LES grid resolution requirements for the modelling of gravity currents

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Highlights

- Grid resolution requirements for LES model of gravity current accessed
- Cannot examine time averaged properties since transient flow
- Metrics for assessing suitable mesh resolution are identified.
Title: LES grid resolution requirements for the modelling of gravity currents

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Abstract

The influence of the grid resolution on the large eddy simulation (LES) of a lock-exchange turbidity current is investigated. The simulations are performed using a finite volume Boussinesq code with a Smagorinsky turbulence model for a range of buoyancy Reynolds numbers, ranging from transitional currents (\(Re_b = 1,000\)) to fully-developed turbulence (\(Re_b = 60,000\)). The general features of the flow and the relative independence of the current front for \(Re_b > 10,000\) are correctly predicted. In agreement with previous research, the spanwise two-point correlations are found to be the most useful quantities to assess the mesh resolution. In addition, velocity power spectrum densities are used to provide information on the maximum cell size required to ensure the LES filter cutoff wavelength is inside the inertial range of the turbulence spectra. We show that at low Reynolds numbers, the turbulence model is too restrictive and direct resolution (DNS) is preferable. For \(10,000 < Re_b < 60,000\), the combination of the different criteria lead to a minimum resolution of \(1140 \times 37 \times 74\) cells for coarse LES, and \(1925 \times 62 \times 125\) cells for well-resolved LES, regardless of the Reynolds number. Finally, recommendations are made on how to achieve a well-resolved LES based on examination of the vertical profiles of
the ratio of SGS viscosity to molecular viscosity, and of the SGS shear-stress to the resolved Reynolds stress.

**Keywords:** Gravity current; lock-exchange; finite volume method; large eddy simulation; grid resolution.

1. Introduction

Gravity currents are a category of flows arising when a higher density fluid starts flowing into a second or identical fluid of lower density. The motion is driven by buoyancy forces that originate in biological, mineral or chemical species concentration and temperature gradients in the fluid. The general theory describing gravity currents is detailed by Ungarish [1]. Gravity currents are commonly observed, exist in a wide range of physical conditions and represent a challenging research topic. In fluvial and marine environments a specific type of gravity current is observed when an accumulation of sediment starts sliding down a slope, taking the form of an underwater avalanche. Those turbidity currents are sustained by the varying concentration of sediment particles in the fluid [2]. The currents can be triggered by natural geophysical events, such as earthquakes or volcanic eruptions [3], as well as human activities, such as bottom trawling (as observed in the Gulf of Maine in [4]). They are known to be a significant factor in sediment transport in rivers and oceans [2], and are an important cause of erosion. They can possess enough energy to cause critical damage to human installations, such as the destruction of submarine telegraph cables after the 1929 Grand Banks earthquake [5].

Historically, the understanding of the dynamics of turbidity currents is closely related to the study of gravity currents. Early works from Schmidt [6], [7] on gravity currents, later extended to turbidity currents [8-10], distinguish two main parts of the flow: a dense head, followed by a thinner decaying body. Experimental studies and shallow water theory predict that the current evolves through three phases, defined by the dominant forces acting upon it. During the initial phase, known as the slumping
phase, the buoyancy forces dominate and the front travels at a quasi-constant velocity. After travelling a certain distance, the current transitions into the self-similar phase, during which the front starts decelerating with the velocity following a $t^{-1/3}$ law [11, 12]. During the final phase, viscous forces start to dominate over the inertial-buoyant forces, and the current enters the buoyant-viscous phase characterised by an even faster deceleration which follows a $t^{-4/5}$ law [13, 14]. Several analytical models based on empirical observations have been derived to describe the dynamics of the currents, as is comprehensively reviewed by Garde and Raju [2].

The temporal evolution of physical quantities at fixed points can be experimentally studied using acoustic and optical measurement techniques such as Laser Doppler Velocimetry (LDV) and Ultrasonic Doppler Velocity Profiling (UDVP) [15]. The interface between the current and the ambient fluid is also trackable with image processing of high resolution camera records [16]. However, insight of the inner dynamics of the current is prevented by its opacity and the intrusive nature of many experimental devices.

CFD modelling is suited for understanding the inner workings of gravity and turbidity currents. Due to the complexity and the mesh requirements, the few attempts that have been conducted to solve geophysical cases, have used depth-averaged formulations of the equations [17, 18] or have solved the Reynolds Averaged Navier-Stokes (RANS) equations [19, 20]. Although some models give good results in terms of the general features of the current, they have the serious drawback of not depicting the turbulent structures sustaining the suspension of the particles. However, the substantial computer cost of methods capable of resolving the inner current turbulence has limited their application to laboratory scale flows. A standard lock-exchange configuration is the typical release mechanism, both experimentally and for numerical models. A common first approach consists in modelling the flow as a gravity current, in which the particles are considered in suspension and the Direct Numerical Simulation (DNS) of Härtel et al. [21] pioneered the use of high resolution simulations to provide a better under-
standing of the dynamic of lock-exchange currents [22, 23]. The models were further improved by Necker et al. [24], who accounted for the settling of turbidity currents particles, which was implemented in the TURBINS CFD code [25-27]. In comparison to DNS, Large Eddy Simulation (LES) has been shown to provide accurate results for a significantly lower computational cost [28-34] for high Reynolds number flows. In contrast to the finite difference and finite volume models of the previous references, Ottolenghi et al. [35] recently demonstrated the application of a Lattice Boltzmann solver to simulate lock-exchange currents, using a LES formulation using a constant Smagorinsky sub-grid-scale model. A detailed review of recent findings and the challenges of modelling gravity and turbidity currents is presented in Meiburg et al. [36], and a review of lock-exchange currents is given by Ooi [23].

