Fitting of extended sub-grid scale models in compressible turbulent MHD

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The use of Large Eddy Simulations in compressible, turbulent MHD is often limited to the implementation of purely dissipative sub-grid scale models. While such models work well in the hydrodynamic case due to the universality of the spectrum, they do not fully describe the complex dynamics of MHD, where the transfer of energy between internal, kinetic and magnetic energies at small scales is less trivial. For this reason, a sub-grid scale model based on the gradients of the fields entering in each non-linear term of the equations has already been proposed and studied in the literature, for the momentum and induction equations. Here, we consider the full set of compressible, ideal MHD equations, with an ideal gas equation of state, and we proposed a generalization of the gradient model, including the energy equation. We focus on the residuals coming from the whole set of equations, by filtering accurate high-resolution simulations of the turbulent Newtonian Kelvin-Helmholtz instability in a periodic box. We employ the same high-resolution shock capturing methods typically used in relativistic MHD, applicable in particular to neutron star mergers. The a-priori test, i.e. the fit between the sub-filter residuals and the model, allows us to confirm that the gradient model outperforms any other, in terms of accuracy of the fit and small deviations of the best-fit pre-coefficient from the expected value. Such results are validated for 2D and 3D, for a range of different problems, and are shown, for the first time, to hold also for the energy evolution equation. This paper is the first step, based on a solid theoretical and numerical basis, towards the near-future extension of the sub-grid scale gradient model to the relativistic MHD, and a future implementation in a full General Relativity LES.

I. INTRODUCTION

In the context of computational fluid dynamics, direct numerical simulations (DNS) are employed to resolve the equations in all the dynamically relevant scales, including the dissipative ones. This means that the numerical grid size $\Delta$ has to be smaller than the dissipative scale. Since the computational cost of DNSs scales as $\Delta^{-3}$ (where $\Delta$ is the Reynolds number), for many problems (including convection zones of stars, planetary atmospheres, accretion disks, and industrial applications such as gas turbines, steady turbulent flows...) it is unfeasible to have a small enough grid size and a large enough domain at the same time, thus representing all the scales of interest. Even though in the near future the increasing computation power will improve the achievable resolution, thus making DNSs feasible for more scenarios, currently there are many cases where we are still very far from it. In astrophysics, one of these cases, which is of particular interest due to the recent discoveries of gravitational waves, is the binary neutron star merger.

The two most widely used numerical approaches to overcome the lack of resolution in turbulent flows are the Reynolds Average Numerical Simulations and the Large Eddy Simulations (LESs). For both cases, the idea is to directly evolve the quantities on the resolved scales, i.e. from the integral scales (the largest ones, corresponding to domain size or to the typical scale where energy is injected), down to the grid scales, and to describe the effect of the smaller ones through a suitable sub-grid scale (SGS) model.

While the purely hydrodynamic turbulence dynamics is relatively well understood due to the universality of the spectral properties, the dynamics becomes more problem-dependent when magnetic fields are included. Magnetic fields tend to break the usually assumed isotropy and self-similarity, and prevent one from defining universal laws, valid for different scenarios. Magneto-hydrodynamic (MHD) turbulence includes a non-linear dynamics, with transfer between magnetic and kinetic energy (dynamo mechanism, when the magnetic energy rises), and, at the same time, between different scales. Such transfers vary locally and in time, so that a statistical evaluation of them represents essential information. In general, the smallest scales are the most interesting ones in terms of interchange of kinetic and magnetic energy.

As a consequence, it is crucial to properly model the unresolved scale dynamics, by means of a SGS modeling, that is incorporated as additional extra terms in the MHD equations. Due to the variety of turbulent scenarios, LESs with SGS models represent an active field of inter-disciplinary research, including engineering, plasma physics and astrophysics (i.e., see for instance a review about the use of LESs in astrophysics, which is also our main interest). A popular SGS model is the dissipative one, introduced by Smagorinsky half a century ago in the context of hydrodynamic direct cascades to mimic the fluid’s viscosity. Other SGS models have also been proposed relying mainly on dimensional analysis or physical assumptions like the dynamo mechanism.

Another branch of SGS models (including the multi-scale and multi-variational ones relies on self-similarity arguments, where basically the loss of information is estimated considering the average spatial correlations of the evolved fields at different scales, and extrapolating such information to infer the fields in the SGSs. These models are used especially in finite-elements schemes.

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On the other hand, the gradient model is based on a mathematical formulation which relates the finite resolution to an effective filtering of the equations. By expanding in Taylor series the non-linear terms in any equation, one can approximate the SGS residuals with a functional form which only relies on mathematical assumptions. The model does not contain any arbitrary physical assumption, and just extrapolates to the SGS the trends seen at the smallest resolved scales.

