

# Enabling the use of unstructured meshes for the Large Eddy Simulation of stable atmospheric boundary layers

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## Abstract

Modeling wind flows in complex terrain under varying atmospheric stability conditions is valuable to better understand its physics and impacts on wind turbines. Yet their numerical simulations are still challenging. Stable boundary layer (SBL) are difficult to model, mostly due to the small size of the characteristic eddies. Complex terrain are hard to match with structured grids. Such constrains require both high fidelity simulations at high resolution and unstructured meshes. This work presents an original numerical framework answering these requirements. It is then validated against the GABLS1 benchmark, a  $400 \times 400 \times 400 \text{ m}^3$  box with periodic walls, cooled by the bottom where surface temperature decrease over time. Induced wall heat flux generates thermal stratification and thus a stable boundary layer. Results with structured and unstructured grids are satisfactory, with both simulations being within the dispersion of previous studies. Minor differences are highlighted. Due to the grid quality, the order of the numerical schemes and the accuracy of the flux estimation, unstructured grids simulations have higher wall heat fluxes than structured grids ones. This gap widens over time, reaching 14%, impacting velocity, temperature, variances and fluxes. Stable boundary layer is found to be around 10% higher. The grid resolution employed highly impacts the accuracy of the SBL modeling. A mesh refine-

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ment study has been carried out with both structured and unstructured grids showing that a  $\Delta x = 6.25$  m grid size is sufficient to correctly reproduce the stable boundary layer.

*Keywords:* GABLS1, Large-eddy simulations, Stable boundary layer, Unstructured grids

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## 1. Introduction

Given today's energy and environmental challenges, increasing the electrical power generated by wind farms is of paramount importance [1]. To this end, the size of wind turbines has significantly increased over the years, with rotors reaching hundreds of meters in diameter. The aforementioned wind turbines are no longer affected solely by micro-scale wind flows that extend well below 1 km. They are also affected by meso-scale processes, ranging from 5 to hundreds of kilometres in size, which influence local weather. They are at the interface between the micro- and meso-scale [2].

The expansion of the scale introduces novel phenomena that modify the overall flow physics. At altitude, we find the geostrophic wind as a result of the balance between the pressure gradient force and the Coriolis force. While pressure gradient is induced by weather systems such as low- or high-pressure areas, Coriolis force is a consequence of the Earth angular momentum conservation. At intermediate heights, we find phenomena that induce a change in the atmospheric boundary layer (ABL) structure. The best known is the thermal stratification. Due to sun's heat, air density varies alternating buoyancy forces. This phenomenon can be either stable or unstable, depending on the direction of the vertical thermal gradient [3].

Finally on the ground, we find terrain effect, which influences horizontal and vertical velocity gradients. Complex terrain can also induce flow separation, re-circulation and roughness change. A finer comprehension of the physics underlying the previously described phenomena is required to better predict the behaviour of wind turbines in complex environments. However, the knowledge of wind flows in such complex environments remains incomplete [2].

This study aims to address this challenge by focusing on one specific aspect: thermal stratification. It is well established that wind turbines performances are significantly influenced by wind shear, with implications on wake recovery, speed deficit, induced turbulence, energy production, loads

31 and fatigue [4]. To gain insight into these phenomena, field measurement  
32 campaigns and wind tunnel experiments can be conducted [5, 6]. Their use  
33 remains constrained by their inherent complexity as well as by the costs as-  
34 sociated to their implementation. In this context, there has been a growing  
35 tendency to rely on numerical simulations as a means of investigation [7].  
36 Nevertheless, while simulations of the convective boundary layer (CBL) has  
37 been widely performed [7], accurate simulation of the stable boundary layer  
38 (SBL) remains a challenging task [7]. The main difficulty lies in the cap-  
39 ture of characteristic vortices, which can be particularly small. Indeed, the  
40 height of the atmospheric boundary layer varies considerably depending on  
41 the thermal stratification [8]. While a CBL can reach altitudes of approxi-  
42 mately 1 km, an SBL is approximately 200 m high. Additionally, CBLs are  
43 driven by large convection vortices, which generate further turbulence. In  
44 contrast, SBLs are driven by wind shear and exhibit lower levels of turbu-  
45 lent kinetic energy. As a result of their reduced height and turbulence, their  
46 vortices characteristic size are also smaller. To accurately capture these  
47 features, high spacial resolution is needed, leading in large computational  
48 resources requirements. The state-of-the-art tool to enable precise numerical  
49 prediction of stable boundary layer flows is the Large Eddy Simulation (LES)  
50 technique [7].

51 To enhance comprehension of stable boundary layers by Large Eddy Sim-  
52 ulation (LES), the Global Energy and Water Cycle Experiment (GEWEX)  
53 initiated the GEWEX Atmospheric Boundary Layer Study (GABLS). The  
54 objective was to enhance comprehension of stable boundary layer and im-  
55 prove its representation by LES models [9]. The focus of GABLS has been  
56 on SBLs over land and the representation of diurnal cycle. Three different  
57 GABLS intercomparisons have already been carried out, focusing on pro-  
58 gressively more realistic cases. These benchmarks are considered important  
59 for improving the modeling of stable atmospheric layers [10]. In this work,  
60 we consider the GABLS1 benchmark targeting an idealized Arctic stable  
61 boundary layer case [11].

62 Initially, a comparison of 11 LES codes was carried out [12]. The GABLS1  
63 setup consists of a periodic box with an uniform initial velocity profile, cooled  
64 by the bottom wall, where the surface temperature decreases over time. The  
65 study has shown that the grid resolution employed highly impacts the ac-  
66 curacy of the SBL modeling. A range of mesh resolution has been given in  
67 order to correctly capture the flow physics behaviour. Subsequent to the  
68 initial study, several LES have been conducted employing the GABLS1 con-

69 figuration with the objective of replicating an SBL scenario. The benchmark  
70 results are used to validate the underlying framework, as well as to investi-  
71 gate the influence of finer grid [13, 14], surface cooling rate [13, 15, 16] or  
72 subgrid-scale (SGS) [17, 18, 19] impact. Other studies have used the GABLS1  
73 configuration to validate their Reynolds Averaged Navier-Stokes equations  
74 (RANS) or pseudo-spectral methods [10, 20]. Regardless of the approach  
75 employed, all of these studies accurately reproduce the physical behaviour of  
76 the stable boundary layer, but the use of finer grids does not prejudice the  
77 quality of the results. It is worth mentioning that all the aforementioned  
78 studies were conducted on structured grids. None have used unstructured  
79 grids since the domain was not requesting.

80 The simulation of wind flows in complex terrain is also a challenging topic  
81 due to the difficulty of creating a mesh that accurately reflects the topogra-  
82 phy [2]. Structured meshes, which are commonly used in atmospheric flow  
83 simulations, tend to encounter difficulties when attempting to follow complex  
84 geometries. For this reason, the use of unstructured grid is mandatory. How-  
85 ever, the complexity of developing high-order flow solvers for unstructured  
86 meshes has limited their use in real atmospheric studies. To address the  
87 reluctance of the research community to employ such meshes, it is essential  
88 to validate their use in simple scenarios before progressing to more complex  
89 studies. Therefore, the aim of this study is to draw analogous conclusions  
90 for simulations using unstructured grids. To the author's knowledge, a Large  
91 Eddy Simulation of a stable boundary layer has never been performed on an  
92 unstructured grid, and this work aims to address this gap in the literature.  
93 Conclusions on the minimum and optimum mesh size [12] for robust LES are  
94 drawn using only a structured grid.

95 The manuscript is structured as follows: the methodology is described in  
96 Section 2. Section 3 first presents the GABLS1 stable boundary layer results  
97 obtained with both structured and unstructured grid having an identical  
98 grid length. Then a sensitivity to resolution study is carried out in the same  
99 section. Finally, conclusions are drawn in Section 4.