As with any CFD model, the accuracy of LES is largely influenced by the quality of the grid resolution. The choice of the grid is complicated by the dependence of LES models on the mesh spacing [37]. Consequently, the grid resolution is typically left to the discretion of the user, and only a few studies provide details of the method used to determine a suitable mesh. For the near-wall region, Chapman [38] derived an estimate of the number of grid cells to correctly represent a turbulent boundary layer, which was later extended to flows at higher Reynolds numbers [39-41]. Outside the boundary layer, attempts have been made to define measures of the general grid resolution errors, such as the subgrid activity parameter \( s \), quantifying the turbulent dissipation in regards to the molecular dissipation [42] and the modified activity parameter \( s^* \) [43]. Celik et al. [43] introduced the relative Kolmogorov scale and SGS viscosity indices of resolution quality \( LES_{IQ_\eta} \) and \( LES_{IQ_\mu} \). Several studies have applied these indices for grid resolution assessment in different fields, such as combustion [44-46] or temperature-driven natural convection [47]. Unfortunately these metrics require the determination of the Kolmogorov length scale \( \eta_k \), which requires experimental or DNS data which is not necessarily available. To overcome this limitation, Celik et al. [43] introduced a third index calculated from
the resolved turbulent kinetic energy \( \text{LES IQ}_k = \frac{k_{res}}{k_{tot}} \). Assuming monotonic convergence of \( k_{res} \), the total turbulent kinetic energy \( k_{tot} \) can be estimated using Richardson extrapolation. While this method has been used in a wide range of studies, its applicability is debatable. Indeed, it does not differentiate the numerical errors from the turbulence modelling errors, which can complicate the extrapolation process [43, 48]. For example, Tóth and Lohász [49] obtain non-monotonic convergence of \( k_{res} \) for a developing axisymmetric shear layer, which is presumed to be the cause of the underestimation of the grid refinement effects by the \( \text{LES IQ}_k \). Manickam et al. [50] also observed the overprediction of \( k_{res} \) on their coarsest mesh due to a low estimate of the dissipation in the early stage of the flow development behind a bluff body.

Richardson extrapolation has been extended into a 3-equations systematic grid and model variation method that aims to dissociate the two errors in the calculation of \( k_{tot} \) [51, 52]. Despite providing a priori better performances in some cases [50, 51], Brandt [53] expresses doubts on the applicability of Richardson’s extrapolation to the quantification of both errors. By varying the filter width of the Smagorinsky model independently from the mesh size, a cross-error due to the coupling of the numerical and modelling errors was identified. Recent work by Tao [54] presented a more detailed verification and validation method to account for the three errors separately, in addition to the temporal error, through a 7-equations estimator. This procedure aims ultimately to derive assessment procedures from 1 to 6-equations estimators, carefully calibrated on the basis of validated sample results from the 7-equations estimator. Despite it being a tedious and time-consuming systematic protocol, it is clear that with sufficient validation this method may allow the generation of a valuable extensive LES database for users. Still, the calculation of the indices is not suitable for gravity currents, since the instantaneous turbulence statistics required for the computation of the turbulent kinetic energy are unavailable for these transiently evolving flows.
Alternatively, one can analyse the flow features and deduct the grid convergence from the comparison. Davidson [55] investigated the impact of grid refinement on a range of turbulence statistics for a hybrid LES-RANS simulation of a fully developed turbulent channel flow. He concluded that, rather than turbulence spectra, the comparison of the two-point correlations, the ratio of the subgrid scale (SGS) viscosity with the molecular viscosity, and the ratio of the SGS shear stresses with the resolved Reynolds stress are the most suitable verification quantities for grid resolution. Similar conclusions have been found from LES of a flow in a plane asymmetric diffuser [56], and the flow around a cubic building [57]. Despite demonstrating its usefulness, Bazdidi-Tehrani et al. [57] observed that the time-averaging required for calculation of two-point correlations of a quasi-steady flow, rendered it a time consuming and inconvenient technique. In addition, their calculation and relevance to non-quasi-steady flows such as turbidity currents is debatable.

To date there has been no published study of the impact of grid resolution on LES solutions of lock-exchange particle-driven currents. The present work aims to quantify the effect of grid resolution on the turbulence characteristics for currents with buoyant Reynolds numbers ranging from 1,000 (weak turbulence) to 60,000 (strong and fully developed turbulence). The study is limited to the case of suspended particles in the fluid, and the current being described as a regular gravity current. First, we assess the impact of the grid resolution on general current features. Then we investigate resolved velocities power spectrum densities, two-point correlations and the ratio of the SGS viscosity to the molecular viscosity. The results provide a guide on how to choose suitable grid resolution for LES modelling of lock-exchange gravity currents and implications are discussed.
2. Problem definition and numerical model

2.1. Lock-exchange configuration and LES governing equations

The study focuses on a typical 3D lock-exchange configuration, as shown in Figure 1. The left box represents the lock of dimensions \( L_{x,l} \times L_{y} \times L_{z} \), initially filled with a fluid of density \( \rho_1 \). The right white part corresponds to the channel of dimensions \( L_{x,c} \times L_{y} \times L_{z} \), filled with water of lower density \( \rho_0 \). At \( t = 0 \), the fluid contained in the lock is released and starts flowing into the channel. The channel is based on the experimental work of Wilson et al. [16] and has the dimensions \( L_{x,l} = 0.58 \text{m}, L_{x,c} = 5.58 \text{m}, L_{c} = 0.4 \text{m} \) and \( H = 0.3 \text{m} \).

![Figure 1](image_url)  
*Figure 1: Representation of the Lock-exchange channel. The left blue part is the lock initially filled with water loaded with particles and the right grey part is the channel initially filled with water.*

A concentration buoyancy driven flow is used as the model. The motion of the fluid is consequently described by the continuity and the momentum equations, together with a transport equation for the particles’ concentration. The difference of density inside the fluid is low enough to remain in the range suitable for the Boussinesq approximation. Thus, the set of equations can be simplified by assuming a constant density equal to the reference density \( \rho_0 \), except in the gravity-buoyancy term of the momentum equations, where the density variations are assumed to show a linear dependency on the particle concentration,
\[(\rho - \rho_0)g = \rho_0 \beta (m - m_0)g \quad (2.1)\]

where \(m\) and \(m_0\) are respectively the concentrations at density \(\rho\) and \(\rho_0\), \(\beta\) is the volumetric coefficient of expansion for the particles, and \(g\) is the acceleration due to gravity. Here, \(\rho_0\) corresponds to the density of the ambient fluid and \(m\) varies between \(m_0 = 0\) and \(m_{\text{max}} = 1\).