In general, two steps can be taken in order to assess and compare the performance of any SGS model:

- **A-priori fitting.** This test requires the post-process filtering of the fields obtained with a relatively high-resolution simulation at a given time. The residuals coming from the filtering (i.e., the non-linear information contained between the filter size \( \Delta_f \) and the original resolution \( \Delta \)) can be fit to a given SGS model, where the only free parameter is a pre-coefficient. The procedure can be easily repeated for different times, resolutions, filter sizes, initial conditions, in order to test the applicability of the tested SGS model. This procedure allows to identify the best-fitting functional form of the SGS model, but does not allow to evaluate the effect of the inclusion of the SGS in a simulation.

- **LES comparison**, including different SGS models. Ideally, a low-resolution LES with a good SGS model should resemble a LES with a higher resolution. The LES comparison is a more demanding test, since it involves the dynamical feedback given by the implemented SGS terms. This test is much more informative and is crucial to evaluate the physical meaning of including a certain SGS tensor in a LES. However, the exploration of parameters is much more computationally expensive.

In this paper, we will perform the first step: an extensive a-priori assessment of the most popular explicit local SGS models present in the literature, leaving a battery of LES comparison tests for a forthcoming paper, which will obviously rely on the results found with the first approach. Works in this sense have been performed in the context of either incompressible or compressible MHD. These studies are among the most detailed in comparing different SGS models, employing either forced or decaying turbulence. Although they consider the momentum and induction MHD equations, the internal energy evolution is not included, since they impose either incompressibility or a polytropic/isothermal equation of state (EoS) as a closure. Here we extend these works by considering instead the compressible MHD equations with an ideal EoS.

We run several bounding box high-resolution simulations of the Kelvin-Helmholtz instability (KHI), which triggers the gradual development of turbulence. We do not include any forcing: we focus on dynamical, decaying turbulence, since we aim at applying them to simulations of astrophysical transient phenomena. We perform a-priori tests, where the filtered residuals are compared to what we would obtain with different SGS models applied to the information available at the filter resolution. We validate both the method and the SGS models, identifying the best-fit coefficients for a variety of initial data, resolutions and filters.

In §II we review and extend the formal description of a LES, seen as a consequence of separating scales by applying a filter to the solution. We describe in some detail the filtered full MHD equations in §III In §IV we introduce different SGS models, with special emphasis on the gradient model. In §V we describe the platform and the numerical methods used in this work (in AppendixA we describe the validation of the code with a set of benchmark tests in 2D). In §VI we present the main highlights of the results coming from 3D KHI simulations, showing a variety of cases. Conclusions are drawn in §VII.

II. EQUIVALENT FILTERING IN LARGE EDDY SIMULATIONS

In a LES, the smallest simulated scales (i.e., the ones corresponding to the grid size \( \Delta \)) are not sufficient to capture entirely all the relevant dynamics, which might occur in the SGS scales. Since the SGS part of the solution is unknown by definition, it can only be either neglected, leading to the so-called implicit LES, where a low-pass filter or the internal numerical dissipation (used for instance in solar physics) act as an intrinsic SGS model, or explicitly modeled through the information which is available, i.e. the one of the resolved scales. This explicit modeling, on which we focus, can be based either on mathematical or physical arguments.

Mathematically, the effect of finite resolution can be thought as equivalent to a low-pass spatial filter, where the filter size, \( \Delta_f \), is given by the grid cell, \( \Delta \). This separates, for a continuous field \( f \), the smoothed (resolved) part, from the sub-filter scale (SFS) fluctuations (or residuals), respectively:

\[
f(x,t) = \bar{f}(x,t) + \hat{f}(x,t)
\]

(1)

Indicating the filter kernel with \( G \), the filtering operator over a field \( f \) can be written as

\[
\bar{f}(x,t) = \int_{-\infty}^{\infty} G(x-x') f(x',t) d^3x'
\]

(2)

An homogeneous isotropic low-pass filter is independent on the direction (i.e., \( G(x-x') = G(|x-x'|) \)) and only smooths out fluctuations on length scales smaller than the filter size \( \Delta_f \), leaving unchanged the variations of the solution at larger length scales. In addition, the filter operator is linear and commutes with spatial derivatives. Generically, it can be written for any dimension \( D \) as

\[
G(|x-x'|) = \prod_{i=1}^{D} G_i(|x_i-x'_i|) ,
\]

(3)

where \( G_i(|x_i-x'_i|) \) is just the one-dimensional kernel function.

