimating error sources by comparing the mean/variances on two different grids
   "two-grid method"

channel flow,
backward-facing step

Past

Future

4. For wall-modeled LES (WMLES)
5. With WMLES and adaptive wall-model "thickness" $h_{\mathrm{wm}}(\mathbf{x}_{\mathrm{walls}})$

Grid-adaptation in LES – error indicators that guide the adaptation

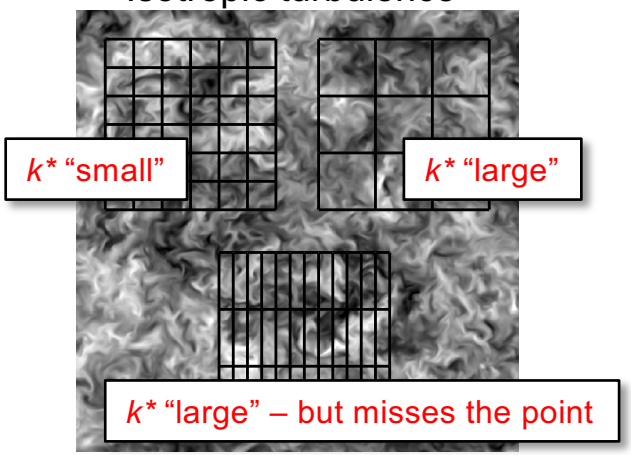
Existing approaches (Pope[1], Bose et al[2]) refine based on the energy in the smallest scales

- E.g. (Bose et al): compute energy in high-pass test-filtered (small scale) velocity field

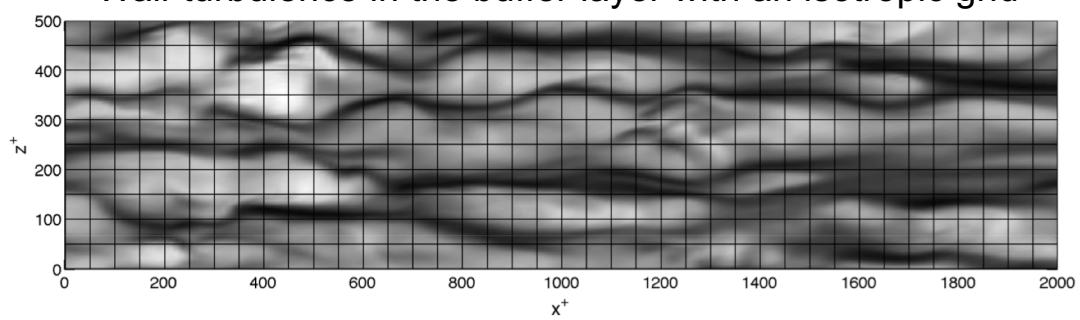
$$\overline{u}_i^* = \overline{u}_i - \widehat{\overline{u}}_i \qquad k^* = \frac{\overline{u}_i^* \, \overline{u}_i^*}{2}$$

and then refine based on *k** – this answers *where* to refine, but not *how to*

Isotropic turbulence[3]



Wall-turbulence in the buffer layer with an isotropic grid



Potential saving of anisotropic grid-adaptation for wall-turbulence starting from isotropic grid:

$$\left(\Delta x^+, \Delta y^+, \Delta z^+\right) \approx (1,1,1) \rightarrow (40,1,20)$$

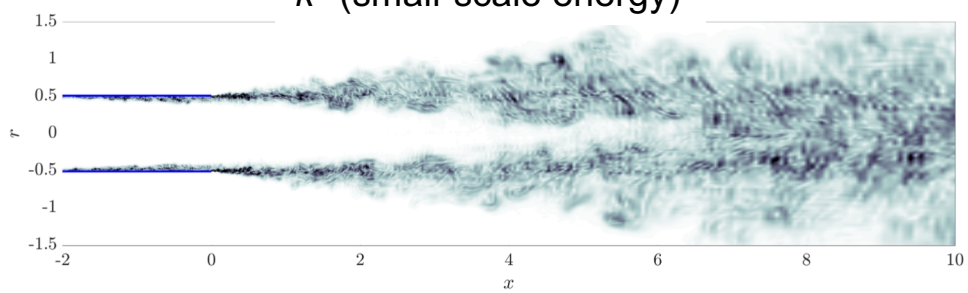
[1] *Pope (NJoP 2004)*
[2] *Bose et al (CTR 2011)*
[3] *Hebert and de Bruyn Kops (PoF 2006)*

In LES, the small-scale energy is not isotropic

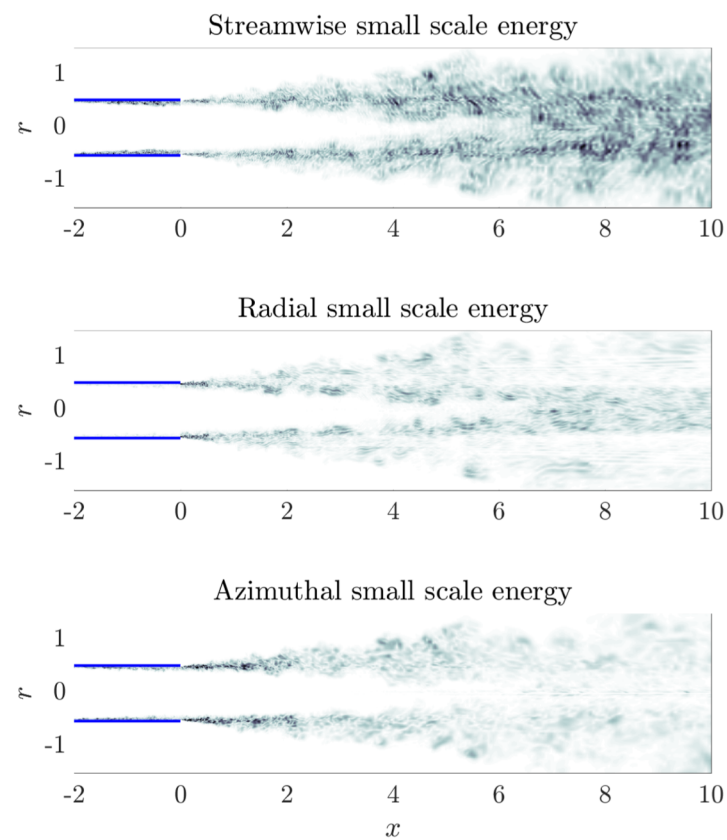
The basic hypothesis of this work:
The directional nature of the smallest resolved scales says something about the required grid-spacing

Example: Mach 0.9 jet by Bres et al[1] on a user-generated unstructured grid

*k** (small-scale energy)



Directional small-scale energy



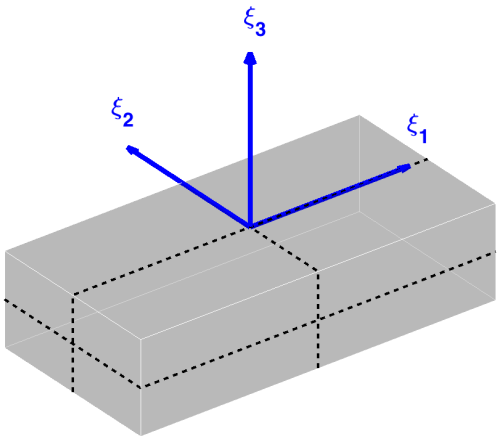
[1] *Bres et al (AIAA 2016-3050)*

Proposed anisotropic error indicator – structured grids (special case)[1]

For structured grid, trivial to implement 1D directional filters:

$$\widehat{\overline{u}}_i^{(\xi_1)}, \widehat{\overline{u}}_i^{(\xi_2)}, \widehat{\overline{u}}_i^{(\xi_3)}$$ (low-pass test-filtered)

$$\overline{u}_i^{(*,\xi_1)} = \overline{u}_i - \widehat{\overline{u}}_i^{(\xi_1)}$$ (high-pass test-filtered)



For example:

$$\widehat{\overline{u}}_i^{(\xi_1)} = \frac{\overline{u}_i(\xi - \Delta\xi)}{4} + \frac{\overline{u}_i(\xi)}{2} + \frac{\overline{u}_i(\xi + \Delta\xi)}{4}$$

Refine in each direction only if

$$\mathcal{A}(\xi_1) = \sqrt{\left\langle \overline{u}_i^{(*,\xi_1)} \overline{u}_i^{(*,\xi_1)} \right\rangle}$$

is larger than some threshold (and similarly in the other directions)

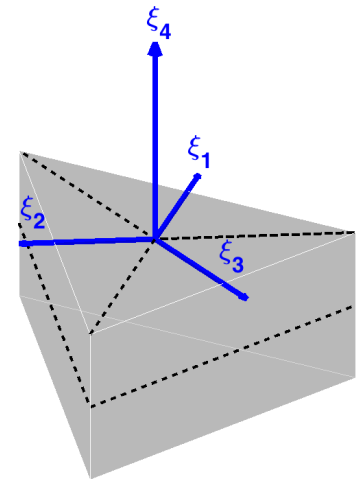
[1] *Toosi and Larsson (AIAA 2017)*

Proposed anisotropic error indicator – general geometries[1]

Key difficulty – how to directionally test-filter in arbitrary geometries?

A differential, directional test-filter:

$$\overline{u}_i = \widehat{\overline{u}}_i^{(\xi)} - \frac{\Delta_\xi^2}{4}\,\xi_j\xi_k\,\frac{\partial^2\,\widehat{\overline{u}}_i^{(\xi)}}{\partial x_j \partial x_k}$$



Approximate inversion[2]:

$$\widehat{\overline{u}}_i^{(\xi)} \approx \overline{u}_i + \frac{\Delta_\xi^2}{4}\,\xi_j\xi_k\,\frac{\partial^2\overline{u}_i}{\partial x_j \partial x_k}$$

High-pass filtered (i.e., small-scale component):

$$\overline{u}_i^{(*,\xi)} = \overline{u}_i - \widehat{\overline{u}}_i^{(\xi)} \approx -\frac{\Delta_\xi^2}{4}\,\xi_j\xi_k\,\frac{\partial^2\overline{u}_i}{\partial x_j \partial x_k}$$

Error indicator in any direction:

$$\mathcal{A}(\xi) = \sqrt{\left\langle \overline{u}_i^{(*,\xi)}\overline{u}_i^{(*,\xi)} \right\rangle}$$

Entirely a post-processing operation!