Introduced by Smagorinsky [58], the LES equations are derived from a truncation of the turbulent energy spectrum by subjecting the governing equations to a high pass filter. Denoting \(\mathcal{F}\) as the filtering operator, each physical quantity can be decomposed as \(X = \overline{X} + X'\), where \(X'\) denotes the contributions eliminated by the filter due to their length scale being smaller than the cut-off length of the filter, and \(\overline{X}\) the filtered largest structures that are resolved by the filter. The equations are presented in their dimensionless form. The length scale is chosen to be half the lock height \(H/2\). The velocity scale is the buoyancy velocity \(u_b = \sqrt{\frac{H}{2} \frac{\rho_1 - \rho_0}{\rho_0}} g\) based on the inertial efforts induced by the density difference between the ambient fluid and the fluid charged in particles inside the lock. The dimensionless variables \(\tilde{X}\) are then related to their physical form \(X\) by

\[x_i = \frac{x_i}{H/2} \quad u_i = \frac{u_i}{u_b} \quad t = \frac{\hat{t}}{(H/2)/u_b} \quad p = \frac{p}{\rho u_b^2} \quad (2.2)\]

In Einstein notation, the LES set of equations is subsequently written in (2.3), (2.4) and (2.5).

\[\frac{\partial \overline{u}_i}{\partial t} = 0 \quad (2.3)\]

\[\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial (\overline{u}_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \frac{1}{\text{Re}_b} \frac{\partial \overline{u}_i}{\partial x_j} \right] - \frac{\partial \tau_{ij}}{\partial x_j} + \overline{m} \epsilon_{i,j} \quad (2.4)\]

\[\frac{\partial \overline{m}}{\partial t} + \frac{\partial (\overline{u}_i \overline{m})}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \frac{1}{\text{Sc} \text{Re}_b} \frac{\partial \overline{m}}{\partial x_j} \right] - \frac{\partial \tau_{ij}^m}{\partial x_j} \quad (2.5)\]
where \( e_{i,g} \) is the normalized gravity vector. The hydrostatic pressure has been subtracted from the static pressure \( p = p_{\text{tot}} - \rho_0 g z \), reducing the rounding error that can occur in the calculation of pressure gradients [59]. The Reynolds number is based on the buoyancy velocity and lock’s half height as \( Re_b = (u_b H / 2)/\nu \). The Schmidt number \( Sc = \nu / \kappa \) is the ratio of the dynamic viscosity \( \nu \) to the particles’ concentration diffusivity \( \kappa \), and can be interpreted as the ratio of the diffusion of the momentum to that of the particles in the flow. Previous studies have shown that the currents properties are insensitive to the Schmidt number when \( Sc \geq 1 \), and in this study its value is set to \( Sc = 1 \) [25, 26, 28, 60].

The influence of the eliminated turbulent structures on the filtered components remains in the equations through the momentum and concentration residual-stress tensors \( \tau_i \) and \( \tau'''_i \).

\[
\tau_j = \frac{u_i u_j - \overline{u_i u_j}}{} \quad (2.6)
\]

\[
\tau'''_i = \frac{mu_i - \overline{mu_i}}{} \quad (2.7)
\]

The closure is made by modelling the residual tensors with the standard Smagorinsky model [58]. The components of \( \tau_j \) are expressed as a function of the corresponding filtered quantities by introducing a SGS eddy-viscosity \( \nu_{SGS} \).

\[
\tau_j = -2 \nu_{SGS} \overline{S_{ij}} \quad (2.8)
\]

\[
\nu_{SGS} = (C_s \Delta)^2 \sqrt{\overline{S_{ij}} \overline{S_{ij}}} \quad (2.9)
\]

\[
\overline{S_{ij}} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.10)
\]

where \( \overline{S_{ij}} \) is the strain tensor of the filtered velocity. The Smagorinsky coefficient \( C_s \) is based on experience and experimental data and commonly lies in the range 0.1 to 0.2; here \( C_s = 0.18 \) is used. \( \Delta \) is
the filter width, taken as $\Delta = \frac{V^{1/3}}{3}$, where $V$ is the volume of a cell. $\tau_i^m$ is modelled in a similar manner, with an eddy-diffusivity $\kappa_{SGS}$ related to $\nu_{SGS}$ through a fixed turbulent Schmidt number $Sc_t = 0.7$.

2.2. Cases definition

2.2.1. Near-wall resolution

Near-wall resolved LES requires a careful treatment of the grid resolution near non-slip walls to ensure the accurate calculation of the turbulent boundary layer. In the studied case, the bottom wall is defined as a non-slip wall. To accurately represent its boundary layer, wall-resolved LES requires that the first off-wall cell lies in the viscous-sublayer of the current’s boundary layer, and that the velocity at the first node from the wall respects the relations stated in (2.13) to (2.16).

$$y^+ < 10 \rightarrow \frac{u_1}{u_r} = y^+ \quad (2.11)$$

$$y^+ = \frac{u_1 \Delta y}{v} \quad (2.12)$$

$$u_e = \sqrt{\frac{\tau_w}{\rho}} \quad (2.13)$$

$$\tau_w = \mu \frac{\partial u}{\partial y}_{\text{wall}} \quad (2.14)$$

$u_i$ is the velocity at the first cell from the wall, $y^+$ is the dimensionless distance from the wall, $\Delta y$ is the height of the first cell adjacent to the wall, $\tau_w$ is the wall shear-stress and $u_r$ is the associated friction velocity. An estimation of the required height of the wall-adjacent cell can be made from experimental correlations describing $\tau_w$ such as (2.17) for $Re_i < 10^6$ [38, 39].

$$\tau_w = \frac{1}{2} c_f \rho U^2 \quad (2.15)$$

$$c_f = 0.0577 Re_x^{1/5} \quad (2.16)$$
\[ \text{Re}_x = \frac{U x}{\nu} \]  

(2.17)

In our case, the velocity length scale is \( U = u_b \). The analytical expression of the average first cell height \( \Delta y_{1,\text{ave}} \) is derived by integrating the local expression of \( \Delta y_{x,i} \) obtained from (2.14) to (2.19) over the channel length.

\[ \Delta y_{l,x} = \sqrt{\frac{0.0577}{2} \frac{y^+ \nu}{u_b} \text{Re}_x^{1/10}} \]  

(2.18)

\[ \Delta y_{1,\text{ave}} = \frac{1}{L_x} \int \Delta y_x dx = \frac{10}{11} \Delta y_{l,x} \]  

(2.19)

Furthermore, it is advised to have 10 to 30 cells within the layer \( 0 < y^+ < 100 \), to correctly resolve the boundary layer [38].