## 100 **2. Methodology**

### 101 *2.1. GABLS1 configuration*

102 The GABLS1 intercomparison is based on an idealized Arctic stable  
103 boundary layer case [11]. A domain of  $400 \times 400 \times 400 \text{ m}^3$  with periodic  
104 walls on both streamwise,  $X$ , and tangential,  $Y$ , direction is employed. The

105 bottom boundary condition is a rough wall with a  $z_0 = 0.1$  m roughness. The  
 106 surface temperature is  $T_w = 265$  K with a cooling rate of  $0.25$  K.h<sup>-1</sup>. The top  
 107 boundary condition is a sleep wall. An imposed uniform geostrophic wind of  
 108  $G_x = 8$  m.s<sup>-1</sup> in the east-west direction at latitude 73° north drives the stable  
 109 boundary layer, corresponding to a Coriolis parameter of  $f = 1.39 \times 10^{-4}$  s<sup>-1</sup>.  
 110 Gravity, reference potential temperature and density as well as the Von Kar-  
 111 man constant are set to  $g = 9.81$  m.s<sup>-2</sup>,  $\theta_0 = 263.5$  K,  $\rho_0 = 1.3223$  kg.m<sup>-3</sup> and  
 112  $\kappa = 0.4$ , respectively. Figure 1 illustrates the configuration of the GABLS1  
 113 setup.

114 Initial velocity profile is set to geostrophic wind, i.e. a uniform  $u_x =$   
 115  $8$  m.s<sup>-1</sup> velocity profile. Initial vertical temperature profile is set uniform to  
 116  $265$  K in the first hundred meters and then increases by  $0.01$  K.m<sup>-1</sup> up to  
 117 the top of the domain, reaching  $268$  K at the top. Random perturbations are  
 118 introduced in the first fifty meters with a  $0.1$  K amplitude as specified in [12].

119 To mitigate gravity-wave reflexion, a sponge layer (SL) is applied above  
 120 three hundred meters. In order to smoothly relax the velocity and the tem-  
 121 perature and thus avoid numerical errors, the sponge layer follows:

$$SL_\phi = \gamma \times \sin^2 \left( \frac{z - Z_{SL}}{L_z - Z_{SL}} \times \frac{\pi}{2} \right) \times (\phi_{target} - \phi), \quad (1)$$

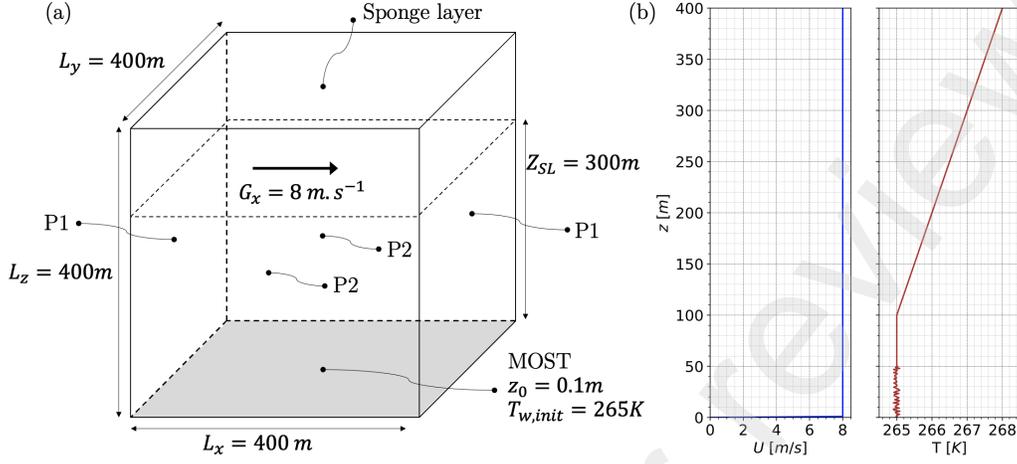
122 where  $\phi$  is the actual velocity or temperature. Here,  $\phi_{target}$  is the target  
 123 velocity or temperature, set to geostrophic wind or linear increasing temper-  
 124 ature respectively.  $\gamma = \frac{1}{5}$  is a time relaxation parameter and  $z$  is the height  
 125 varying between the SL bottom height  $z_{SL} = 300$  m and the domain top  
 126 height  $z_{top} = 400$  m. The sponge layer is then smoothed over time and over  
 127 space.

## 128 2.2. Flow solver

129 LES are performed with the incompressible flow at constant density solver  
 130 from the YALES2 platform [21]. YALES2 is a massively parallel finite vol-  
 131 ume flow library able to process structured and unstructured meshes. Spatial  
 132 fourth-order central scheme and time fourth order Runge-Kutta-like integra-  
 133 tion method are used [22]. In this work we solve the filtered Navier Stokes  
 134 equations, expressed using Einstein's notation where  $\tilde{\bullet}$  is the low-pass spatial  
 135 filtering operator, as:

### 136 Continuity equation

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \quad (2)$$



**Figure 1:** (a): GABLS1 setup configuration scheme.  $P1$  and  $P2$  for periodic walls in pairs. (b): initial velocity and temperature vertical profiles.

137

### Momentum-conservation equation

$$\frac{\partial \tilde{u}_j}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_i} = \nu \frac{\partial^2 \tilde{u}_j}{\partial x_i \partial x_i} + \frac{1}{\rho_0} \frac{\partial}{\partial x_i} \tau_{ij}^R - \frac{1}{\rho_0} \frac{\partial \tilde{P}}{\partial x_j} + \frac{\tilde{\rho} g}{\rho_0} - 2\Omega(G_i - \tilde{u}_i), \quad (3)$$

138 where  $u$  is the fluid velocity,  $\nu$  the kinematic viscosity,  $\rho_0$  the reference air  
 139 density,  $\tau_{ij}^R$  the residual stress tensor and  $P$  the pressure. The last two terms  
 140 are the Boussinesq approximation [23] to account for the gravitational effect  
 141 induced by thermal stratification and the Coriolis effect, respectively. In  
 142 these terms,  $\rho$  is the local density,  $g$  the Earth gravitational constant,  $\Omega$  the  
 143 Earth angular velocity and  $G$  is the geostrophic wind.

### 2.3. Wall model

145 As the mesh resolution is not enough to capture the boundary layer, one  
 146 must employ a wall model in order to predict momentum and heat flux at  
 147 the wall. The most common atmospheric flow wall model is based on the  
 148 Monin-Obukhov Similarity Theory [24, 25] and assumes classical logarithmic  
 149 profiles for both temperature and velocity. It is capable of accommodating  
 150 all three atmospheric thermal configurations: neutral, stable, and unstable.  
 151 This is made possible by the presence of correction terms whose intensity  
 152 and shape vary depending on the thermal state [3].

153 The velocity and temperature profiles can be expressed as follows:

$$\frac{\bar{u}(z)}{u_*} = \frac{1}{k} \left[ \ln \left( \frac{z}{z_0} \right) - \psi_m \left( \frac{z - z_0}{L} \right) \right], \quad (4)$$

$$\frac{\theta(z) - \theta_w}{\theta_*} = \frac{1}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) - \psi_h \left( \frac{z - z_0}{L} \right) \right], \quad (5)$$

154 where  $u_* = \sqrt{\tau_w/\rho}$  is the friction velocity with  $\tau_w$  the local shear stress at  
 155 the wall.  $\theta_* = -q_w/u_*$  is the friction temperature where  $q_w$  is the kinematic  
 156 surface heat flux and  $\theta_w$  is the wall temperature.  $\kappa$  is the Von Karman con-  
 157 stant and  $z_0$  the roughness length.  $L$  the Obukhov length which represents  
 158 the height above the surface from where buoyancy first dominates shear com-  
 159 puted as  $L = -\frac{u_*^3 \theta_0}{\kappa g q_w}$ .  $\theta_0 = 263.5$  K is the reference potential temperature.  
 160

161 The correction functions  $\psi_m$  and  $\psi_h$  are set to zero for neutral cases, lead-  
 162 ing to a classical logarithmic velocity profile. For non-neutral configurations,  
 163 they can be expressed as:

$$\psi_{m/h}(\xi) = \int_{z_0/L}^{\xi} \frac{1 - \phi_{m/h}(\xi)}{\xi} dz, \quad (6)$$

164 where  $\xi = z/L$ . Furthermore,  $\phi_m$  and  $\phi_h$  are referred to as the stability  
 165 functions. They are empirically determined and can be expressed depending  
 166 on the stability condition as:

167  
 168 **Unstable cases**

$$\begin{aligned} \phi_m &= (1 - \gamma_m \xi)^{-1/4}, \\ \phi_h &= (1 - \gamma_h \xi)^{-1/2}, \end{aligned} \quad (7)$$

169 **Stable cases**

$$\begin{aligned} \phi_m &= 1 + \beta_m \xi, \\ \phi_h &= 1 + \beta_h \xi, \end{aligned} \quad (8)$$

170 Various parameterizations were introduced over the years [26, 27]. In  
 171 this work, we use the one prescribed in the GABLS1 setup:  $\beta_m = 4.8$  and  
 172  $\beta_h = 7.8$ .