The simplest low-pass filter is the mean value in a cubic domain with size \( \Delta_f \) in each Cartesian direction \( \{x_i\} \), described by the normalized kernel
Despite the appealing simplicity of the box filter, which makes it very useful to perform numerical calculations, we will see below that it is not suitable for analytical calculations involving its derivatives, since they are not continuous. Therefore, at a formal level, it is more practical to introduce the normalized Gaussian kernel, which in the space domain can be written as

\[ G_i(|x_i - x_i'|) = \begin{cases} 1/a & \text{if } |x_i - x_i'| \leq \Delta f/2 \\ 0 & \text{otherwise} \end{cases} \]  

where \( a \) defines the effective filtering width. Besides having the same zeroth and first moments, Gaussian and box filters have the same second moment if we set \( a = \Delta f/2 \).

\[ \int_{-\infty}^{\infty} x^2 G(x) dx = 2a = \frac{\Delta^2 f}{12}. \]

The filter is a useful mathematical tool to analyze not only the SFS residuals, that is, the loss of small-scale information due to the filtering process related to the non-linear terms of the equations. Since the filtering operator has a-priori choice of a given SGS physics.

Regardless of the specific equations considered, these new terms always appear due to the non-commutativity of the filtering operator with the non-linear terms of the equations. In a LES, which effectively only evolves \( \bar{u} \) and cannot simulate the unresolved scales, the explicit expression of \( \tau \) is a-priori unknown, and needs to be written as a function of the filtered fields in order to close the system of equations.

There are several ways of doing that, based mostly either on physical arguments or on an expected self-similarity of the solution. For instance, a popular, historical approach to fluid dynamics SGS models in compressible MHD is the setup of an artificial viscosity \( \nu \), namely

\[ \tau = \bar{u}^2 - \bar{u}^2 \approx \nu \partial_i \bar{u}, \]

The viscosity parameter is often taken to be proportional to \( \Delta^2 f |\partial_i \bar{u}| \) due to dimensional reasons and in order to ensure that this term vanishes in the continuum limit, thus guaranteeing numerical convergence to the continuum (or DNS) solution. The numerical value of the proportionality coefficient can be fixed by hand or estimated by means of dynamical procedures which assume self-similarity (thus similar to a multiscale/multivariational approach).13 Regardless of the value of \( \nu \), this functional form of \( \tau \) is equivalent to the viscous Burger’s equation, where the viscosity is the numerical SGS model.

However, in many cases the physics involved does not consist only in dissipation, but can involve, for instance, inverse cascade, and scale-dependent transfers of energy between the fluid kinetic energy and the magnetic one. Therefore, in those cases any result coming from the LES will be biased by the a-priori choice of a given SGS physics.

If one wants to avoid introducing arbitrary physical assumptions, it is possible to compute these terms relying only on mathematical arguments by considering the analytical Taylor expansion of the SFS terms. The main hypothesis is that the discretization of the equations over a finite-size grid is approximated by a filtering operator acting on the equations, with a Gaussian kernel equivalent to a box filter with width \( \Delta f \), eq. (5). Its D-dimensional Fourier transformed function is

\[ \hat{G}(k) = \exp(-ak^2), \]

The main idea is to compute an approximation of the inverse filtering operator based on gradient expansion of the filter kernel \( G \), that is, an approximation of the inverse Fourier transform of \( 1/\hat{G} \). The first step is to perform a Taylor expansion of the transformed function and its inverse in terms of the filter scale, that is,

\[ \hat{G}(k) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (ak^2)^n, \]

Consider the expansions to the fields \( \hat{f} \) and \( \hat{f} \), the application of the inverse Fourier transformation yields to an infinite series representation of the filter operator and its inverse in terms of gradient operators acting on the fields, namely

\[ \hat{f} \equiv G^{-1} \ast \hat{f} = \sum_{n=0}^{\infty} \frac{1}{n!} (a \nabla^2)^n \hat{f}, \]

These expressions are absolutely convergent and formally accurate at all orders, since the Gaussian kernel is infinitely differentiable and with unbound support. In fact, it was found that these series converges for all canonical filters.

The unknown components of the SFS tensors usually have the form \( \hat{f} \) and \( \hat{f} \). Applying the relations in Eq. (14) results in a series in terms of the individual fields, namely

\[ \hat{f} = \hat{f} + 2a \delta^k i \partial_i \hat{f} \partial_k \hat{f} \]

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The viscosity parameter is often taken to be proportional to \( \Delta^2 f |\partial_i \bar{u}| \) due to dimensional reasons and in order to ensure that this term vanishes in the continuum limit, thus guaranteeing numerical convergence to the continuum (or DNS) solution. The numerical value of the proportionality coefficient can be fixed by hand or estimated by means of dynamical procedures which assume self-similarity (thus similar to a multiscale/multivariational approach).13 Regardless of the value of \( \nu \), this functional form of \( \tau \) is equivalent to the viscous Burger’s equation, where the viscosity is the numerical SGS model.