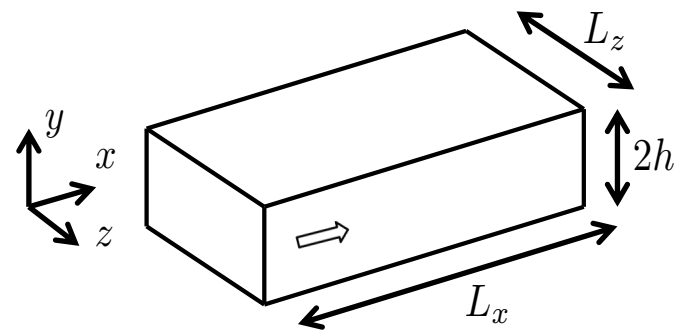
[1] *Toosi and Larsson (AIAA 2017)*
[2] *van Cittert (1931)*

Test on channel flows – where the “optimal” grid is known

$$(L_x, L_y, L_z) = (10h, 2h, 3h)$$

$$Re_b = 30000 \ , \ Re_\tau \approx 830$$

$$M = \frac{U_b}{c_w} = 0.8$$



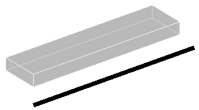
Solution-adaptive finite-difference code,
6th-order central / 5th-order WENO, minimal numerical dissipation

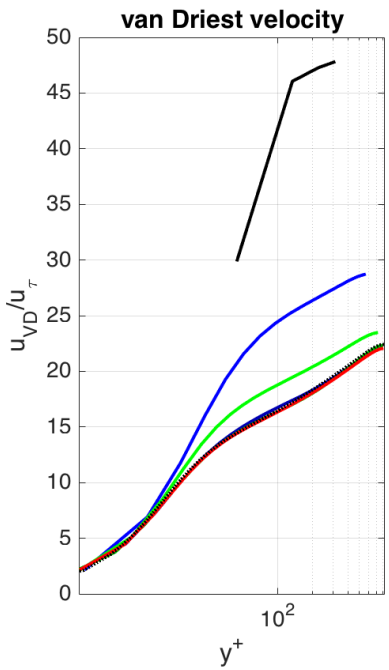
Dynamic Smagorinsky model

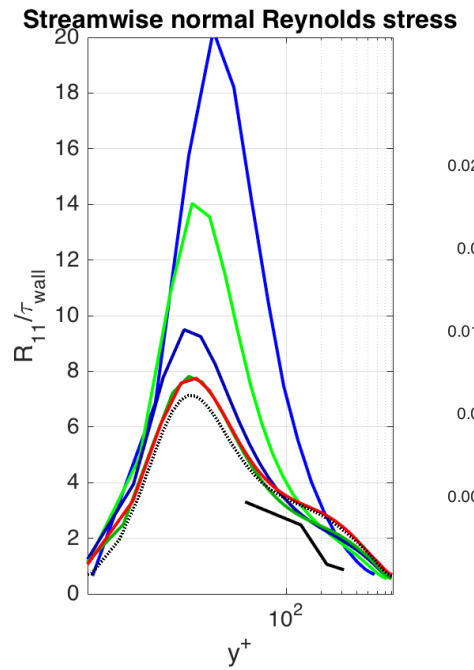
Constant mass flux

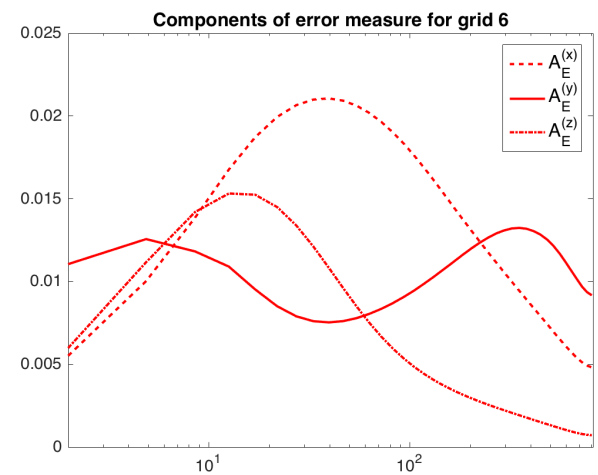
Convergence metric: $$\varepsilon_{\text{prev}} = \frac{1}{5}\frac{\int_a^b \left|U_1^+ - U_{1,\text{prev}}^+\right| d\left(\ln y^+\right)}{\int_a^b U_{1,\text{prev}}^+ \, d\left(\ln y^+\right)} + \sum_{R_{ij}} \frac{1}{5}\frac{\int_a^b \left|R_{ij}^+ - R_{ij,\text{prev}}^+\right| d\left(\ln y^+\right)}{\int_a^b R_{kk,\text{prev}}^+/2 \, d\left(\ln y^+\right)}$$

Channel flow: LES with dynamic Smagorinsky model







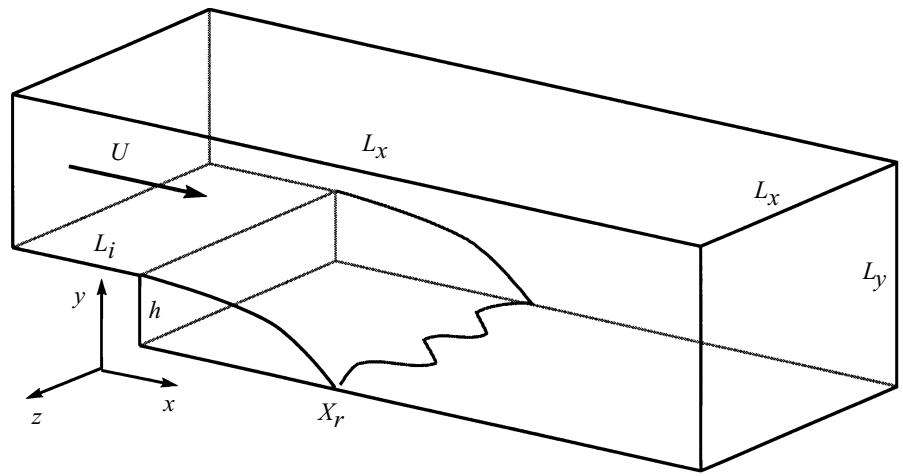


	Grid	(N_x, N_y, N_z)	$(\Delta x, \Delta y_c, \Delta z)/\delta$	$(\Delta x^+, y_1^+, \Delta z^+)$	Re_τ	$\varepsilon_{\text{prev}}$ (%)
	LES-1	$(40, 8, 12)$	$(0.25, 0.25, 0.25)$	$(89, 45, 89)$	356	-
	LES-2	$(35, 32, 15)$	$(0.29, 0.14, 0.20)$	$(170, 2.2, 120)$	611	200
	LES-3	$(60, 50, 40)$	$(0.17, 0.090, 0.075)$	$(130, 1.7, 57)$	758	17
	LES-4	$(96, 60, 96)$	$(0.10, 0.075, 0.031)$	$(85, 1.6, 26)$	820	13
	LES-5	$(152, 72, 180)$	$(0.066, 0.063, 0.017)$	$(54, 1.3, 14)$	822	5.8
	LES-6	$(220, 80, 270)$	$(0.046, 0.052, 0.011)$	$(38, 1.5, 9.2)$	827	2.1

LES of the flow over a backward-facing step

Experiment by Jovic & Driver[1]

$Re_h \approx 5000$



Taken from Le et al (JFM 1997)

DNS by Le et al[2]:

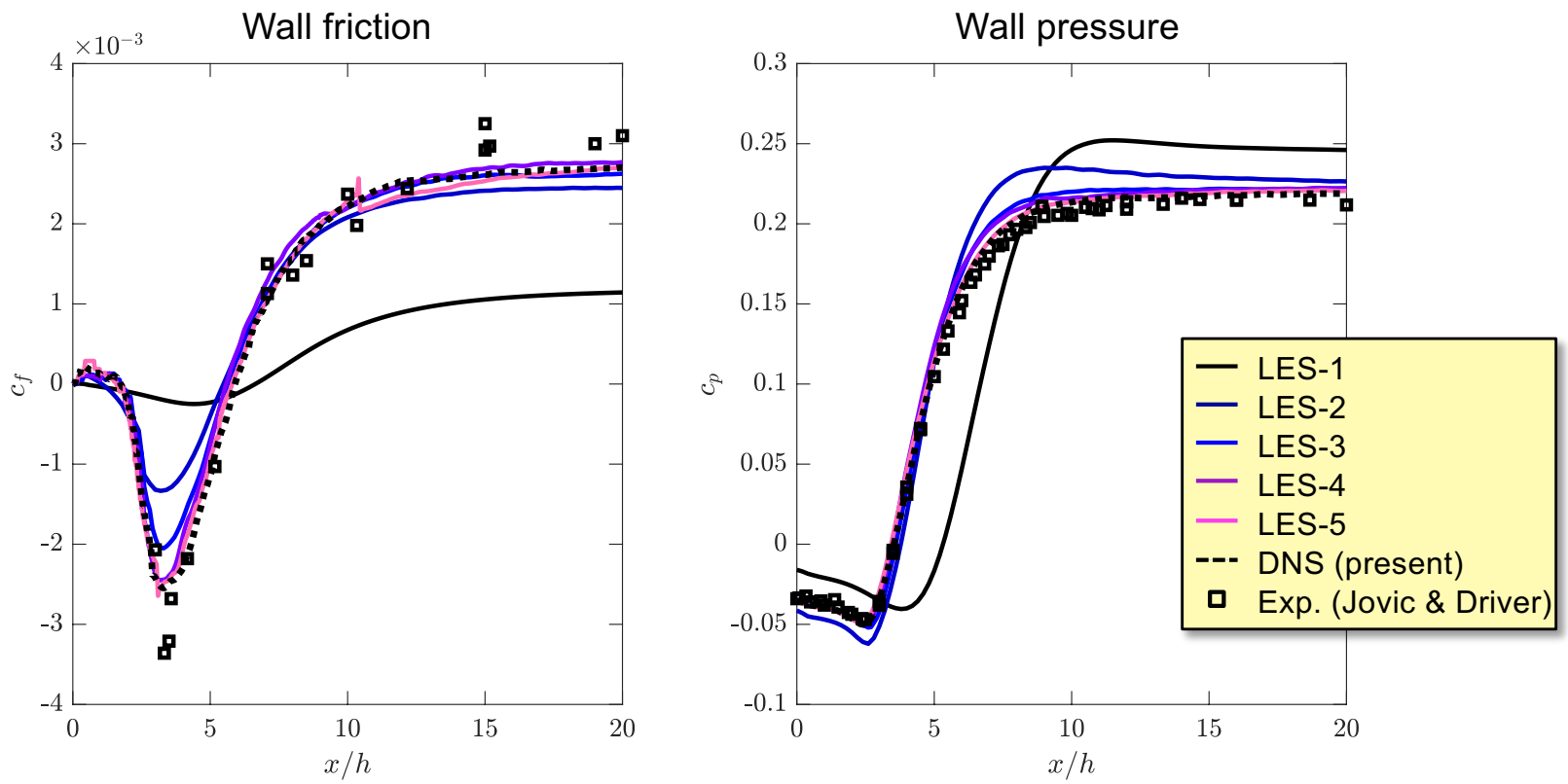
- domain [-10h, 20h] x [0, 6h] x [0, 4h]
- about 9.4M grid points, deemed borderline in their paper