### 2.2.2. General grid resolution

The cell size for wall bounded flows is limited by the geometric and flow features of the case studied. On one hand, the size of the largest spanwise structures is restricted by the presence of the walls, to a maximum size \( H \). It is recommended to have a minimum of eight cells to represent the largest structures for an LES [55], but this number is insufficient for a well-resolved LES and more than 16 cells is typically assumed to be a minimum for an accurate LES. Therefore the maximum mesh size scales with \( H/16 \). On the other hand, the minimum mesh size of an LES should be, by definition, considerably higher than the dissipative Kolmogorov length scale, which, according to the energy cascade theory of homogeneous turbulence [37], scales with \( (H/2) \text{Re}^{-3/4} \). The mesh size \( h \) should consequently respect \( (H/2) \text{Re}^{-3/4} \ll h < H/16 \). If both boundaries are of the same scale, DNS should be preferred to LES. A minimum Reynolds’ scale to perform LES is defined by \( [ (H/16) / (H/2) ]^{4/3} = (1/8)^{-4/3} \approx 20 \) which is generally true for the cases we have studied. Consequently, the domain is divided into two regions; 1) A near wall region to account for the no slip bottom boundary layer of size
(L_{x,d} + L_{x,c}) \times h_w \times L_z \), with $h_w = H / 3$, and 2) a region with a uniform grid resolution in each axis with $\Delta x \approx \Delta y \approx \Delta z$. In the near wall region, the horizontal grid resolution is constant and the vertical grid is refined using a logarithmic distribution going from $\Delta y_1$, the size of the first cell at the wall, to $\Delta y$, the vertical grid size outside this region. The total number of cells can be written $N = N_w + N_d$, where $N_w = N_x \times N_{y,w} \times N_z$ corresponds to the number of cells in the near-wall layer, and $N_d = N_x \times N_{y,d} \times N_z$ is the uniform homogeneous grid resolution in the rest of the domain.

2.2.3. Reynolds number dependency

Flows have been studied for $Re_b$ varying between 1,000 to 60,000. Using the above specifications, six grid resolutions were chosen which are listed in Table 1. From (2.21), an estimation of the position of the first vertical node was determined to ensure $y^+ \approx 5$, and the actual $\Delta y_1$ was chosen by applying a factor of safety. The grid repartition was chosen to keep the ratio of mesh spacing between two consecutive cells below 1.2.
The flow is non-steady with the position and the structure of the current changing with time, and therefore the calculation of the time averaged quantities is not relevant. However, in case of sufficiently homogeneous turbulence, the turbulence statistics can be obtained through averaging in space over a sufficiently large region. The region of the body of the current directly following the head is the region of the current that experiences the highest shear and shows its most critical turbulent aspects, while being in the self-similar phase of the propagation of the current. Therefore, the turbulence statistics were calculated inside the current’s body at time $t = 29.1$. We observed large differences in instantaneous fields for different simulations of currents with the same Reynolds number. This limitation was overcome by averaging on the streamwise and spanwise direction in the red region shown on Figure 2.

To account for the differences in the predicted position of the current, the front position is used as the reference location for the definition of the averaging region. Those observed differences are due to refinement and differences in Reynolds numbers. The calculations are performed sufficiently far from the front. The front position $x_f$ is determined from the concentration fields averaged in the spanwise direction of the channel, and is chosen to be the maximum value of $x$ on the concentration isocontour.
\( c = 0.1 \). The front velocity is calculated from the front position by computing its derivative using a central differencing scheme.

\[ \frac{\Delta x}{\Delta t} = \frac{x_f - x_f - H}{\Delta t} \]

**Figure 2**: Representation of the averaging box used for the calculation of the turbulence statistics.

### 2.3. Numerical model and computational platform

The simulations are carried out using the structured non-staggered Cartesian finite volume SnS code, described in [59]. The filtered equations are solved using a fractional-step method with the advection terms discretized in time using an Adams-Bashforth scheme and the diffusion terms using the Crank-Nicolson scheme. Second order central differencing is used for the spatial discretization of the advection and diffusion terms. The momentum and Poisson equations are solved using a bi-conjugate gradient stabilised (BICGSTAB) method [61], with a strongly implicit procedure [62] preconditioner, and a Jacobi method is used for the transport equation. The time step is varied to maintain the value of the Courant-Lewy-Friedrich number \( (CFL = u \Delta t / \Delta x) \) in the range \( 0.15 – 0.25 \). The code was originally written for the efficient simulation of buoyancy-driven convective flows [63, 64], has been applied to
the modelling of wind turbine farms [65], and has been updated to model concentration driven convection.

To account for the mixing of the fluid done to homogenise the lock concentration in experimental work, the fluid filling the lock is initialised with a random repartition of velocity respecting $-0.45 < u_i < 0.45$. The fluid inside the channel is left at rest. The initial fluid’s motion before its release in the channel greatly accelerates the turbulence generation and the formation of the instabilities at the front of the current.

All the computations were performed on a high performance computational cluster provided by the New Zealand eScience Infrastructure (NeSI) consortium. Each node of the cluster had two Intel Xeon E5-2680 Sandy Bridge 2.70 GHz CPUs, each of which had 8 cores, with an infiniband interconnection. Simulations on grids G5 and G6 where computed with 128 cores, while 64 cores were used for the rest of the simulations. The total CPU time is plotted as a function of the number of mesh points in Figure 3 for the simulations of the flow at $Re_b = 25,000$.

![Figure 3](image)

*Figure 3: Total CPU time as a function of the number of mesh points for $Re_b=25,000$.***
3. Results

3.1. Front features

The profiles of front position $x_f$ and velocity $u_f$ are shown on Figure 4 for each $Re_b$. The charts are presented for a grid resolution fine enough to perform a well resolved LES. The chart for the laminar case $Re_b = 250$ has also been plotted for comparison purposes. As $Re_b$ increases, the front (Figure 4a) advances at a faster rate until its propagation becomes almost independent of the Reynolds number for $Re_b > 10,000$.