173 As mention in [28], surface temperature is prescribed as boundary con-  
 174 dition instead of surface sensible heat flux. Thus we have a two-unknown

Mesh name	S1	U1	S2	U2	S3	U3	S4	U4
$\Delta x$ [m]	12.5		6.25		3.125		2.0	
$N_{elem}$ [ $\times 10^3$ ]	32.8	148.2	262.1	1186	2097.2	9487.9	8000.0	35972.8
$N_{node}$ [ $\times 10^3$ ]	45.4	41.8	366.3	337.8	2919.7	2659.1	11255.5	10042.7
$\Delta t$ [s]	0.2		0.1		0.05		0.032	

**Table 1:** Case set-up with  $\Delta x$  the mesh cell size,  $N_{elem}$  the number of mesh elements and  $\Delta t$  the time step.

175 problem,  $u_*$  and  $q_w$ . We therefore use a double Newton-Raphson conver-  
176 gence method [29] for its quadratic convergence speed.

177 As wall models are derived from averaged Navier-Stokes equations, quan-  
178 tities such as velocity and temperature must be spatially filtered [30]. For  
179 structured grids, averaging the quantities on the horizontal plane passing  
180 through the 1st node is straightforward. For unstructured grids, the 1st  
181 node plane does not exist. To overcome this problem a filtering operator is  
182 applied to the latter as well as to the first node velocity and temperature  
183 used to build the momentum and heat flux at the wall.

#### 184 2.4. Numerical set-up

185 Structured (S) and unstructured (U) meshes with 4 different resolutions  
186 are used in this study. Tab. 1 gathers the mesh characteristics for these  
187 cases. The number of elements varies significantly between the structured  
188 and unstructured meshes of the same resolution but the number of nodes is  
189 similar. Since the control volumes are defined at the nodes into YALES2,  
190 the number of degrees of freedom remains approximately the same and so  
191 the mesh type comparison is fair.

192 Subgrid scale modelling is performed using the dynamic Smagorinsky  
193 model [31, 32]. Even though different models are sometimes used to better  
194 model anisotropic flows [19], Smagorinsky models are still the most commonly  
195 used in the literature and has been proven to perform reasonably well [33].  
196 In addition, dynamic Smagorinsky model has shown to be more effective at  
197 sustaining deeper SBLs relative to the Smagorinsky model [12].

198 Simulations are ran out for a total of 8 hours of physical time, representing  
199 a diurnal cycle. Statistics are collected on the last hour i.e. between the 7th  
200 and the 8th hour. Our results are compared with the eleven LES codes from

201 the first GABLS1 intercomparison [12] but also with various studies who  
202 compared themselves to the first study [15, 16, 17, 13, 34, 18, 19, 35].

### 203 2.5. Time discretization

204 Flow solver time step is here imposed to respect the Courant-Fredrichs-  
205 Lewy  $CFL = U\Delta t/\Delta x$  condition. Due to the explicit integration of the  
206 Coriolis force, the time step is chosen following [36] such that  $\Delta t = \frac{CFL \times \Delta x}{\|U\| + \sqrt{gH}}$   
207 with  $H$  the vertical depth of the fluid, i.e. the stable boundary layer height.  
208 The imposed time step is evaluated to ensure  $CFL < 0.9$  with a convective  
209 velocity  $\|U\| = 9 \text{ m.s}^{-1}$  and a boundary layer height  $H = 200 \text{ m}$ . All time  
210 steps used in this study are summarized in Table 1.

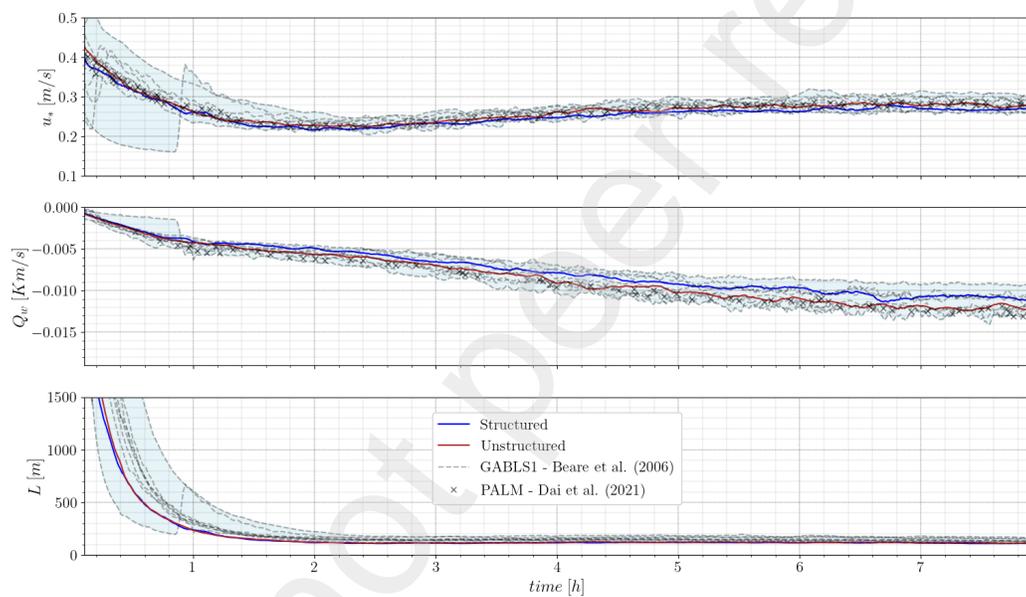
## 211 3. Results

### 212 3.1. Unstructured and Structured grid comparison

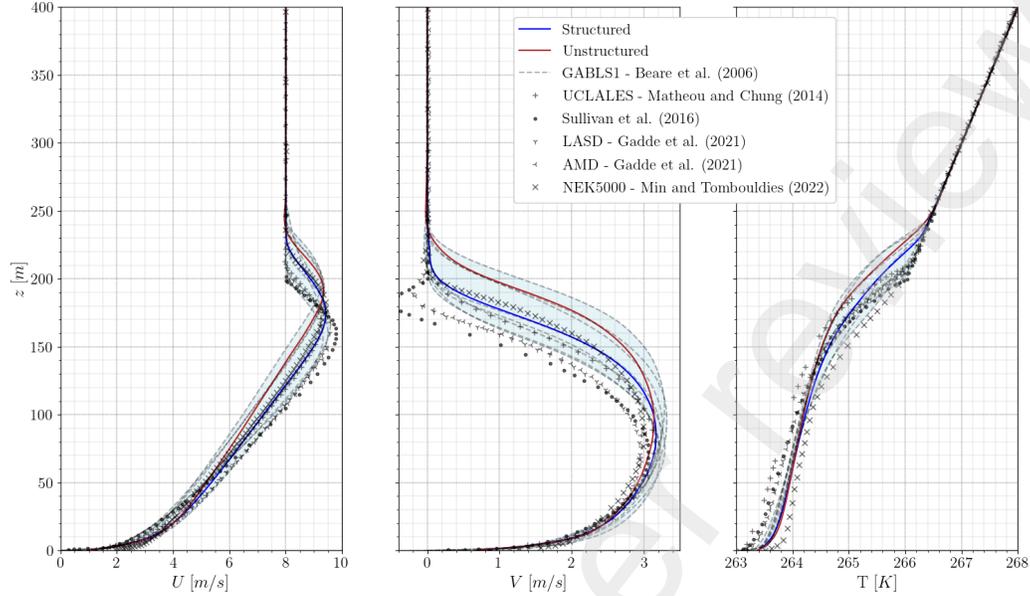
213 To validate the use of unstructured meshes for the simulation of atmo-  
214 spheric flows, the first step is to assess the mesh type impact by comparing  
215 results from both unstructured and structured grids. The mesh resolution is  
216 chosen as advised by [12] to be optimal for robust LES, i.e.  $\Delta x = 3.125 \text{ m}$   
217 for an isotropic grid. Grids are referred as  $S3$  and  $U3$  for structured and  
218 unstructured grids, respectively, according to Tab. 1.