Current LES:

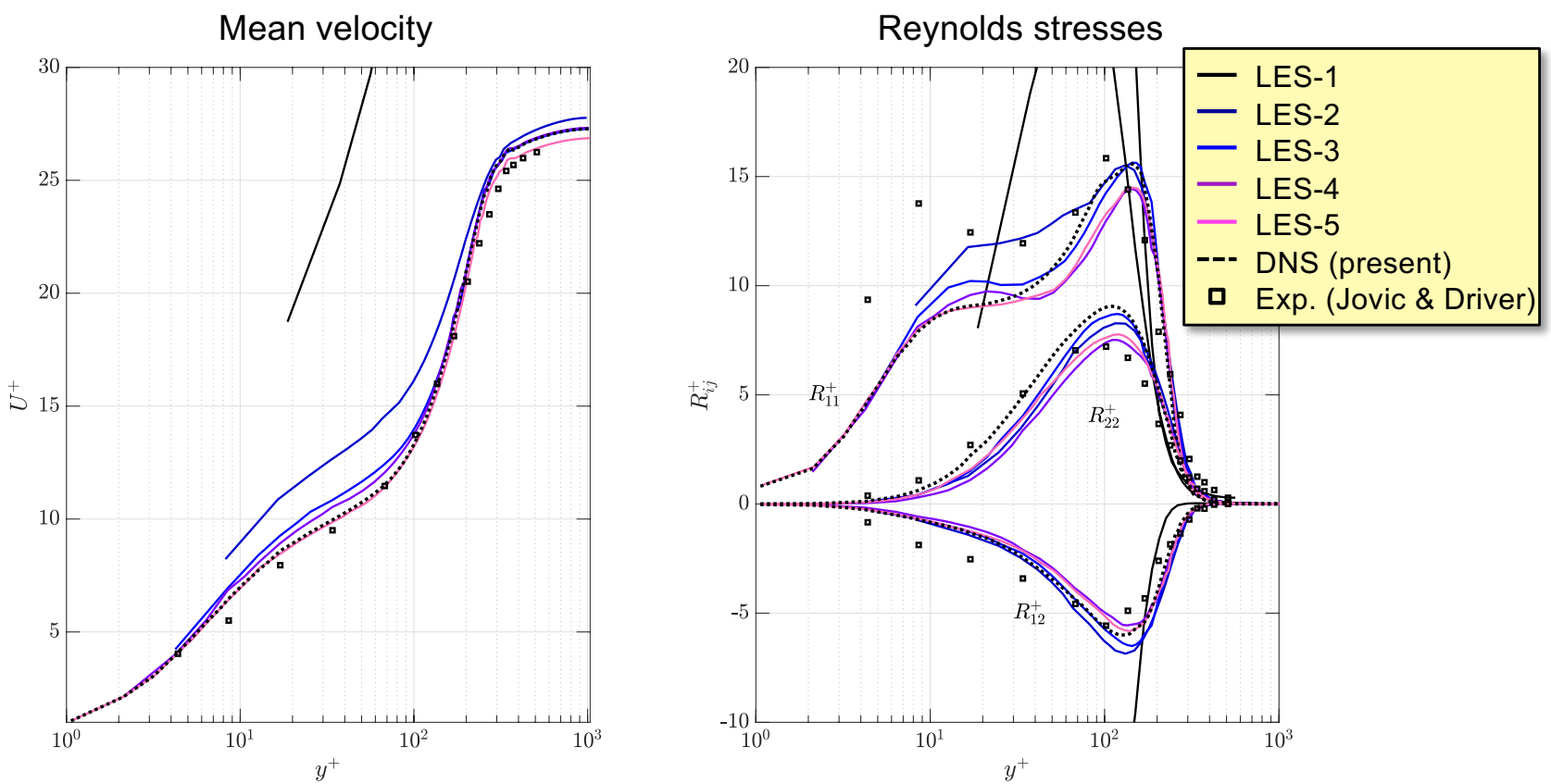
- OpenFOAM with dynamic k-equation subgrid model, central 2nd-order numerics
- domain [-20h, 25h] x [0, 6h] x [0, 4h] – 50% larger than Le et al.
- initial grid ("LES-1"): cubic cells with size 0.2h (125K cells)

[1] *Jovic & Driver (NASA report 1994)*
[2] *Le et al (JFM 1997)*

LES of backward-facing step: wall quantities



LES of backward-facing step: at x/h = 10 (after reattachment)



LES of backward-facing step: sequence of grids

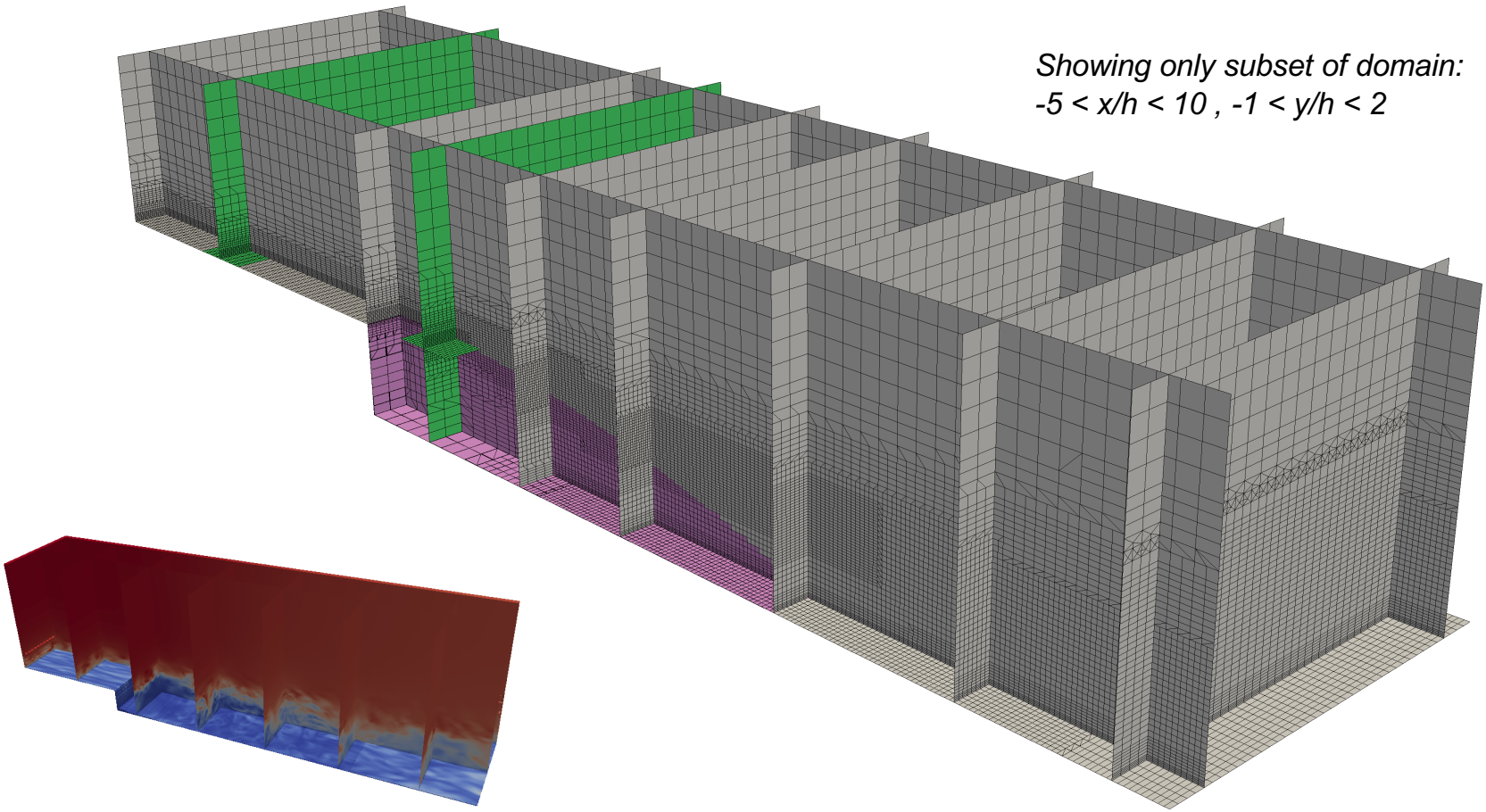
Grid	N_{tot}	N_{struc}	at *x/h* = -3 (upstream of step) $(\Delta x^+, y_1^+, \Delta z^+)$	middle of detached shear layer $(\Delta x, \Delta y, \Delta z)/\delta_{\text{shear}}$	$\varepsilon_{\text{prev}}$ (%)	ε_{ref} (%)
LES-1	125k	125k	$(28, 14, 28)$	$(0.5, 0.5, 0.5)$	-	29
LES-2	273k	517k	$(40, 2.5, 20)$	$(0.4, 0.1, 0.2)$	23	12
LES-3	694k	2.3M	$(46, 2.9, 12)$	$(0.14, 0.036, 0.071)$	8.0	5.2
LES-4	1.7M	11.2M	$(24, 1.5, 6.0)$	$(0.071, 0.018, 0.036)$	3.2	4.9
LES-5	3.2M	16.2M	$(24, 1.5, 6.1)$	$(0.036, 0.018, 0.036)$	3.1	3.3
DNS	9.1M	70M	$(12, 0.76, 6.1)$	$(0.036, 0.0089, 0.036)$	-	-