![Figure 4](image)

*Figure 4*: Temporal evolution of the front position (a) and velocity (b) for cases [G2; Re$=1,000$], [G3; Re$=10,000$], [G4; Re$=25,000$] and [G5; Re$=60,000$].

The different phases of the current are correctly predicted as shown by their front propagation on Figure 4b. The quasi-constant front velocity observed during the slumping phase at the early stage of propagation increases to $u_f \sim 0.65$ to 0.7 for $Re_b > 10,000$ and the current starts decelerating after $t \sim 20$. The transition occurs within the range of 5 to 10 times the lock-length, as observed by Rottman and Simpson [14]. For $Re_b = 250$, the deceleration matches the $t^{-4/5}$ power law predicted for the buoyant-viscous phase [13], in agreement with the laminar nature of the current dominated by the viscous effects. The flows at other $Re_b$ show a deceleration consistent with the $t^{-1/3}$ power law character-
istic of the self-similar phase [11, 12], the final transition to the buoyant-viscous phase being observed only during the last stage of the front propagation ($t > 50$).

3.2. Current structure

Figure 5 shows an isosurface of concentration for $c = 0.1$ together with a contour plot of the 2D vorticity field on the symmetry plane for $Re_b = 1,000$ and $Re_b = 60,000$ at a short interval after the release of the lock ($t = 9.3$), while Figure 6 shows them for when the flow is fully developed ($t = 50.1$). The two instabilities characteristic of gravity currents are noticeable shortly after the gate opening (Figure 5). At the upper boundary between the current and the ambient fluid, large billows of dense vorticity characteristic of a Kelvin-Helmholtz instability are created and sustained over time (Figure 6). Due to greater mixing, the billows tend to be less pronounced at higher $Re_b$ and are made of the aggregation of smaller vortex structures. The lobe and cleft instability is also observed at the front of the head. For $Re_b = 1,000$ the lobes decay with time (Figure 6) but at higher $Re_b$ they are maintained showing the dominance of buoyancy-inertial forces over viscosity for longer periods and the ability of the resulting flow to propagate for longer times at high $Re_b$.

![Figure 5](attachment:image.png)  
*Figure 5: Concentration isocontour $c=0.1$ and vorticity field on the symmetry plane $z=0$ at $t=9.3$ after the lock release for the cases [G2;Re$_b$=1,000] (a), [G5;Re$_b$=60,000] (b).*
Figure 6: Concentration isocontour $c=0.1$ and vorticity field on the symmetry plane $z=0$ at $t=50.1$ after the lock release for the cases \([G2; Re_b=1,000]\) (a), \([G5; Re_b=60,000]\) (b).

Figure 7 presents the vertical profiles of streamwise velocity, its fluctuations, the spanwise shear-stresses and the vorticity magnitude inside the head of the current at $t = 23.1$ for the different grid resolutions, and Figure 8 presents the equivalent concentration statistics. Regardless of the Reynolds number, the averaged characteristics of the current behaves similarly inside the head (shown for $Re_b = 25,000$). Their behaviour with grid refinement is presented in the next section. The simulations calculated on different meshes predict similar streamwise velocity profiles, with slight differences being observed. As expected, the averaged streamwise velocity shows a strong gradient in the bottom near-wall region. This strong gradient is similar to the high vorticity and the local peak of the turbulent velocity fluctuations encountered in a turbulent boundary layer. Inside the current, the velocity increases at a nearly-constant rate. A layer of strong mixing occurs between the current and the ambient reverse flow. This mixing layer exhibits strong turbulence, as shown by the increase of the resolved
perturbations and vorticity in the region \(0.4 < y < 1.2\), where the resolved velocity decreases at a constant rate. At the centre of the layer (\(y \approx 0.9\)), the resolved perturbations reach a maximum, and the resolved Reynolds stresses as well as the SGS stresses (shown in Figure 16) increase to balance the strong velocity gradient in the energy budget.

\[ \text{Figure 7: Vertical profile of the averaged streamwise component of the resolved velocity (a), streamwise component of the resolved velocity fluctuations (b), shear-stresses (c) and vorticity magnitude (d) at } t=23.1 \text{ inside the body of the current } (x = x_f - H) \text{ for } Re_b=25,000, \text{ and grids } G2, G3, G4, G5 \text{ and } G6.\]

The thickness of the mixing layer corresponds to the range of concentration \(0 < m_{\text{ave}} < 0.8\) (Figure 8.a) for \(Re_b > 10,000\). The maxima of the concentration fluctuation (Figure 8.b) and advection rate (Figure 8.c) are at a slightly higher location than their velocity equivalents (\(y \approx 0.97\)).
3.3. Qualitative comparison of the grid resolution

Refining the grid has a significant effect on the simulations and an initial approximation of their quality can be provided by the qualitative observation of the simulated current. The refinement has a similar impact on the structure of the current, regardless of the value of $Re_b$. The current shape and vorticity fields generated for grids G2 to G6 are compared in Figure 9 for $Re_b = 25,000$ at $t = 29.1$. The distribution of vorticity and the roughness of the current shape shows that smaller turbulent structures are refined as the grid is refined. Nevertheless, the size of the lobes seem to remain the same for grid G4 and finer. The qualitative observation of the flow indicates a poor representation by grids G2 and G3.
Figure 9: Concentration isocontours with $c=0.1$ at $t=29.1$ with $Re_B=25,000$ for the grids $G2$ (a), $G3$ (b), $G4$ (c), $G5$ (d) and $G6$ (e). The improvement of the current’s representation induced by refinement is noticeable on the size of the turbulent structures.

Lock-exchange gravity currents do not have quasi-steady features. This limits the ability to use local values of the current to assess the grid resolution. The resolved averaged velocities, perturbations and shear-stresses (see Figure 7.a, b, c) do not seem to be relevant by themselves. Even if the near-wall velocity gradient seems to converge when the grid is refined for this specific Reynolds number, as shown by the increase of the local maximum near $y = 0.1$ (Figure 7.a), this behaviour is not consistent for different Reynolds numbers. Taking the most refined cases as references, the gradients alternate from overprediction to underprediction, without showing a clear trend (not shown), and similarly, the
velocity fluctuations and shear-stresses do not show any clear trend with refinement. However, refining the mesh leads to higher vorticity inside the mixing layer, as observed on Figure 7.d.