219 Time series of frictional velocity, wall heat flux and Monin-Obukhov  
220 length are shown in Fig. 2. All of these variables fall within the dispersion  
221 envelope of the original GABLS1 study results [12]. As far as the frictional  
222 velocity is concerned, the results are quite similar for both kind of grids even  
223 if the  $S3$  grid results are slightly lower. Particularly interesting, the  $U3$   
224 results fit its counterpart obtained with the state-of-the-art and commonly  
225 used tool PALM [35].

226 The same observation can be made for the Monin-Obukhov length, which  
227 is similar for both grids. After a strong decrease during the first hour, it  
228 quickly converges to  $O(100) \text{ m}$ . Wall heat fluxes for the  $S3$  and  $U3$  cases  
229 exhibit similar physical behaviour and decrease with time due to the cool-  
230 ing rate. However, a gap starts developing after 1 h, reaching a maximum  
231 between the 7th and 8th hour where a 14% average wall heat flux difference  
232 is measured. This gap could be explained by a numerical effect of the mesh  
233 type. Some time after the initialisation where the flow is laminar, a flow  
234 destabilization process occurs leading to the development of the stable tur-  
235 bulent boundary layer. This development is directly impacted by the initial



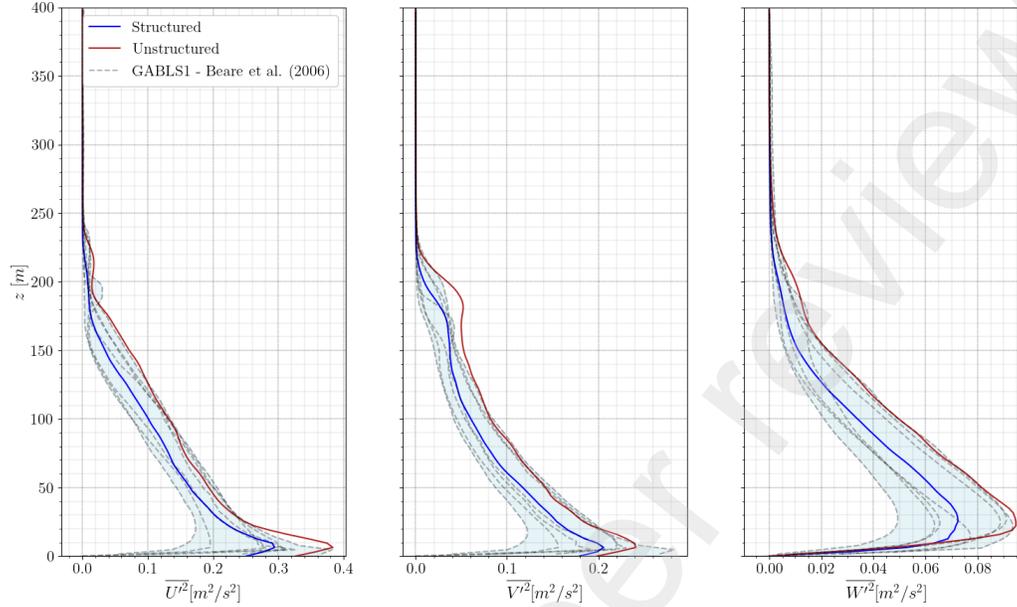
**Figure 2:** Frictional velocity, wall heat flux and Monin-Obukhov length with  $S3$  and  $U3$  grids, compared to original GABLS1 results dispersion [12] and PALM results [35].



**Figure 3:** Streamwise and tangential velocities and temperature profile for meshes  $S3$  and  $U3$  with cell size  $\Delta x = 3.125$  m. Blue shaded area stands for the original GABLS1 study results dispersion [12] and symbols for more recent studies [17, 13, 19, 14].

236 temperature field which contains random values, and so is different from one  
 237 simulation to another. More information on these sources of errors are given  
 238 into Appendix 4. This destabilisation process could also explain the strong  
 239 jump in some GABLS1 original results of Fig. 2. Consequently, mesh type  
 240 and resolution will have an impact on the flow development which cannot  
 241 converge to the same results since the boundary conditions are unsteady.

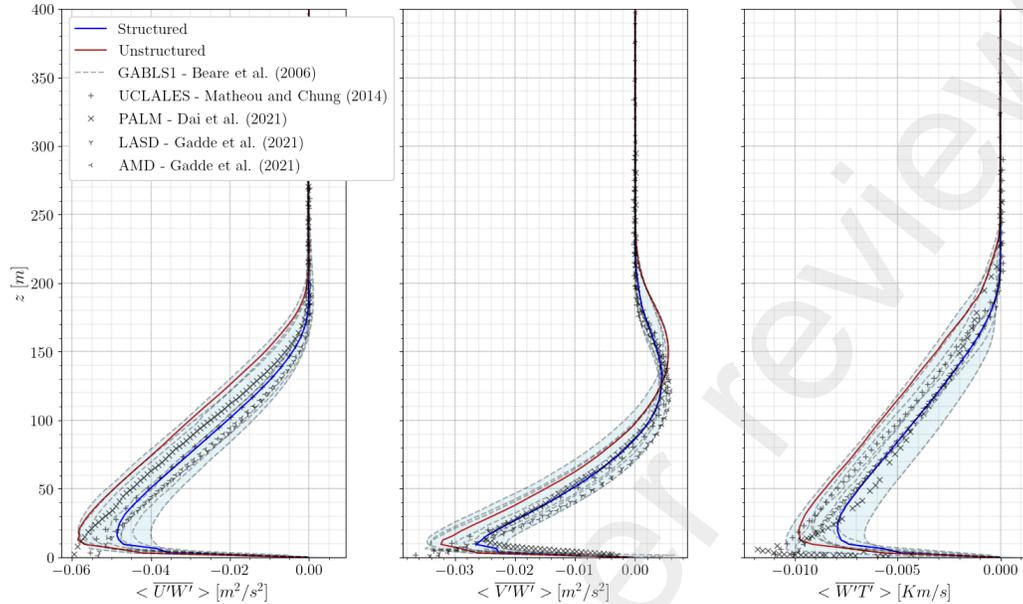
242 Following the GABLS1 recommended post-processing procedure, the pro-  
 243 files are spatially averaged over horizontal planes and temporally averaged  
 244 between the 7th and 8th hour. The streamwise velocity  $U$ , tangential velocity  
 245  $V$  and temperature  $T$  profiles are plotted in Fig. 3 and compared to the orig-  
 246 inal GABLS1 results [12] as well as more recent studies [17, 13, 35, 19, 14].  
 247 The streamwise velocity is zero at the bottom of the domain and is set to the  
 248 geostrophic wind at the top. The stable boundary layer is developed with  
 249 a velocity peak between 160 and 200 m. The tangential velocity, being zero  
 250 in the geostrophic wind, starts to grow by descending into the domain due  
 251 to the Coriolis effect. In the vicinity of the wall, where the friction effect is



**Figure 4:** Streamwise, tangential and vertical velocity variances with  $S3$  and  $U3$  of cell size  $\Delta x = 3.125$  m. Blue shading stands for the original GABLS1 study results dispersion [12].

252 dominant, the tangential velocity is reduced to zero. The temperature pro-  
 253 file shows a behaviour correlated with both velocity profile with an increase  
 254 with height and a bend between 150 and 200 m. All three profiles show dif-  
 255 ferences between  $S3$  and  $U3$  simulations but remain within the dispersion  
 256 of the GABLS1 results. The  $U3$  simulation has a streamwise velocity peak  
 257 offset of 20 m compared to  $S3$ , also visible on the tangential velocity pro-  
 258 file and on the temperature inflection point. More recent studies are also  
 259 compared, most of which show a similar behaviour but also expand the origi-  
 260 nal results dispersion. For example, Sullivan [13] exhibits an unexplained  
 261 negative tangential velocity near the top of the boundary layer. This results  
 262 spreading enlargement show the difficulty in having reference data but assure  
 263 some confidence in our results with both meshes.

264 Variance of streamwise  $\overline{U'^2}$ , tangential  $\overline{V'^2}$  and vertical  $\overline{W'^2}$  velocities are  
 265 plotted in Fig. 4. All three velocity variances are zero in the geostrophic  
 266 region due to the imposition of the sponge layer and increase by decreasing  
 267 the height. In the vicinity of the wall the variances dampen through the wall  
 268 model impact. For all three components, the  $U3$  configuration always shows



**Figure 5:** Momentum and heat fluxes for meshes  $S3$  and  $U3$  with cell size  $\Delta x = 3.125$  m. Blue shading stands for the original GABLS1 study results dispersion [12] and symbols for more recent studies [17, 35, 19].