Convergence metric:
(-5 < x/h < 20, -1 < y/h < 1)

$$\varepsilon_{\text{prev}} = \frac{1}{3}\sum_{U_i}\frac{1}{2}\frac{\iint_\Omega |U_i - U_{i,\text{prev}}|\,dxdy}{0.2U_\infty A_\Omega} + \frac{1}{3}\sum_{R_{ij}}\frac{1}{4}\frac{\iint_\Omega |R_{ij} - R_{ij,\text{prev}}|\,dxdy}{0.015U_\infty^2 A_\Omega}$$
$$+ \frac{1}{6}\frac{\int_\Psi |c_f - c_{f,\text{prev}}|\,dx}{0.002\,L_\Psi} + \frac{1}{6}\frac{\int_\Psi |c_p - c_{p,\text{prev}}|\,dx}{0.1\,L_\Psi},$$

LES of backward-facing step: the converged grid LES-4

- 1.7M cells, generated “automatically” from the isotropic initial grid
- 5% error compared to DNS



The different approaches to grid-adaptation that we have tried…

1. Estimating error sources from the energy in the smallest scales
   $\mathcal{A}(\mathbf{x}, \mathbf{n})$
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   $\mathcal{G}(\mathbf{x}, \mathbf{n})$
3. Estimating error sources by comparing the mean/variances on two different grids
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channel flow,
backward-facing step

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4. For wall-modeled LES (WMLES)
5. With WMLES and adaptive wall-model "thickness" $h_{\mathrm{wm}}(\mathbf{x}_{\mathrm{walls}})$

A error indicator derived from the evolution equation

LES evolution eqn:

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^{\mathrm{mod}}(\overline{u}_i)}{\partial x_j}$$

Test-filtered eqn:

$$\frac{\partial \widehat{\overline{u}}_i^{(\mathbf{n}_0)}}{\partial t} + \frac{\partial \widehat{\overline{u}_i \overline{u}_j}^{(\mathbf{n}_0)}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{p}}^{(\mathbf{n}_0)}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{u}}_i^{(\mathbf{n}_0)}}{\partial x_j \partial x_j} - \frac{\partial \widehat{\tau_{ij}^{\mathrm{mod}}(\overline{u}_i)}^{(\mathbf{n}_0)}}{\partial x_j}$$

Eqn at the test-filter level:

$$\frac{\partial \widehat{\overline{v}}_i^{(\mathbf{n}_0)}}{\partial t} + \frac{\partial \widehat{\overline{v}}_i^{(\mathbf{n}_0)} \widehat{\overline{v}}_j^{(\mathbf{n}_0)}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{q}}^{(\mathbf{n}_0)}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{v}}_i^{(\mathbf{n}_0)}}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^{\mathrm{mod}}\left(\widehat{\overline{v}}_i^{(\mathbf{n}_0)}\right)}{\partial x_j}$$

Difference between the eqns:

$$\widehat{\overline{e}}_i^{(\mathbf{n}_0)} = \widehat{\overline{v}}_i^{(\mathbf{n}_0)} - \widehat{\overline{u}}_i^{(\mathbf{n}_0)} \quad , \quad \widehat{\overline{\Pi}}^{(\mathbf{n}_0)} = \widehat{\overline{q}}^{(\mathbf{n}_0)} - \widehat{\overline{p}}^{(\mathbf{n}_0)}$$

$$\underbrace{\frac{\partial \widehat{\overline{e}}_i^{(\mathbf{n}_0)}}{\partial t} + \widehat{\overline{u}}_j^{(\mathbf{n}_0)} \frac{\partial \widehat{\overline{e}}_i^{(\mathbf{n}_0)}}{\partial x_j}}_{T_1} - \underbrace{\nu \frac{\partial^2 \widehat{\overline{e}}_i^{(\mathbf{n}_0)}}{\partial x_j \partial x_j}}_{T_2} + \underbrace{\frac{\partial \widehat{\overline{e}}_i^{(\mathbf{n}_0)} \widehat{\overline{e}}_j^{(\mathbf{n}_0)}}{\partial x_j}}_{T_3} + \underbrace{\widehat{\overline{e}}_j^{(\mathbf{n}_0)} \frac{\partial \widehat{\overline{u}}_i^{(\mathbf{n}_0)}}{\partial x_j}}_{T_4} + \underbrace{\frac{1}{\rho}\frac{\partial \widehat{\overline{\Pi}}^{(\mathbf{n}_0)}}{\partial x_i}}_{T_5} = \widehat{\overline{\mathcal{F}}}_i^{(\mathbf{n}_0)}$$

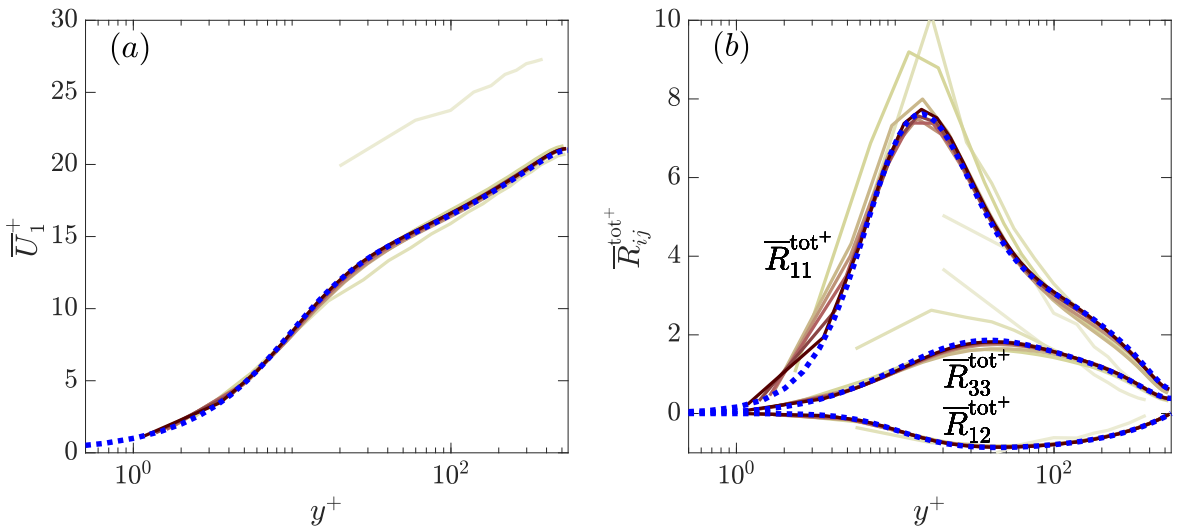
Source in difference eqn:

$$\widehat{\overline{\mathcal{F}}}_i^{(\mathbf{n}_0)}(\mathbf{x}) = \frac{\partial}{\partial x_j}\left(\widehat{\overline{u}_i \overline{u}_j}^{(\mathbf{n}_0)} - \widehat{\overline{u}}_i^{(\mathbf{n}_0)} \widehat{\overline{u}}_j^{(\mathbf{n}_0)}\right) + \frac{\partial}{\partial x_j}\left(\widehat{\tau_{ij}^{\mathrm{mod}}(\overline{u}_i)}^{(\mathbf{n}_0)} - \tau_{ij}^{\mathrm{mod}}\left(\widehat{\overline{v}}_i^{(\mathbf{n}_0)}\right)\right)$$

Error indicator:

$$\overline{\mathcal{G}}(\mathbf{x}, \mathbf{n}) = \sqrt{\left\langle \widehat{\overline{\mathcal{F}}}_i^{(\mathbf{n})}(\mathbf{x}) \widehat{\overline{\mathcal{F}}}_i^{(\mathbf{n})}(\mathbf{x}) \right\rangle}$$

Assessment on channel flow



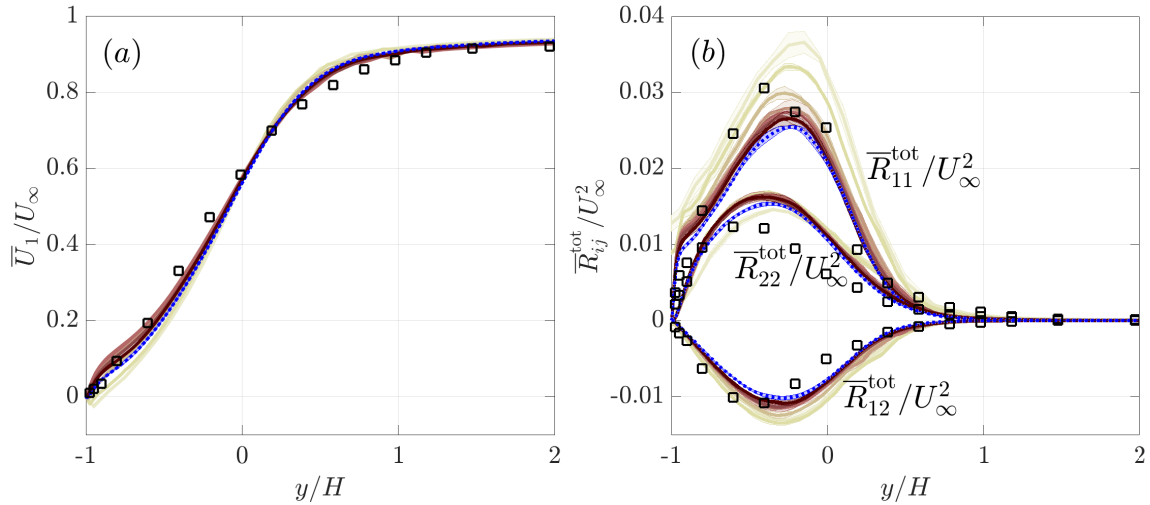
Grid	N_{tot}	N_y	$(\overline{\Delta}_x^+, \overline{y}_1^+, \overline{\Delta}_z^+)$	$(\overline{\Delta}_x, \overline{\Delta}_{y,c}, \overline{\Delta}_z)/H$	Re_τ	$e_{\mathrm{QoI}}^{\mathrm{DNS}}$ (%)	$\mathcal{A}(\mathbf{x},\mathbf{n})$	$e_{\mathrm{QoI}}^{\mathrm{prev}}$ (%)
DSM-1	$15k$	20	$(80, 20, 80)$	$(0.20, 0.10, 0.20)$	398	32	32	–
DSM-2	$74k$	34	$(77, 5.6, 55)$	$(0.14, 0.099, 0.010)$	553	12	9.2	27
DSM-3	$251k$	44	$(53, 2.3, 29)$	$(0.098, 0.091, 0.054)$	536	6.5	7.9	8.8
DSM-4	$514k$	50	$(45, 1.7, 19)$	$(0.082, 0.080, 0.035)$	544	3.3	5.2	4.5
DSM-5	$1.18M$	60	$(34, 1.4, 13)$	$(0.063, 0.065, 0.024)$	544	1.8	4.3	2.1
DSM-6	$2.53M$	72	$(25, 1.6, 10)$	$(0.046, 0.052, 0.018)$	542	1.5	2.7	< 1
DSM-7	$5.80M$	90	$(18, 1.4, 7.6)$	$(0.033, 0.041, 0.014)$	540	< 1	< 1	< 1
DSM-8	$11.1M$	108	$(14, 1.2, 6.3)$	$(0.025, 0.033, 0.012)$	541	< 1		< 1

$$\delta Q_1^{\mathrm{ref}} = \frac{\int_a^b \left| \overline{U}_1^+ - \widetilde{U}_{1,\mathrm{ref}}^+ \right| d\left(\ln y^+\right)}{\int_a^b \widetilde{U}_{1,\mathrm{ref}}^+ \, d\left(\ln y^+\right)}$$

$$\delta Q_{2\text{-}5}^{\mathrm{ref}} = \frac{\int_a^b \left| \overline{R}_{ij}^{\mathrm{tot}+} - \widetilde{R}_{ij,\mathrm{ref}}^{\mathrm{tot}+} \right| d\left(\ln y^+\right)}{\int_a^b \widetilde{R}_{kk,\mathrm{ref}}^{\mathrm{tot}+}/2 \, d\left(\ln y^+\right)} \quad , \quad (i,j) = (1,1),\ (2,2),\ (3,3),\ (1,2)$$