3.4. Near-wall resolution

In this study, the near-wall resolution verification has been limited to the validation of the $y^+$ condition stated by (2.13). The maximum wall shear-stresses, and consequently the maximum of $y^+$, are observed near the lobes at the head of the current on Figure 10.a. To ensure $y^+ < 10$ for all of the bottom wall, the temporal evolution of the maximum $y^+$ is plotted on Figure 10.b for each $Re_b$. The initial random definition of the velocity fields inside the lock necessarily induces differences on the $y^+$ values for the different grids, however the maximum values are in the same range and the trend is shown to be grid independent. Thus, the charts have been extracted from case $G_2$ at $Re_b = 1,000$ and $G_5$ for $Re_b$ of 10,000 to 60,000. The maximum $y^+$ remain in the acceptable range $2 < y^+ < 7$ for each Reynolds number. The empirical correlation (2.17) allows a good estimation of the first vertical mesh size at the bottom wall. Nevertheless, it is advised to apply a factor of safety in order to ensure that $y^+ < 10$. 
3.5. Turbulence statistics

Figure 11 presents the streamwise power spectrum densities of the streamwise and spanwise resolved velocity components \( PSD_x(U) \) and \( PSD_z(W) \), plotted on log-log axes for each grid. They show similar forms regardless of \( Re_b \) and are therefore only plotted for \( Re_b = 10,000 \). Their values are computed by generating the discrete Fourier transform on each \( x \)-lines of the discretized domain and are finally averaged over the \( y \) and \( z \)-directions. For the whole range of \( Re_b \), both \( PSD_x \) feature a broad linear decaying range corresponding to the inertial range with a slope smaller than the typical -5/3 law, indicating the choice of the cutoff wavelengths is in the inertial range and that good resolution has been achieved on all grids. As with the physical viscous dissipation observed in DNS or experimental spectra, the steeper decay at high wavelengths occurs in the SGS dissipation range caused by the numerical SGS viscosity of the turbulence model. With grid refinement, the transition into the dissipation range occurs at shorter wavelengths, as smaller turbulent structures are resolved. However, the \( PSD_x(U) \) does not show a clear dissipation range, with a minimal pile-up at the largest wavenumbers. No obvious conclusions can be drawn to assess the grid resolution from the analysis of the \( PSD_z \). However, a
sufficient grid resolution for all the grid resolutions is achieved, although the observation of the current structure shows poor resolution for the coarsest grid at high Re_b.

![Figure 11: Averaged streamwise power spectrum densities of the streamwise (left) and spanwise (right) components of the velocity at t=29.1 for Re_b = 25,000.](image)

The averaged spanwise power spectrum densities of the streamwise velocity $PSD_z\{U\}$ (Figure 12) and spanwise velocity $PSD_z\{W\}$ (Figure 13) gives more information about the quality of the simulations. Not all the grid data reach the expected -5/3 decaying range. In this case, the requirement imposing the filter’s cut-off wavelength in the inertial range cannot be assured, resulting in a poor resolution on the corresponding grid. Grids G1 and G2 do not resolve enough wavenumbers to represent the decaying range and appear as too coarse for Re_b = 1,000. The quantity of wavenumbers of the $PSD_z\{U\}$ are barely sufficient to reach a potential linear decaying range. In another hand, the $PSD_z\{W\}$ do not exhibit a proper -5/3 range compared to higher Reynolds values. From this observation, it is fair to assume that LES is not appropriate for this range of Re_b.

The three remaining grid resolutions exhibit similar behaviour. At a fixed grid resolution, increasing Re_b only has a limited impact on the $PSD_z$, except at high wavenumbers. The greater the Re_b, the more energy is stored in the high wavenumbers. Also the pile-up of the $PSD_z\{U\}$ tend to be converted
into a pile-up of the $PSD_z[W]$ as $Re_b$ increases, an observation that is also true for the DNS case. By only accounting for the $PSD_z$, grids G1 to G3 do not reach the linear decaying range and are consequently too coarse. Moreover, grid G4 barely reaches the -$5/3$ range on $PSD_z[W]$ limiting its use to coarse LES, but grids G5 and G6 lead to solutions with a large inertial range and can be considered sufficiently fine for a well-resolved LES according to the $PSD_z$ observation.

Figure 12: Averaged power spectrum densities of the streamwise components of velocity along the spanwise $z$-direction at $t=29.1$ for $Re_b=1,000$ (a), $Re_b=10,000$ (b), $Re_b=25,000$ (c) and $Re_b=60,000$ (d).
Figure 13: Averaged power spectrum densities of the spanwise components of velocity along the spanwise $z$-direction at $t=29.1$ for $Re_b=1,000$ (a), $Re_b=10,000$ (b), $Re_b=25,000$ (c) and $Re_b=60,000$ (d).

Figure 14 presents the spanwise two-point correlations of the streamwise and spanwise resolved velocity components $R_{uu}$ and $R_{ww}$. It enables the qualitative estimation of the number of cells composing the largest structures of the flow and is defined as the inverse discrete Fourier transform of the kinetic energy spectrum. Typically, it is advised to have at least 8 cells to accurately represent the largest flow structures \cite{55}. The $R_{uu}$ and $R_{ww}$ have only slight differences for $Re_b > 10,000$, so that only $Re_b = 1,000$ and $Re_b = 60,000$ are plotted. Furthermore and for the purpose of clarity, only the coarsest grid size are shown, as the finest grids are necessarily satisfying the requirement if a coarser one respects it. The conclusions on the poor refinement of the coarse grid G1 to G3 are supported by Figure 14. For $Re_b = 1,000$ $R_{uu}$ and $R_{ww}$ decrease to 0.1 within only ~ 8 cells for the grid G2. At high $Re_b$, G3 would only result in a poor representation of the driving structures, with $R_{uu}$ and $R_{ww}$ going...
to 0 within 11 and 9 cells. Grid G4 is the first that provides a sufficient number of cells for LES with 
$R_{uu}$ and $R_{ww}$ decreasing to 0.1 within 17 and 14 cells respectively. However with 14 cells, it can only
be considered adequate for a coarse LES regardless of the Reynolds number.