269 higher values than  $S3$ , regardless of the ground distance, showing a higher  
 270 fluctuation level with the unstructured mesh.

271 The momentum fluxes  $\langle U'W' \rangle$ ,  $\langle V'W' \rangle$  and the heat flux  $\langle W'T' \rangle$  are plot-  
 272 ted in Fig. 5. Similar global behaviour is observed for all fluxes. Nevertheless,  
 273 a similar vertical offset for the  $U3$  mesh compared to  $S3$  is observed, here  
 274 due to the higher level of fluctuations. These results are again well within  
 275 the GABLS1 scatter and similar to recent studies.

276 To summarize, both  $S3$  and  $U3$  simulations bring similar results as other  
 277 studies, even though differences are noticeable among them. Firstly, the  
 278 temperature profile presents a lower temperature inflection. This gap is the  
 279 source of the difference in the averaged velocity profile. Secondly, a lower  
 280 wall heat flux, but higher in norm, generates more turbulent kinetic energy  
 281 and thus more velocity variances.

282 The gap on heat flux profile might be the cause of the total wall heat  
 283 flux time deviation. Indeed, a different momentum flux at the wall implies a  
 284 different scalar flux, thus a different wall heat flux. Three causes have been  
 285 identified for this phenomenon: the grid quality, the order of the numerical

286 schemes and the accuracy of the flux estimations. For the grid quality, both  
287 grids have the same characteristic cell size but not the same quality. As the  
288 *S3* mesh is structured and possesses uniform hexahedron, its quality is good  
289 and homogeneous. On the contrary, the *U3* grid is unstructured and so each  
290 tetrahedron constituting the mesh can vary locally.

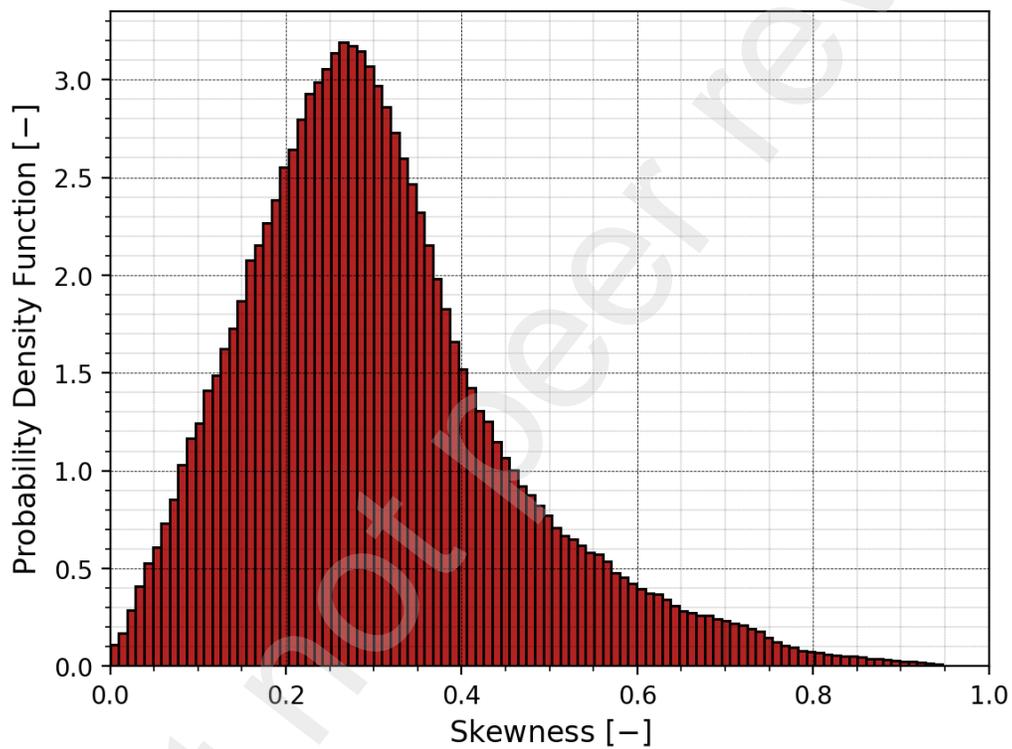
291 Grid quality can be evaluated via the skewness parameter, which mea-  
292 sures the deviation between the existing cell and an optimal cell. Figure 6  
293 shows the *U3* grid skewness distribution. The *U3* skewness is mainly around  
294 0.3, but reaches locally values of 0.96 with 0.5% of elements with a skewness  
295 higher than 0.8. Other unstructured meshes follow the same distribution.  
296 Spatial numerical schemes commit interpolation and approximation errors  
297 while transporting the velocity and the temperature variables. A poor grid  
298 quality will increase these errors, leading to more numerical diffusion errors  
299 and so affecting the results.

300 Moreover, while YALES2 spatial numerical scheme are 4<sup>th</sup> order, this is  
301 only true on uniform and regular grid. Due to the cell size variations of the  
302 *U3* mesh, this integration drops to 3<sup>rd</sup> order, leading to higher numerical  
303 error level and so may cause different flow behaviour. Finally estimating the  
304 flux at the wall is known to be quite an arduous task. For unstructured grids,  
305 the estimation gets even more complex if the mesh is irregular, causing face-  
306 to-face flux irregularities related to the wall mesh. Because of these three  
307 sources of error, each grid type simulation deviates from each other, ending  
308 on different wall fluxes and as a result different velocity and temperature  
309 fields.

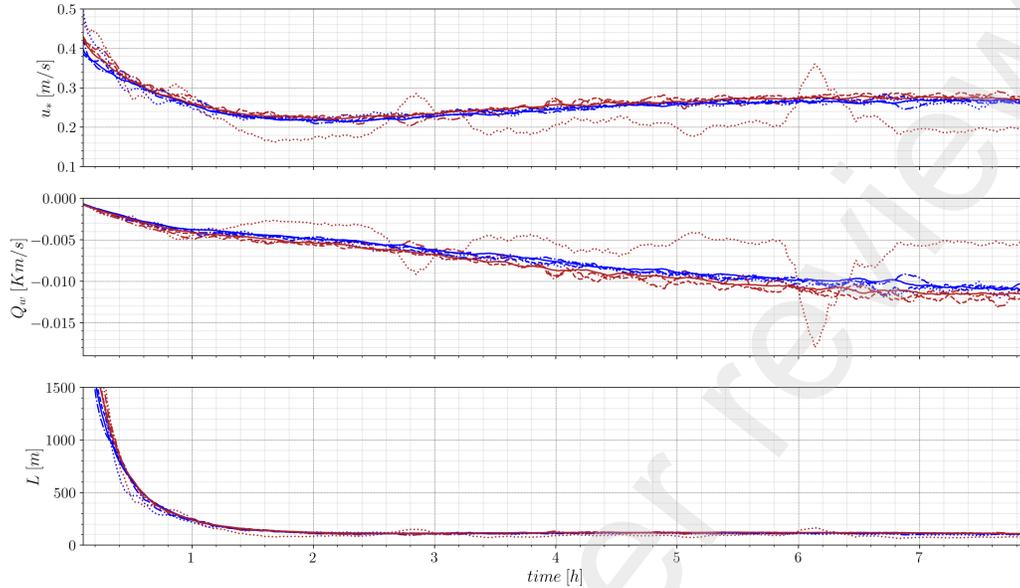
310 Nevertheless, it can be concluded that both structured and unstructured  
311 grids simulations are correctly reproducing the SBL of the GABLS1 config-  
312 uration. All studied quantities are well within previous studies data spread.  
313 Minor differences between *S3* and *U3* have been highlighted particularly in  
314 the wall heat flux and three sources of error have been highlighted: the grid  
315 quality, the order of the numerical schemes and the accuracy of the flux  
316 estimation.