Assessment on backward-facing step

At *x/h*=6



$$\delta Q_{1\text{-}2}^{\mathrm{ref}} = \frac{\iint_\Omega \left|\overline{U}_i - \widetilde{U}_{i,\mathrm{ref}}\right| dxdy}{0.2U_\infty\, A_\Omega}; \quad i = 1,\, 2$$

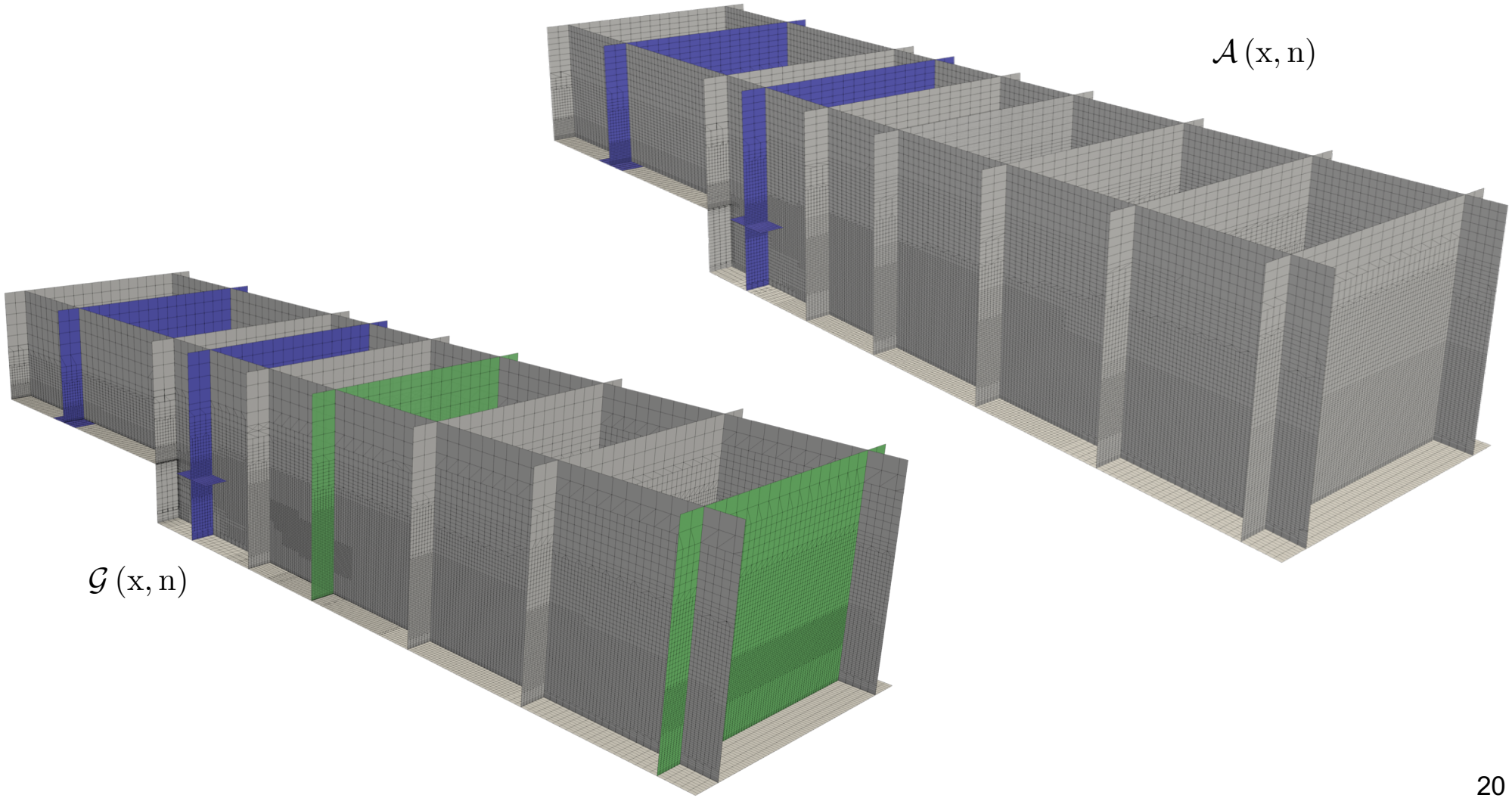
$$\delta Q_{3\text{-}6}^{\mathrm{ref}} = \frac{\iint_\Omega \left|\overline{R}_{ij}^{\mathrm{tot}} - \widetilde{R}_{ij,\mathrm{ref}}^{\mathrm{tot}}\right| dxdy}{0.015U_\infty^2\, A_\Omega}; \quad (i,j) = (1,1),\, (2,2),\, (3,3),\, (1,2)$$

$$\delta Q_7^{\mathrm{ref}} = \frac{\int_\Psi \left|\overline{c}_f - \widetilde{c}_{f,\mathrm{ref}}\right| dx}{0.002\, L_\Psi};$$

$$\delta Q_8^{\mathrm{ref}} = \frac{\int_\Psi \left|\overline{c}_p - \widetilde{c}_{p,\mathrm{ref}}\right| dx}{0.1\, L_\Psi}.$$

Grid	N_{tot}	$(\overline{\Delta}_x^+, \overline{y}_1^+, \overline{\Delta}_z^+)$	$(\overline{\Delta}_x, \overline{\Delta}_y, \overline{\Delta}_z)/\delta_{\mathrm{shear}}$	$e_{\mathrm{QoI}}^{\mathrm{DNS}}$ (%)	$\mathcal{A}(\mathbf{x},\mathbf{n})$	$e_{\mathrm{QoI}}^{\mathrm{prev}}$ (%)
G-1	149k	$(42, 10, 42)$	$(0.21, 0.17, 0.33)$	11.1	11.1	–
G-2	297k	$(42, 2.6, 21)$	$(0.16, 0.078, 0.16)$	10.5	11	5.3
G-3	611k	$(45, 1.4, 11)$	$(0.16, 0.049, 0.078)$	5.6	6.4	6.4
G-4	1.32M	$(47, 1.5, 12)$	$(0.076, 0.038, 0.076)$	4.9	6.8	3.8
G-5	2.13M	$(25, 0.77, 6.2)$	$(0.070, 0.035, 0.035)$	5.4	4.5	2.8
G-6	3.41M	$(25, 0.77, 6.1)$	$(0.068, 0.034, 0.034)$	3.5	4.7	3.4
G-7	6.72M	$(12, 0.76.6.0)$	$(0.034, 0.017, 0.034)$	2.5	2.3	2.2
DNS	54M	$(6.0, 0.38.3.0)$	$(0.017, 0.0086, 0.017)$	0		–

Comparison of the final grids



The different approaches to grid-adaptation that we have tried…

1. Estimating error sources from the energy in the smallest scales
   $\mathcal{A}(\mathbf{x}, \mathbf{n})$
2. Estimating error sources from the test-filtered evolution equation
   $\mathcal{G}(\mathbf{x}, \mathbf{n})$
3. Estimating error sources by comparing the mean/variances on two different grids
   "two-grid method"

channel flow,
backward-facing step

Past

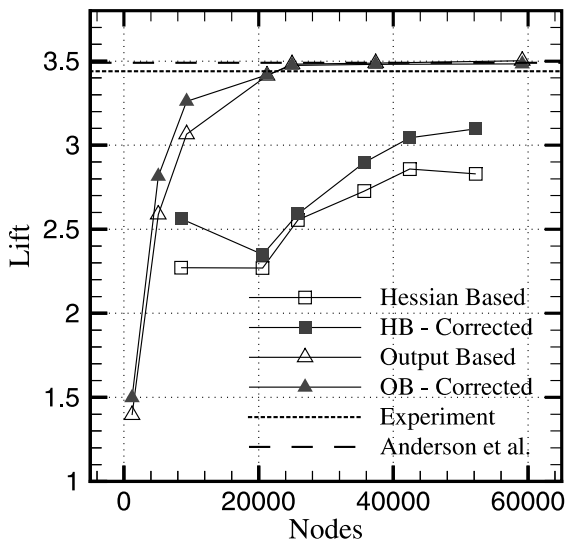
Future

4. For wall-modeled LES (WMLES)
5. With WMLES and adaptive wall-model "thickness" $h_{\mathrm{wm}}(\mathbf{x}_{\mathrm{walls}})$