Figure 14: Averaged two-point correlations along the spanwise z-direction of the streamwise velocity components for $Re=1,000$ (a) and $Re=60,000$ (b) and spanwise velocity components for $Re=1,000$ (c) and $Re=60,000$ (d) components of velocity at $t=29.1$.

According to Davidson [55] and Bazdidi-Tehrani et al. [57], the two most practical parameters for
evaluating mesh quality are the ratios of the SGS shear-stresses to the resolved stresses 
$N_S = \tau_{SGS,xx}/(u' v')_{ave}$, and SGS viscosity to the molecular viscosity $N_v = \nu_{SGS}/\nu$.

The vertical profiles of the ratio of the SGS viscosity to the molecular viscosity $N_v$ averaged in the
spanwise direction in the head are shown in Figure 15 for each $Re$. Logically, $N_v$ should increase
with increasing Reynolds number. Two main elements are noticeable. Outside the mixing layer, $N_v$
diminishes, following the fading of the resolved velocity perturbations (Figure 7.b). The globally low value of $N_v$ for $Re_b = 1,000$ again questions on the relevance of LES at such low Reynolds numbers. For higher $Re_b$, the SGS viscosity falls below one third of the molecular viscosity for grids G3 and finer for $Re_b = 10,000$, G4 at $Re_b = 25,000$ and G5 at $Re_b = 60,000$. Similar to the two-point correlations and the velocity PSD, the other combinations of grid and Reynolds number demonstrate a poorly resolved LES. Strong peaks of $N_v$ are seen inside the mixing layer. Improving the grid resolution towards the finer grid reduces the amplitude of the peak, and the reduction of the SGS viscosity, due to its dependence on the cell size in (2.9), is respected. Although large values reflect a poorly resolved LES, to the best of our knowledge there are no published recommendations on what is a typical acceptable level of $N_v$. 
The ratio of the SGS shear-stress to the resolved Reynolds stress $N_S$ is presented on Figure 16. High values of $N_S$ means that a large part of the turbulence is modelled and is proof of a poorly resolved LES. Thus, this quantity is of interest inside the mixing layer where the turbulent shear-stresses become important and is plotted in the range $0.4 < y < 1.2$. As with the ratios of viscosities, refining the grid diminishes the ratios of shear-stresses. The global ratios achieved remain fairly low for grid G3 and finer, for which the modelled shear-stresses on average remain less than 10% of their resolved counterparts. Refining the grid resolution further than G4 for $\text{Re}_b > 10,000$ does not lead to significant changes and the SGS shear-stresses remain, on average, less than 5% for grid G4 and 3% for grids G5.
and G6. As with the ratio $N_v$, no guidance exists to define a satisfactory level of $N_s$ for a well-resolved LES.

![Graph showing shear stress profiles](image)

**Figure 16**: Spanwise averaged shear stress vertical profiles at $t=29.1$ at the position $x=xf-H$ for $Re_b=25,000$. The vertical line corresponds to $N_s = 0.05$.

4. **Discussion**

This study aims to qualify the relevance of different parameters in determining a suitable grid resolution for a LES of a lock-exchange gravity current, for buoyancy Reynolds numbers ranging from 1,000 to 60,000, as commonly studied in laboratory experiments.

With regard to the current behaviour, the expected features of the current are represented. The lobe and cleft instabilities at the head of the current and the Kelvin-Helmholtz billows are correctly depicted. The slumping and deceleration phases [11, 12] are predicted with the transition between the two occur-
ring at $t = 12$ [66]. For $Re_b = 1,000$, the viscous effects are strong enough to transition the current into the buoyant-viscous phase with no intermediate self-similar phase, which agrees with the observations of Cantero et al. [66] for gravity currents with $Re_b < 10,000$. Above this Reynolds number the self-similar phase front velocity laws of Huppert and Simpson [11] are observed. The relatively low dependency of the propagation and shape of the current on the Reynolds number in fully-developed turbulent currents [28] is illustrated by the similarity of the front velocities, the front positions and the total resolved kinetic energies depletion for $Re_b > 10,000$. Consequently, lower Reynolds number simulations can lead to useful predictions of high Reynolds flows so as long as the self-similar phase is maintained. Others have found that the size of the mixing region between the two fluids [67] and the magnitude of the lift and drag forces generated by a current interacting with square obstacles [68] are similarly independent of Reynolds number.

The impact of the Reynolds number is mainly observed on the dynamics of the interface between the two fluids as shown by the vorticity profiles and the isosurfaces of concentration. Even if the coherency of the Kelvin-Helmholtz structures are maintained, the large two-dimensional billows break up into smaller three-dimensional eddies along with the development of lobes of shorter spanwise wavelength. The Kelvin-Helmholtz billows have been shown to be the consequence of the roll-up of the thin shear layer that develops at the front during the initial stage of the current [69], and Ooi et al. [28] demonstrate that those two phenomena are interdependent since the deformation of the billows is the direct consequence of the propagation of shear effects due to the lobe and cleft instability at the front.

Focusing on the assessment of grid resolution, a typical first approach lies in the qualitative observation of the current’s flow distribution. The finer structure of the vorticity and concentration isosurfaces reflect the improvement in the prediction of the dynamics of the current and the shrinking of the resolved turbulent structures as the resolution is refined. However, it only provides a limited indi-
cation of the quality of the simulations and one should use them only to ensure that the sizes of the resolved structures are consistent with the level of detail required for the physical phenomena studied.

The spanwise averaged velocity, fluctuations, shear-stresses and profiles inside the head of the current are not useful for gravity currents. Those components are usually considered in the case of quasi-steady flows and time averaging is performed to compare the results [41, 55-57, 70]. The non-quasi-steady nature of gravity currents and the variability in the prediction of the current position and internal dynamics naturally causes too large a discrepancy between profiles for their use.