### 317 3.2. Sensitivity to resolution

318 After assessing the impact of the use of unstructured meshes on a recom-  
319 mended mesh resolution, the impact of the grid resolution on the simulation  
320 results is now studied. Hence, a sensitivity to resolution study with a grid  
321 resolution varying from  $\Delta x = 12.5$  m to  $\Delta x = 2$  m is performed. Simulations  
322 are referred as *S1* to *S4* and *U1* to *U4* for structured and unstructured grids,



**Figure 6:** Probability density function (PDF) of the skewness distribution for  $U3$  mesh.

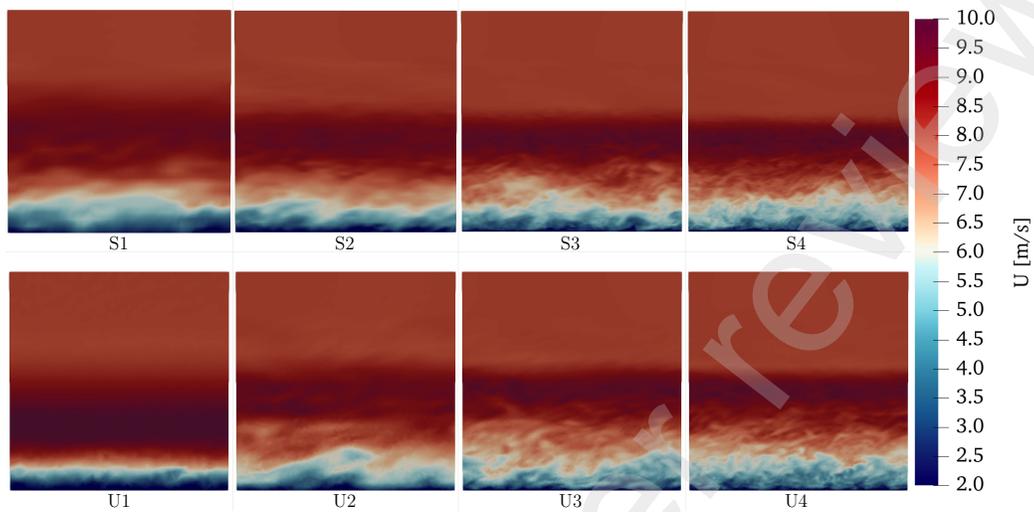


**Figure 7:** Frictional velocity, wall heat flux and Monin-Obukhov length time series. Blue and red lines stand for structured and unstructured grids, respectively. 4 resolutions are plotted:  $\Delta x = 12.5$  m (.....),  $\Delta x = 6.25$  m (-...),  $\Delta x = 3.125$  m (- - -) and  $\Delta x = 2$  m (—).

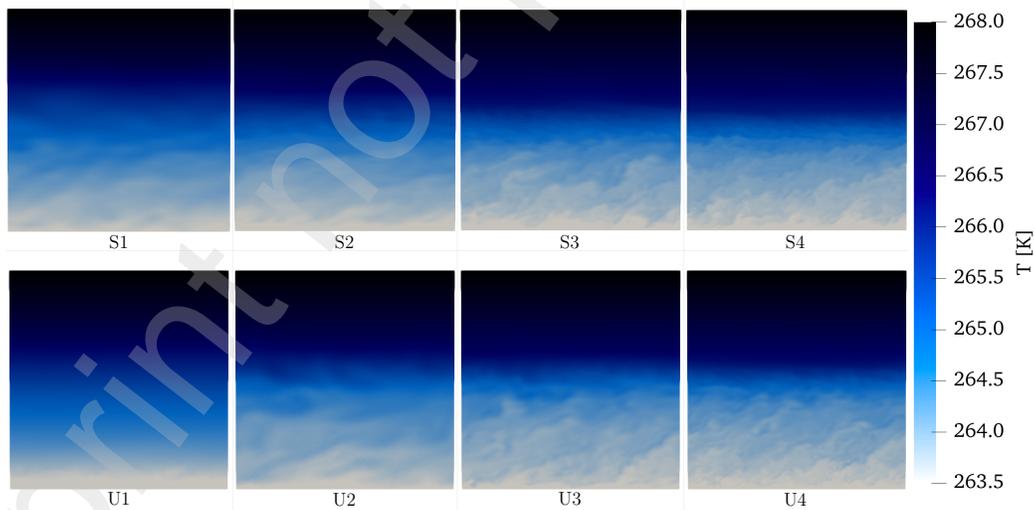
323 respectively. Each number corresponds to the resolution level according to  
 324 Tab. 1.

325 Wall integrated quantities time series are shown in Fig. 7. All results be-  
 326 have similarly except for  $U_1$ , which gives results that are irrelevant. While the  
 327 friction velocities for the structured grid simulations show slightly lower and  
 328 more noisy values, the differences in the wall heat flux are more pronounced.  
 329 Unstructured grids simulations show a greater heat flux with respect to the  
 330 structured grids. This difference has an impact on the temperature, veloc-  
 331 ity and flux profiles as seen in Section 3.1. However, finer meshes tend to  
 332 converge to a similar value, although not perfectly matching, reducing the  
 333 numerical diffusion and allowing for better gradient estimation. This be-  
 334 haviour supports the destabilization process influence caused by numerical  
 335 error as the source of the gap between the two grid types. For the Monin-  
 336 Obukhov length, which is a more global variable, all simulations are nearly  
 337 identical.

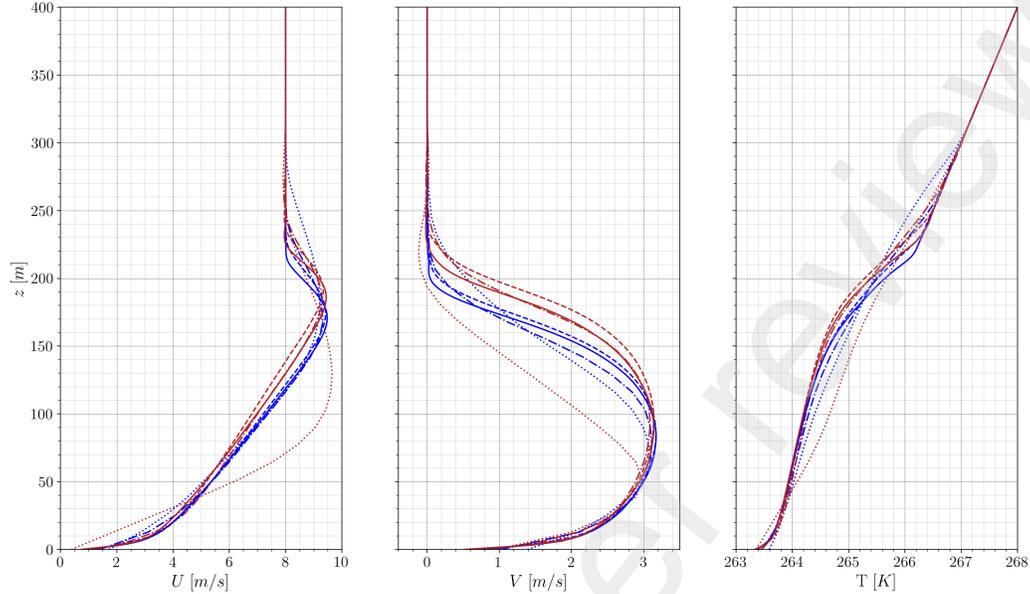
338 Figs. 8 and 9 show instantaneous velocity and temperature planes, re-



**Figure 8:**  $XZ$  velocity planes at  $Y = 200$  m. Top: structured cases, bottom: unstructured cases. From left to right mesh resolution increases.



**Figure 9:**  $XZ$  temperature planes at  $Y = 200$  m. Top: structured cases, bottom: unstructured cases. From left to right mesh resolution increases.