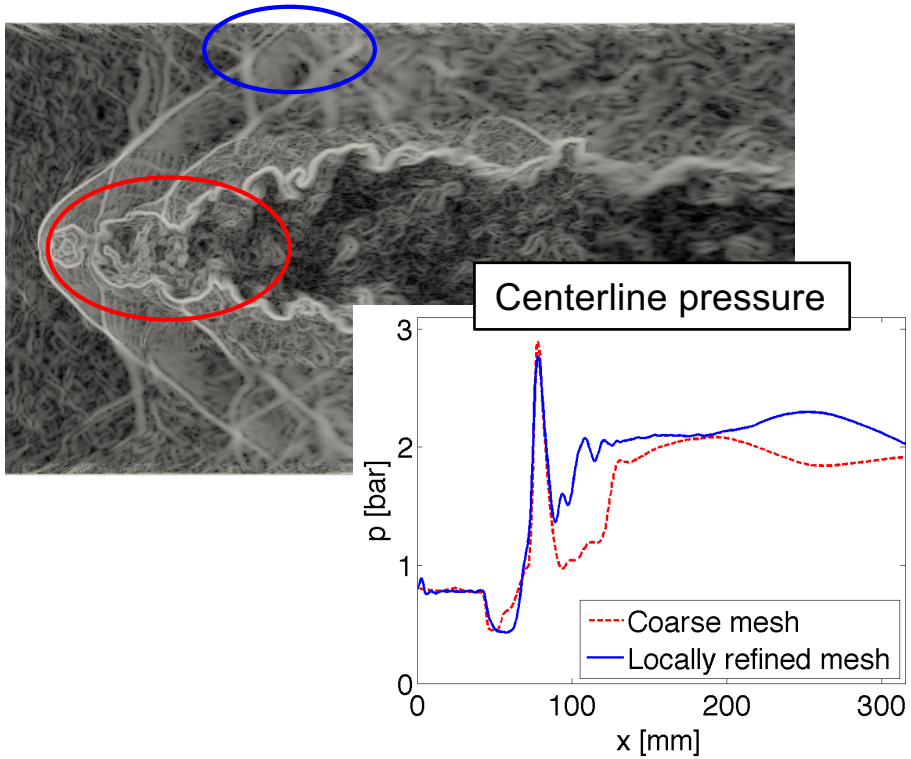
Can a sequence of adapted grids be used to prove grid-convergence?

Not in general – if the error indicator missed some important region, those errors are the same, thus preventing convergence to the *true* solution

Convergence of lift coefficient using different adaptation methods[1]



LES of a scramjet combustor



[1] *Venditti & Darmofal (JCP 2003)*

How to verify grid-convergence in LES?

Chaotic + modeled unresolved scales => can't speak of point-wise convergence
But all meaningful outputs must converge – if not, why use LES?

Focus on outputs:

Adjoint-weighted residual (AWR)[1]: $J(u_h) - J(u) \approx \langle \text{adjoint}, \text{trunc. error} \rangle$

AWR applied to LES: $J(u_h) - J(u) \approx \langle \text{adjoint}, \text{trunc. error} + \text{model error} \rangle$

Can modeling error be estimated with 100% confidence?
If not, we can NOT verify grid-convergence in this way (with 100% confidence)!

What's a meaningful definition of grid-convergence for LES?

"If the grid-spacing is changed everywhere by a constant factor, no output quantities-of-interest should change by more than some tolerance"

Given a grid with Δ_h and u_h, need a second grid with $\Delta_H = \kappa\Delta_h$ and u_H, and $J(u_H) - J(u_h) \leq \text{tol.}$

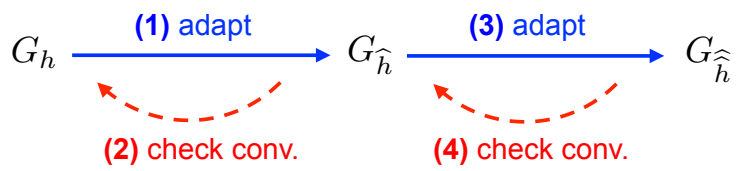
This changes the whole verification/adaptation framework (compared to AWR):

- Twice as much information going into the grid-adaptation problem
- Adjoint used only for "optimal" grid-adaptation, not to also verify grid-convergence

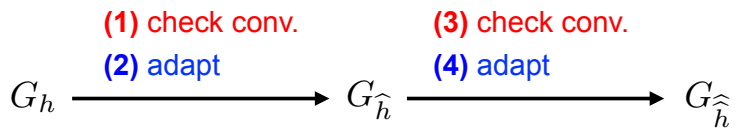
[1] *cf. Fidkowski and Darmofal (AIAA J, 2011) and others*

Combined adaptation and verification (grid-convergence) process

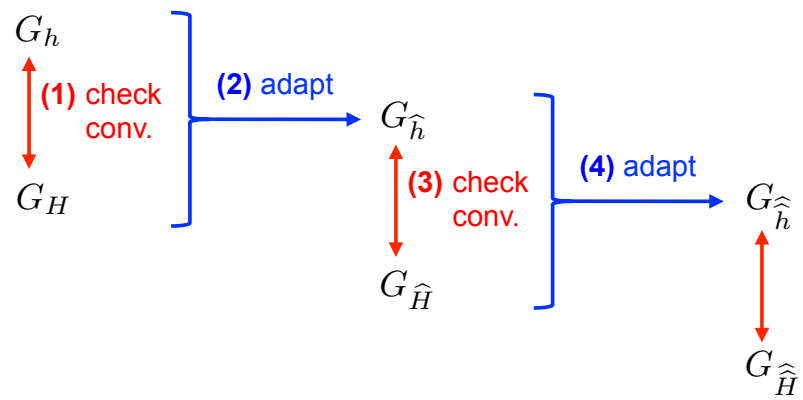
0. <u>Without adjoint (non-rigorous):</u>
non-rigorous convergence check
by comparing with the adapted grid



1. <u>Adjoint-weighted residual (non-chaotic):</u>
rigorous convergence check by the
estimated output error



2. <u>Proposed (chaotic):</u>
rigorous convergence check by the
uniformly refined/coarsened grid;
adaptation using all available information



When combined with rigorous verification, the grid-adaptation problem becomes:
- given solutions on two related (sibling) grids, how should the grid optimally be modified?

Proposed new formulation or meta-algorithm[1]

Verification-driven grid-adaptation:
Suppose we have a grid G_h with grid-spacing $\Delta_h(x,t)$ and solution $u_h(x,t)$. We then first ask whether this solution is grid-converged.

Step 1 – verification (is the solution grid-independent on G_h?):
Create the uniformly coarsened (or refined) grid G_H with $\Delta_H(x,t) = \kappa\Delta_h(x,t)$ and solve for $u_H(x,t)$. Compute the difference in the outputs and check whether

$$|J_i(u_H) - J_i(u_h)| \leq dJ_{i,\text{conv-crit}} \quad , \quad \forall i = 1, \ldots, N_{\text{outputs}} \,. \tag{5}$$

If criterion (5) is satisfied, the solution u_h is considered converged and grid-independent; if not, we proceed to create a new grid.

Step 2 – adaptation (create the new grids $G_{\widehat{h}}$ and $G_{\widehat{H}}$):
Using all available information, i.e., the solutions and grid-spacings on both the G_h and G_H grids, seek a new grid $G_{\widehat{h}}$ and it's uniformly coarsened (or refined) sibling $G_{\widehat{H}}$ that

1. has as few grid points as possible; and
2. satisfies the convergence criteria, i.e., for which

$$\boxed{\left|J_i(u_{\widehat{H}}) - J_i(u_{\widehat{h}})\right|} \leq dJ_{i,\text{conv-crit}} \quad , \quad \forall i = 1, \ldots, N_{\text{outputs}} \,. \tag{6}$$

Notes:

- J_i are important output quantities (e.g., lift and drag, or the solution in some location)
- Key difficulty – must estimate the sensitivity of the outputs on all possible candidate grids

[1] *Larsson (AIAA SciTech 2018)*

Estimating the output error on the adapted grid

For non-chaotic problems – straightforward, and computationally efficient with adjoints:

$$J_i\left(u_{\widehat{H}}\right) \approx J_i\left(u_{\widehat{h}}\right) + \left\langle \frac{\partial J_i}{\partial u}, u_{\widehat{H}} - u_{\widehat{h}} \right\rangle$$

For chaotic problems, difference between instantaneous fields is not meaningful.
Proposed approach: expand outputs in terms of deterministic statistics of the solution, e.g.:

$$J_i(u_{\widehat{H}}) \approx J_i(u_{\widehat{h}}) + \left\langle \frac{\partial J_i}{\partial \overline{u}}, \overline{u}_{\widehat{H}} - \overline{u}_{\widehat{h}} \right\rangle + \left\langle \frac{\partial J_i}{\partial \overline{u'u'}}, \overline{u'u'}_{\widehat{H}} - \overline{u'u'}_{\widehat{h}} \right\rangle + \ldots ,$$

Model difference in statistics in a mean sense, from exact corresponding equations (mean, variance, etc) with modeled source terms

The corresponding adjoint equations are steady in time, and deterministic – very cheap to solve… but possibly poorly linking local errors to the outputs

Application to incompressible large eddy simulation (LES)

LES evolution equation:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_j}\left(\nu \frac{\partial u_i}{\partial x_j}\right) + \frac{\partial \tau_{ij}^{\text{model}}}{\partial x_j} = f_i^{\text{err-num}} + f_i^{\text{err-mod}}$$

Mean equation (RANS momentum eqn):

$$\mathcal{M}\left(\overline{u}_i, \overline{u_i' u_j'}\right) = \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} + \frac{\partial \overline{u_i' u_j'}}{\partial x_j} + \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial}{\partial x_j}\left(\nu \frac{\partial \overline{u}_i}{\partial x_j}\right) + \frac{\partial \overline{\tau_{ij}^{\text{model}}}}{\partial x_j} = \overline{f_i^{\text{err}}} \approx 0$$

Variance equation (Reynolds stress eqn):

$$\mathcal{R}\left(\overline{u}_i, \overline{u_i' u_j'}\right) = \text{Conv}_{ij} + \text{Diff}_{ij} + \text{Prod}_{ij} = Q_{ij} \approx c_{ij}\Delta^2$$

"Error source density": $c_{11}(\mathbf{x}) = \dfrac{\mathcal{R}\left(\overline{u}_H, \overline{u'u'}_H\right) - \mathcal{R}\left(\overline{u}_h, \overline{u'u'}_h\right)}{\Delta_H^2 - \Delta_h^2}$