In agreement with Davidson [55], [56] and Bazdidi-Tehrani et al. [57], the two-point correlations are seen to be particularly useful quantities. The spanwise velocity spectra also provide interesting data for a lock-exchange gravity current, unlike the near-wall modelled LES of a channel flow at Re = 4,000 [55] and the flow in a plane asymmetric diffuser at Re = 18,000 [56]. Both spectra and two-point correlations show a weak sensitivity to the Reynolds number. Grids G1 to G3 are found to be far too coarse for the LES of fully turbulent gravity currents. Less than 10 cells are used to represent the largest structures of the flow, far from the recommended 16 cells for a well-resolved LES [55], and the spectra fail to reach the typical -5/3 inertial range, indicating too large a filter width. The spectra of grid G4 hardly reach the -5/3 range and the spanwise structures are represented by 14 cells so that it can barely be considered acceptable for a well-resolved LES but suitable for a coarse LES. The pile-up of the PSD,\text{U} at high wavelength is similar to that observed by Davidson [55] in his energy spectra.

From the analysis of the velocity gradient PSD and the dissipation spectra, he explains it as a consequence of a decrease of the SGS dissipation at very high wavelengths, which supposedly takes place preferably at lower wavelengths, and he attributes this misprediction to inaccuracies in the turbulence model.
The ratio of the SGS viscosity to the molecular viscosity, $N_v = \nu_{SGS}/\nu$, and of the SGS shear-stress to the resolved Reynolds stresses, $N_s = \tau_{SGS,12}/(u'v')_{ave}$, inside the mixing layer seem to be the most practical and accessible quantities for assessing the grid resolution. Both parameters show good convergence with grid refinement. In the mixing region, despite observing the decrease of the peak amplitude of $N_v$ when the grid is refined, no guidelines is found for an acceptable level in the literature and the definition of threshold values is difficult [56]. In contrast, the region above the current is subject to a low level of turbulence as shown by the reduced shear-stresses (see Figure 7.c) and it is reasonable to assume that the flow should be fully resolved in this region. The SGS viscosity becomes negligible in comparison to its molecular counterpart and, consequently $N_v << 1$, in agreement with the reduction of $N_v$ above the mixing layer. Knowing that a grid of G5 and finer are suitable for a well-resolved LES from the two-point correlations and the PSDs, $N_v < 0.3$ seems suitable as a limiting condition to have a proper representation of the region above the current. This condition is less restrictive at low Reynolds numbers, and grids G3 and finer respect it for $Re_b = 10,000$. It is more limiting at high Reynolds numbers as clearly only the ratios of grids G5 and G6 become sufficiently low for $Re_b = 60,000$. An in-depth study to determine the Reynolds number at which grids G5 and G6 remain sufficiently fine to correctly compute the flow in the low turbulence areas would be challenging. Likewise, the ratio of the shear-stresses $N_s$ reduces inside the mixing layer as the resolution is improved with little variation in its magnitude for grids finer than G4. As with $N_v$, no recommendations are given in the literature for an acceptable level of $N_s$, but the grids found to be fine enough from the two-point correlations and the velocity PSD (G5 and G6) have $N_s$ less than 5%. Based on this observations, the criteria $N_s < 0.05$ can reasonably be set as a requirement for a well-resolved LES of a lock-exchange configuration.
The present paper does not aim to provide a detailed analysis of the turbulence dynamic of the current, and, for simplicity, the simulations have been carried out using the standard Smagorinsky turbulence model. While this model has been shown to be inferior in the prediction of developing turbulent mixing layers than the dynamic Smagorinsky model [71] and the model proposed by Vreman [72], it predicts well the qualitative behaviour of the statistics throughout the layer in the presence of a fully turbulent mixing layer when benchmarked against DNS [71, 72] and experimental [73] data. Nonetheless, the increase of the SGS viscosity in the near-wall region shows the difficulty the standard Smagorinsky model has in damping the SGS viscosity in the near-wall region [37], limiting this study to regions of the current far from the wall. The thorough analysis of the internal dynamics of the current and the effect of grid refinement in the near-wall region, such as the maxima of mean wall shear-stress at the lobes, and the areas of light fluid overlapping by the current, would require the use of a more accurate turbulence model. For this reason, the dynamic Smagorinsky model has been mainly preferred in recent LES studies of lock-exchange currents.

5. Conclusions

Several grid resolution assessment methods have been compared to quantify the quality of large eddy simulations of a typical laboratory lock-exchange gravity current for buoyancy Reynolds numbers varying from 1,000 to 60,000. The unsteady and dynamic nature of gravity currents requires the averaging and turbulent statistics to be obtained from double spatial-averaging over the complete spanwise direction, for a highly energetic region of the current head over the streamwise direction.

Insights on the impact of the grid refinement are obtained with a qualitative comparison of the concentration isosurfaces, the vorticity fields and vertical profile inside the current head. The standard approach of comparing the averaged quantities of the current at specific locations of the current is found to be inappropriate. We found that the averaged velocity and concentration profiles are comparable for all grid resolutions we tested. Although the rms velocities and the resolved shear-stresses behave simi-
larly, they do not monotonically converge on the finer grids. Unlike their streamwise equivalent, spanwise two-point correlations are affected by changes of the buoyant Reynolds number. A comparison shows that DNS should be preferred to LES for transitional flows, such as a buoyancy Reynolds number of 1,000. In the cases where the Reynolds number is over 60,000, a coarse LES is obtained for 1140×37×74 cells (grid G4) outside the near-wall layer, whilst a well-resolved LES has resolutions finer than 1925×62×1251 (grid G5). The results from the spanwise two-point correlations inform on the number of grid points needed to resolve the largest structures, and whether the cell size is small enough to satisfy the placement of the LES filter width inside the inertial range of the spectra distribution.

Finally, we show that the ratio of the SGS viscosity to the molecular $N_v = \nu_{SGS} / \nu$, and the ratio of the SGS shear-stress to the resolved $N_s = \tau_{SGS,12} / (u'v')_{ave}$ decrease with grid refinement inside the current head. However, threshold values for a well-resolved LES are difficult to define. From the two-point correlations and the power spectrum densities we can conclude that a complete resolution of the flow in the low turbulence region above the upper boundary of the current is achieved when $N_v < 0.3$. The ratios of shear-stresses inside the turbulent mixing layer is recommended to converge to values below $N_s < 0.05$ to achieve a well-resolved LES.

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