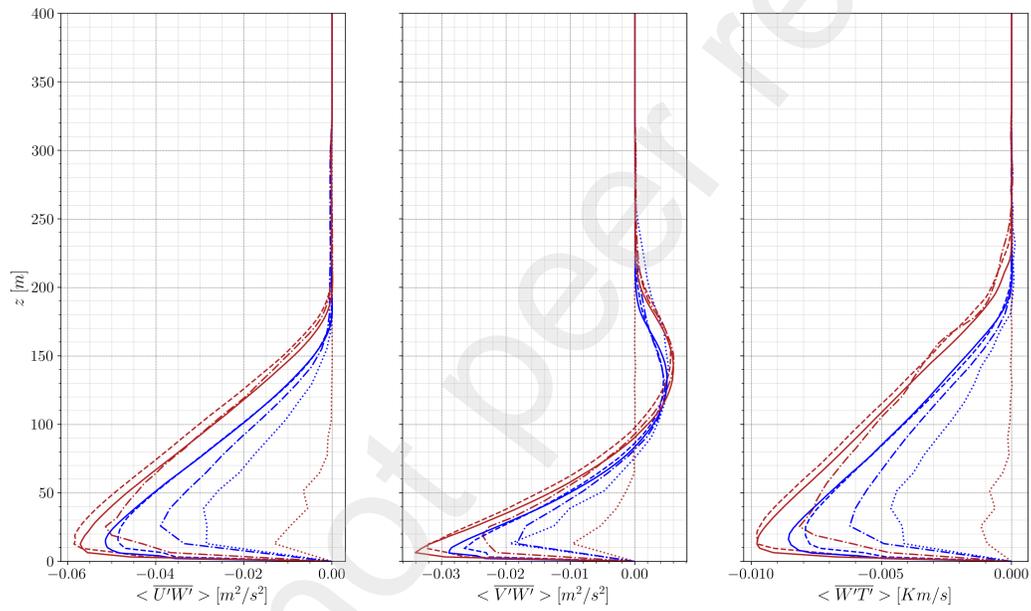


**Figure 10:** Average velocity and temperature profile. Blue and red lines stand for structured and unstructured grids, respectively. 4 resolutions are plotted:  $\Delta x = 12.5$  m (.....),  $\Delta x = 6.25$  m (-.-.),  $\Delta x = 3.125$  m (- - -) and  $\Delta x = 2$  m (—).

339 spectively. These planes are normal to the  $Y$  direction, at  $Y = 200$  m. This  
 340 qualitative display shows the impact of the mesh resolution on the flow. By  
 341 refining, more vortices are captured. At a glance, there is a noticeable dif-  
 342 ference between the resolution levels, but not between the structured and  
 343 unstructured cases.

344 Figure 10 presents the velocity and temperature profiles spatially aver-  
 345 aged over horizontal planes and temporally averaged between the 7th and 8th  
 346 hour. Again, except for  $U1$ , all other grids show similar behaviour. The trend  
 347 highlighted in Section 3.1, where the unstructured grid has a temperature in-  
 348 flection above the one of the structured case, is confirmed for all resolutions.  
 349 The streamwise and tangential velocities return to the geostrophic wind at  
 350 higher altitudes.

351 The momentum and heat flux profiles for all meshes are shown in Fig. 11.  
 352 For all resolutions except the coarsest, the unstructured grids exhibit stronger  
 353 fluxes. For the coarsest resolution, fluxes are near zero because the flow  
 354 behaviour is far from expected with a boundary layer that no longer resembles  
 355 a stable atmospheric layer. Fluxes are stronger with a finer mesh with both



**Figure 11:** Average momentum and heat fluxes profile. Blue and red lines stand for structured and unstructured grids, respectively. 4 resolutions are plotted:  $\Delta x = 12.5\text{ m}$  (.....),  $\Delta x = 6.25\text{ m}$  (-.-.),  $\Delta x = 3.125\text{ m}$  (-.-) and  $\Delta x = 2\text{ m}$  (—).

356 structured and unstructured grids. As expected, a finer grid is less dissipative  
357 and captures more turbulent kinetic energy. Again, the difference in wall heat  
358 fluxes leads to differences in momentum and heat fluxes profiles along the  
359 height. Stronger heat flux observed with the unstructured grid simulations  
360 leads to more fluctuations. Finally, all cases give satisfactory results except  
361 the structured and unstructured coarsest meshes, which will not be further  
362 considered into the analysis.

363 The boundary layer height was measured to evaluate the LES quality [12].  
364 The calculation of the boundary layer height is based on the turbulent  
365 stress [11]. Its disappearance means a transition to a non-turbulent layer, i.e.  
366 the top of the ABL. It is worth noting that the calculation of the boundary  
367 layer height is often based on the heat flux. However, it may be inaccurate  
368 if the heat flux is affected by gravity waves, which predominate at the top  
369 of the ABL. Following this definition, the SBL top height is defined as the  
370 one where the tangential turbulent stress is reduced to  $\alpha = 5\%$  of its sur-  
371 face value. Linear extrapolation is then used to evaluate the boundary layer  
372 height:

$$h = \frac{z|_{\langle \overline{U'W'} \rangle = \alpha u_*^2}}{1 - \alpha}. \quad (9)$$

373 Table 2 summarizes the boundary layer height from different studies with  
374 different codes and grid resolution. In both of our simulations as well as  
375 in other studies, the boundary layer heights tend to decrease with the grid  
376 resolution, converging towards  $\sim 160-175$  m. As more turbulent fluctuations  
377 are captured as shown in Fig. 11. It is noted that simulations based on  
378 unstructured grids provide a boundary layer that is 10% higher.

379 The original GABLS1 study [12] used their most refined mesh simula-  
380 tions, with a grid cell size of  $\Delta x = 1$  m, as references. The average boundary  
381 layer height at this resolution is 157 m. Compared to this reference, all com-  
382 putations showing an ABL height difference of less than 20% are considered  
383 accurate. Following this criterion, both structured and unstructured grids  
384 present an accurate behaviour, i.e. from 3.8% to 2.5% deviation for the  
385 structured grid and from 18% to 14% deviation for the unstructured one.  
386 This is in line with the original study advised requirements: a minimum grid  
387 length of  $\Delta x = 6.25$  m to obtain a stable boundary layer height accuracy of  
388 20%.

389 Quantifying the height of the boundary layer is essential, but not suffi-  
390 cient. While interesting, a similar boundary layer height does not reflect the

$\Delta x$ [m]	12.5	6.25	3.125	2
GABLS1 [12]	215	188	182	174
Cuxart et al. [37] - LES	-	-	177	-
Stoll and Porté-Agel [38]	-	-	173	-
Huang and Bou-Zeid [16]	-	-	-	158
Abkar and Moin [34]	168	165	169	-
Gadde et al. [19]	-	-	-	166 – 176
Min et al. [14]	-	-	160	-
Current work - Unstructured	149	180	186	179
Current work - Structured	149	163	162	161

**Table 2:** Boundary layer heights in various studies, depending on the grid resolution.

Mesh type	Quantity	$\Delta x$ [m]			
		12.5	6.25	3.125	2
Unstructured	$\langle U \rangle$	9.2	4.8	5.9	4.6
	$\langle T \rangle$	0.09	0.08	0.09	0.07
Structured	$\langle U \rangle$	5.3	2.9	2.7	1.9
	$\langle T \rangle$	0.09	0.06	0.05	0.03

**Table 3:** Relative  $L2$  norm error in % of the horizontal average velocity and temperature profiles compared to the reference profiles from [12].

391 global behaviour of the boundary layer or the amplitude of the over-speed  
392 region. To be more quantitative in this respect, another criterion have been  
393 used. The relative  $L2$  norm error. The simulation designed as a reference  
394 in [12] have been used as reference. The relative  $L2$  norm error have been  
395 measured on horizontal average velocity and temperature profiles. Values  
396 are gathered in Tab 3. Excluding the coarsest meshes, the  $L2$  norm error  
397 on streamwise velocity does not exceed 6%, while on temperature it remains  
398 under 0.1%. By refining the mesh, the  $L2$  norm error decreases but is within  
399 an envelope, showing a grid convergence below  $\Delta x = 6.25$  m. Overall, the  
400 obtained results present a very good agreement to the original study, proving  
401 the validity of the methodology to correctly reproduce the stable atmospheric  
402 boundary layer dynamics.

#### 403 4. Conclusions and openings

404 A high-order incompressible Navier-Stokes solver able to perform LES  
405 of a stable boundary layer on unstructured meshes was developed, which is  
406 not straightforward. It takes into account the Coriolis force, the Boussinesq  
407 approximation for buoyancy-driven flows and the Monin-Obukhov similarity  
408 theory for wall modeling. This framework was validated against the GABLS1  
409 setup. Time-averaged and variance of quantities like velocity, temperature  
410 and fluxes were compared with both structured and unstructured meshes of  
411 similar advised homogeneous cell size  $\Delta x = 3.125$  m. Very good agreement  
412 was obtained with both meshes compared to the initial and to more recent  
413 studies. Minor differences between the two setups were highlighted: the un-  
414 structured grid produces slightly more numerical diffusion of the temperature  
415 scalar than the structured grid.