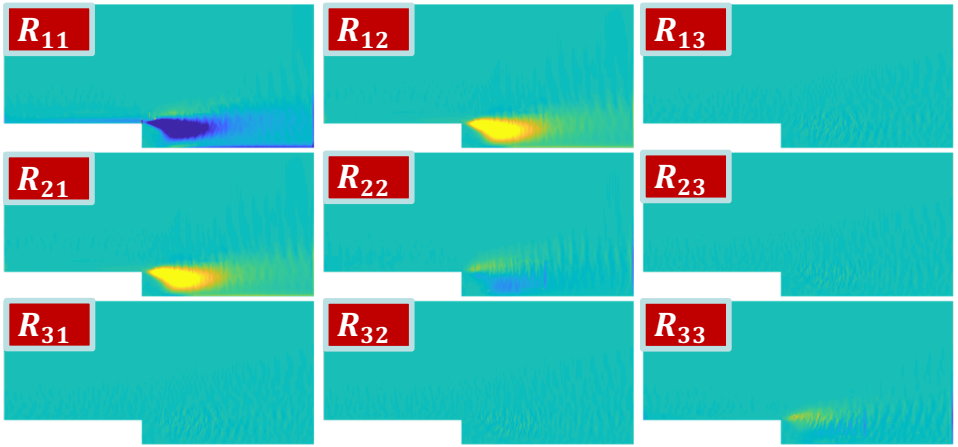
Find the grid by minimizing

$$\left|J(u_{\widehat{H}}) - J(u_{\widehat{h}})\right| \approx \left|\left\langle \frac{\partial J}{\partial \overline{u}}, \overline{u}_{\widehat{H}} - \overline{u}_{\widehat{h}} \right\rangle + \left\langle \frac{\partial J}{\partial \overline{u'u'}}, \overline{u'u'}_{\widehat{H}} - \overline{u'u'}_{\widehat{h}} \right\rangle + \ldots\right|$$

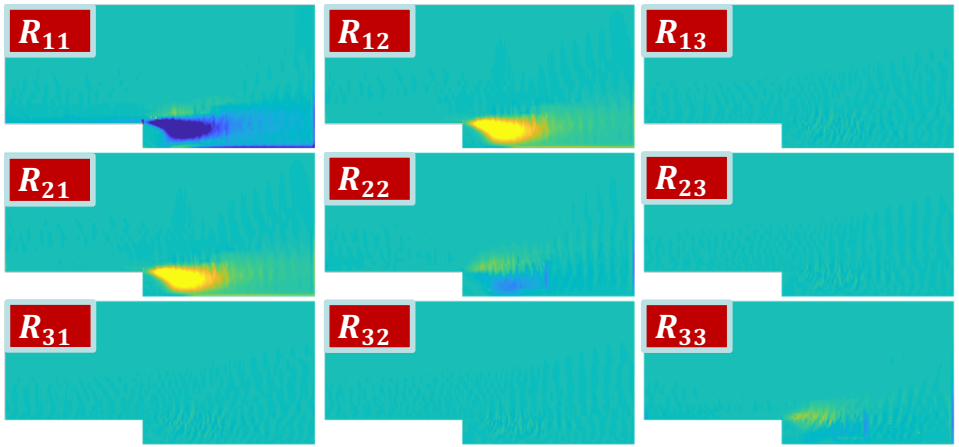
$$\approx \left|\langle \text{adjoint}_{\mathcal{M}}, 0\rangle + \left\langle \text{adjoint}_{\mathcal{R}}, \underbrace{c_{11}(\mathbf{x})\left(\Delta_{\widehat{H}}^2 - \Delta_{\widehat{h}}^2\right)}_{c_{11}(\mathbf{x})\left(\kappa^2 - 1\right)\Delta_{\widehat{h}}^2(\mathbf{x})} \right\rangle\right|$$

Assessment on the flow over a backward-facing step

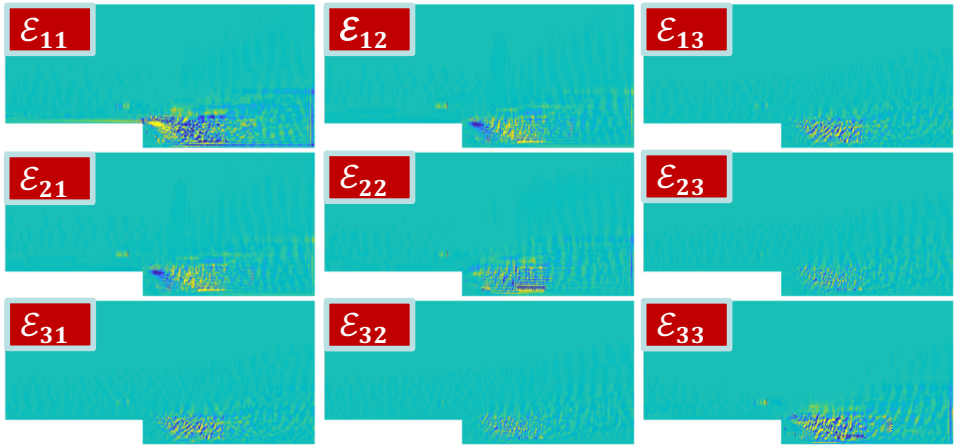
$Q_{ij,h}$



$Q_{ij,H}$



$Q_{ij,h} - Q_{ij,H} \approx c_{ij}\left(\Delta_h^2 - \Delta_H^2\right)$

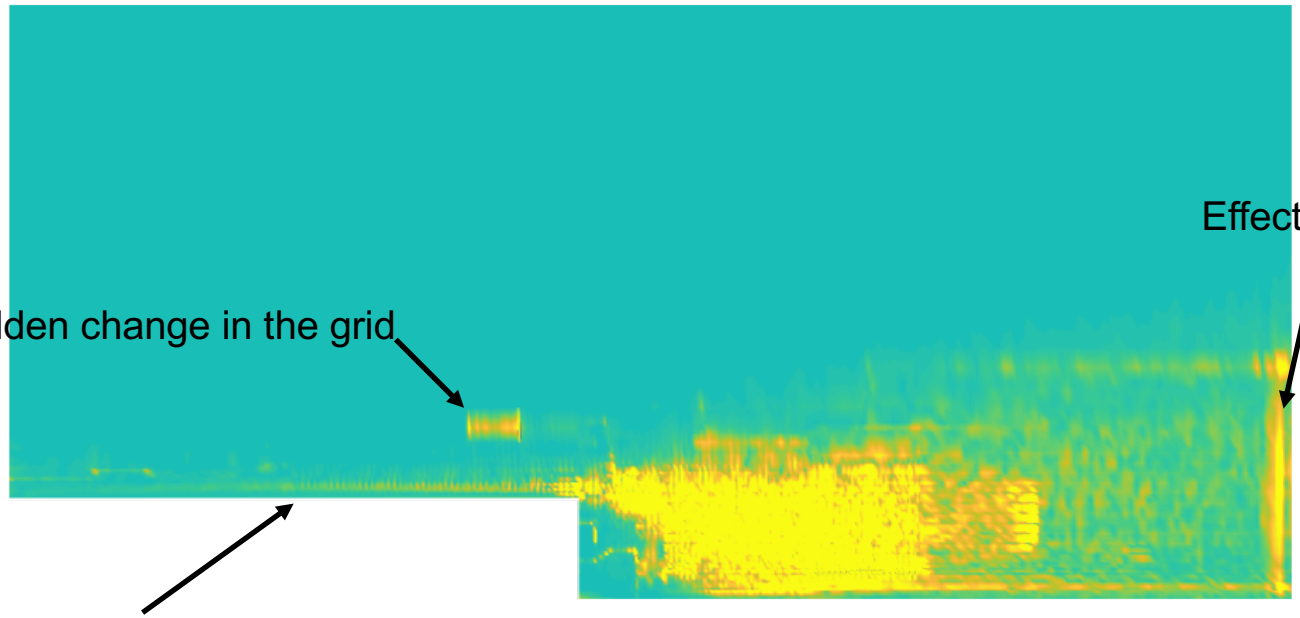


c_{ij}

Assessment on the flow over a backward-facing step

Inferred error on the base grid:

$$|Q_h| = \sqrt{Q_{ij,h} Q_{ij,h}}$$



Effect of outflow condition

Sudden change in the grid

Small error in incoming boundary layer since the base grid is already good enough there

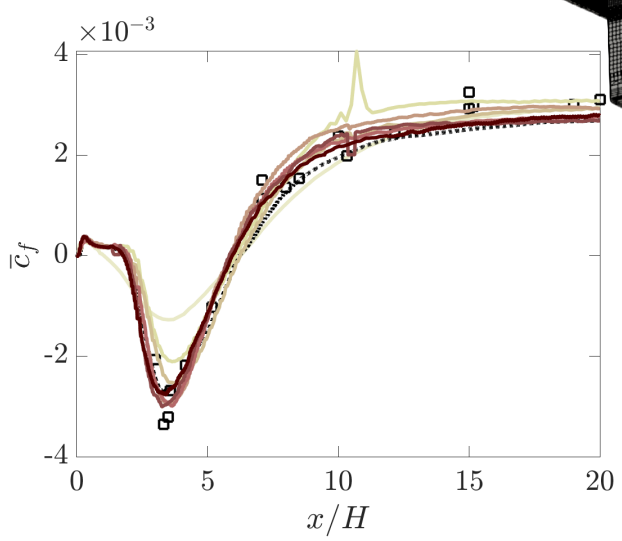
Assessment on the flow over a backward-facing step