416 Moreover, the gradient estimation is also more difficult in the unstruc-  
417 tured formalism, leading to a less accurate prediction of the flux. As a con-  
418 sequence, the destabilization of the stable boundary layer occurs differently,  
419 resulting in a slight gap between the results at the end of the simulation.  
420 The boundary layer height is 10% higher with the unstructured grid, with  
421 stronger velocity variances as momentum and heat fluxes. However, these  
422 differences remain small compared to the range of results from other studies.  
423 It appears that the subgrid scale models [19], numerical methods [10, 20],  
424 and grid resolutions [35] have more influence on the results than the use of  
425 an unstructured grid.

426 A sensitivity to grid resolution study was also performed. The boundary  
427 layer height was measured and showed that a grid length of  $\Delta x = 6.25$  m is  
428 sufficient to obtain a 20% accuracy. The relative  $L2$  norm errors of stream-  
429 wise velocity and temperature profiles to a reference high resolution study  
430 were also calculated for both structured and unstructured grids with less than  
431 6% for both meshes. Thus, a  $\Delta x = 6.25$  m grid size for both structured and  
432 unstructured meshes is sufficient to produce a simulation with a reasonable  
433 accuracy, but a  $\Delta x = 3.125$  m grid size is ideal for a robust LES.

434 To conclude, properly reproducing a stable boundary layer using unstruc-  
435 tured grid has been performed for the first time to the author's knowledge.  
436 More geometrically complex cases will then be investigated where structured  
437 grids are unqualified like complex terrain simulations.

#### 438 **acknowledgements**

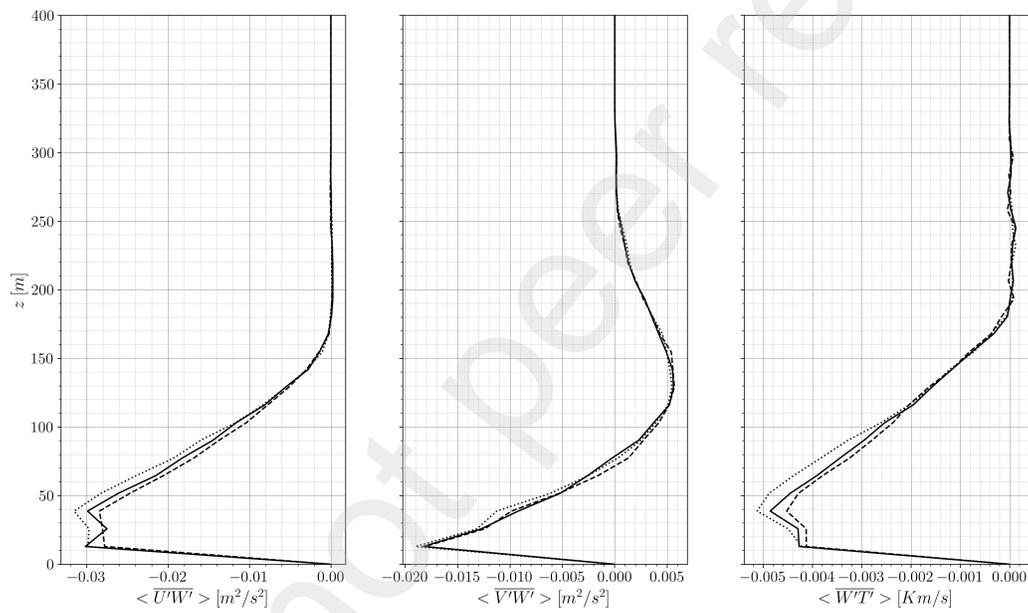
439 This work has been initiated during the Extreme CFD Workshop &  
440 Hackathon (<https://ecfd.coria-cfd.fr>). This project was provided with com-  
441 puter and storage resources by GENCI at TGCC thanks to the grant 2023-  
442 A0142A11335 on the supercomputer Joliot Curie's ROME partition and to  
443 CRIANN resources under the allocation 2012006.

#### 444 **Appendix 1: GABLS1 source of errors**

445 Two sources of debate can be highlighted in the design of the GABLS1  
446 benchmark [12]: initial condition definition and numerical errors accumula-  
447 tion.

##### 448 *Initial condition definition*

449 . The initial condition vertical temperature profile of the GABLS1 bench-  
450 mark is spatially uniform, set to  $T = 265$  K from the ground up to  $z = 100$  m  
451 and then increases by 1 K/100 m. To help the flow destabilization process,  
452 a random potential temperature perturbation of 0.1 K amplitude is super-  
453 posed to the profile between  $z = 0$  m and  $z = 50$  m. The definition of this  
454 random perturbation is left to the user's discretion, which is questionable.  
455 Commonly, users add a randomly generated noise on each control volume  
456 which is spatially uncorrelated. This can clearly have an impact on the flow  
457 evolution and will depends on the mesh resolution and grid partitioning.



**Figure 12:** Horizontally averaged momentum and heat fluxes vertical profile s on S3 mesh. Results with seed 1 and 1 CPU core (—), seed 2 and 1 CPU Core (---) and seed 1 and 4 CPU cores(.....).

458 To quantify its impact on the flow behaviour, two identical simulations  
459 based on the  $\Delta x = 12.5$  m structured grid are performed with the only dif-  
460 ference being the random number seeds. Figure 12 shows the momentum  
461 and heat fluxes profiles spatially averaged over horizontal planes and tempo-  
462 rally averaged between the 7th and the 8th hour, so long after initialization.  
463 Results present a clear dependency on the random seed, with noticeable dif-  
464 ferences, showing a different flow evolution between the initialisation and the  
465 8th hour. Similar gaps are observed for average velocity, temperature and ve-  
466 locity variance and these results are reproducible for different grid resolutions  
467 and numerical schemes, but not shown here for the sake of clarity.

468 This effect means that a small change in the initial profile affect the  
469 behaviour of the flow and so the collected statistics. It can distort the com-  
470 parison between codes since the random number generation will necessarily  
471 be different. Moreover, this random number is only determined by an ampli-  
472 tude and a mean, analogous to a white noise without spatial coherence. As  
473 different grid resolution were used in all GABLS1 studies, different fluctua-  
474 tion frequency were added. Since the flow behaviour is sensitive to this initial  
475 profile, part of the differences obtained when comparing two resolutions can  
476 be explained by this phenomenon. Similarly, it could also explain differences  
477 between structured and unstructured grids. Adding constraints on the ran-  
478 dom number, such as giving the fluctuation frequency or giving some spatial  
479 correlation, would help in having similar initial condition, whatever the mesh  
480 type and resolution. The perturbation would then be analogous to pink noise  
481 instead of white noise. The results would still depend on the random num-  
482 ber seed but at least would minimize differences when comparing different  
483 resolutions.

#### 484 *Numerical errors accumulation*

485 . Theoretically, a deterministic behaviour of the simulation is expected, since  
486 the resolution of the Navier-Stokes equations is fully deterministic. Simula-  
487 tions are reproducible and all states can be derived from the input data.  
488 However, numerical errors can lead to non-deterministic flows, i.e. different  
489 results can be obtained with identical input data. The sources of numerical  
490 errors are various: node reordering, machine precision, operation orders, etc.  
491 In this respect, the grid partitioning and so the number of CPU cores used in  
492 a LES can cause variations in the results. It has been demonstrated that the  
493 propagation of numerical errors is linear for laminar flows but exponential  
494 for turbulent flows [39]. This difference between laminar and turbulent flows

495 is due to the true chaotic nature of turbulence.

496 To illustrate this effect, two identical simulations were performed on the  
497  $\Delta x = 12.5$  m structured grid with different number of CPU cores: one simu-  
498 lation with 1 CPU, the other with 4 CPUs and by keeping the same random  
499 generator seed). Figure 12 shows the momentum and heat fluxes profiles for  
500 both cases. Momentum and heat fluxes profiles show discrepancies depending  
501 on the number of CPUs used. Similar gaps are observed for other quantities  
502 and is reproducible with other grid resolutions and numerical schemes but  
503 are not shown for the sake of brevity. As the errors accumulate quickly,  
504 working with higher machine precision will not suppress the error propaga-  
505 tion but only delay it. Since error propagation is exponential, the flow paths  
506 will always diverge [39]. To circumvent this effect, several simulations with  
507 different random number generations could be performed and averaged to  
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