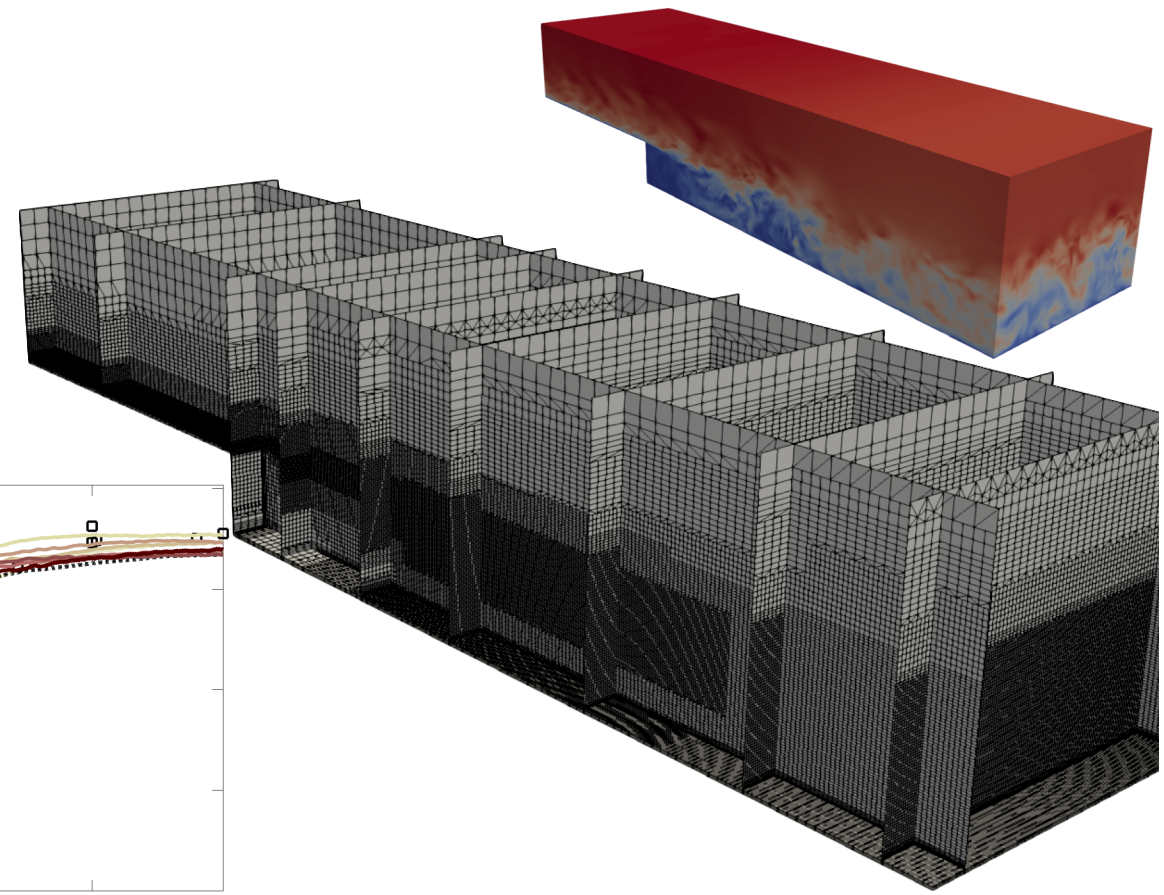
Error metric ϵ including c_f, c_p, $\bar{u}_i$, and $\overline{u'_i u'_j}$.

Comparing Δ_h and Δ_H

Comparing Δ_h to DNS

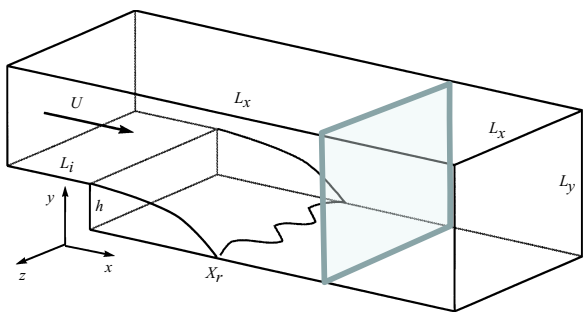
#	N_{tot}	ϵ'%	ϵ%
1	149k	9.4	12
2	292k	7.8	12
3	596k	6.9	7.9
4	1.31M	6.3	8.1
5	2.13M	6.5	5.3
6	3.78M	3.9	5.0
7	6.69M	3.9	4.7





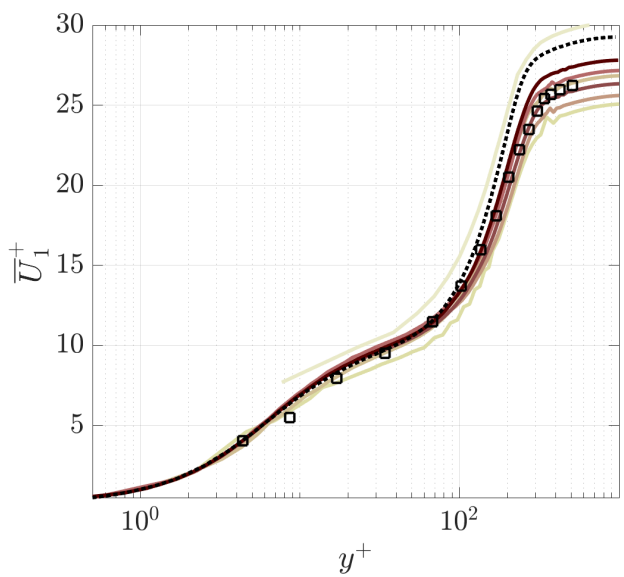
Symbols: experiment
Dotted line: DNS

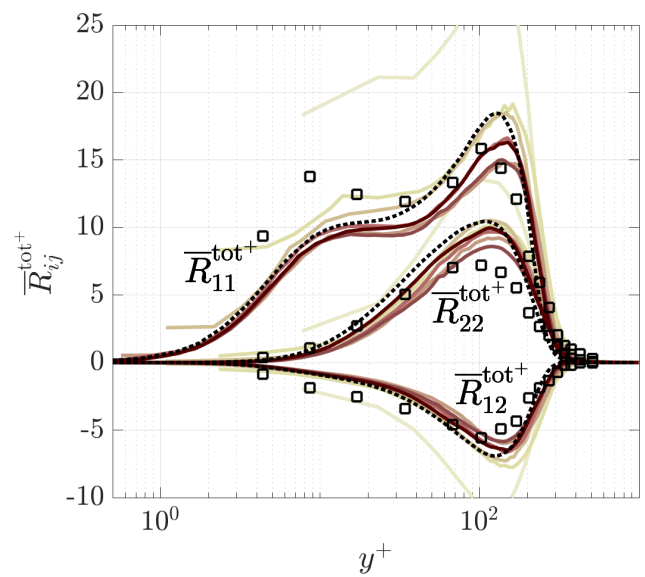
Assessment on the flow over a backward-facing step



#	N_{tot}	ϵ'%	ϵ%	Color
1	149k	9.4	12	
2	292k	7.8	12	
3	596k	6.9	7.9	
4	1.31M	6.3	8.1	
5	2.13M	6.5	5.3	
6	3.78M	3.9	5.0	
7	6.69M	3.9	4.7	

Symbols: experiment
Dotted line: DNS





Cost of the full algorithm

Base grid Δ_h

Sibling grid Δ_H

#	N_{tot}	$\epsilon'\%$	$\epsilon\%$	N'_{tot}
1	149k	9.4	12	75k
2	292k	7.8	12	158k
3	596k	6.9	7.9	308k
4	1.31M	6.3	8.1	685k
5	2.13M	6.5	5.3	1.10M
6	3.78M	3.9	5.0	1.90M
7	6.69M	3.9	4.7	3.42M

Cost = 1.23C

The cost of avoiding grid-generation by user-expertise – presumably pays off with a more optimal final grid

Cost C

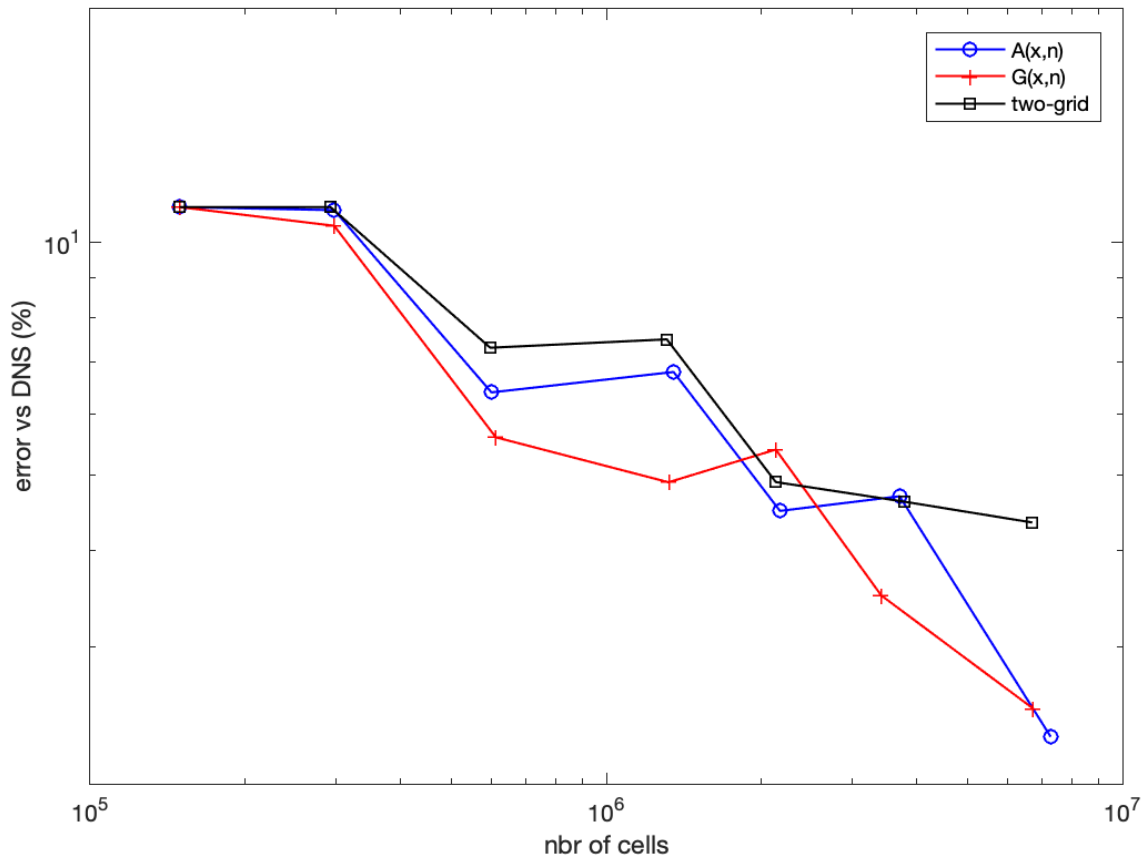
Cost = 0.54C

Additional cost of always computing on a "sibling" grid

Cost = 0.43C

Unavoidable if you want to verify grid-convergence – which you do!!!

Comparing all 3 algorithms for the backward-facing step



Summary

Have developed 3 different methods for grid-adaptation in LES:

- Based on the directionally small scale energy
- Based on the test-filtered evolution equation
- Based on comparing means and variances on two related grids

All 3 methods seem to find the accepted “best practice” grid for channel flows, even when starting from extremely coarse and ignorant initial grids

All 3 methods are post-processing only – no changes to the LES solver are needed

Computational cost:

- Generally no more than twice the cost of the final grid -- it’s totally worth it!
  - Presumably more “optimal” grids than a human could do
  - Much less human grid-generation

Ongoing/future work:

- Grid-adaptation combined with wall-modeled LES, and with adaptive wall-model thickness
- Would love to collaborate with grid/solver people!