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which is accurate up to $O(a^2)$. The first order terms scale with the second moment of the filter, eq. (6). With this expansion is easy to model the SFS terms appearing in Eq. (8), namely

$$\tau \equiv \frac{1}{2} - \frac{u^2}{2} \approx -2a \partial_t \pi \partial_t \pi. \quad (16)$$

For a Cartesian grid with step $\Delta_j$, the pre-factor can be set to the equivalent value $a = \frac{\Delta_j}{2}$, according to eq. (6). In principle, corrections to these expression are expected due to the form factor (due to the kernel shape) and the contribution from higher orders. As a matter of fact, if the range of modeled SFSs, $a$, becomes large, then the higher-order terms can be important. In other words, this approximated expression can help as long as we can capture most of the dynamics with our LES, leaving to the SGS the task of mimicking the small-scale contributions.

Regardless of these quite obvious caveats, notice that this prescription is very different from the viscous one given by eq. (6): one arises from physical considerations, while the other just from mathematical ones. After this simple example, we pass to the application of this formalism to the MHD equations.

### III. FILTERING THE NEWTONIAN COMPRESSIBLE MHD EQUATIONS

#### A. Compressible MHD equations

We consider the conservative formulation of the ideal Newtonian compressible MHD equations, consisting of the continuity, Euler, induction and energy evolution equations, respectively:

$$\partial_t \rho + \partial_i \left[ \rho \partial^i \right] = 0 \quad (17)$$

$$\partial_t (\rho v^i) + \partial_j \left[ \rho v^i v^j - B^i B^j + \delta^i \left( p(\rho, e) + \frac{B^2}{2} \right) \right] = 0 \quad (18)$$

$$\partial_t B^i + \partial_j \left[ \nu B^i - v^j B^j \right] = 0 \quad (19)$$

$$\partial_t E + \partial_k \left[ \left( E + p(\rho, e, B^k) + \frac{B^2}{2} \right) v^k - (v_j B^j) B^k \right] = 0 \quad (20)$$

where the magnetized fluid is described by the total energy density defined as

$$E = e + \frac{\rho v^2}{2} + \frac{B^2}{2}, \quad (21)$$

the mass density $\rho$, the fluid pressure $p$, the internal energy density $e$, and the velocity $v^k$ and magnetic field $B^k$ vectors, being $\delta^k$ the standard Kronecker delta. For simplicity, we have set the speed of light and the magnetic permeability $c = \mu_0 = 1$. The conserved quantities of the equations $\{ \rho, \rho v^k, B^i, E \}$, in their discretized versions, are numerically evolved. At each step of a simulation, the internal energy is recovered by inverting eq. (18).

The pressure, required to close the system of equations, is defined by an EoS, which in general can read $p = p(\rho, e, B^k)$. In this paper, we will present results with the ideal gas EoS, namely

$$p = (\gamma - 1)e \quad (22)$$

where $\gamma > 1$ is the ideal gas adiabatic index. However, our formalism is general and can extend to any EoS.

#### B. Filtered continuity equation and variable inversion

The filtered continuity equation is simply

$$\partial_t \bar{\rho} + \partial_k \left[ \bar{\rho} \bar{v}^k \right] = 0. \quad (23)$$

where the Favre-filtered velocities, i.e., weighted by density $\bar{\rho}$

$$\bar{v}^k = \frac{\rho v^k}{\rho} \quad (24)$$

are the natural choice in compressible MHD, where the momenta $\rho v^k$ are the evolved fields. Therefore, and are simply written as $\bar{\rho} \bar{v}^k = \bar{\rho} \bar{v}^k$ under the filtering operation.

We will use the same notation $\bar{f}$ whenever we indicate an auxiliary field as a function of evolved filtered fields only. Specifically, in our case we can express the internal energy density as a function of the evolved filtered variables, eq. (18), defining

$$\bar{e} = E - \frac{B^2}{2} - \frac{\bar{\rho} \bar{v}^2}{2} \quad (25)$$

Note that there is a difference between what can be numerically evaluated with the resolved fields only, $\bar{e}$ (i.e., combining the filtered evolved fields), and what cannot be, $\bar{e}$ (i.e., filtering the local non-linear combinations of the variables):

$$\bar{e} - \bar{\bar{e}} = - \left( \frac{\bar{\rho} \bar{v}^2}{2} - \frac{\rho v^2}{2} \right) - \left( \frac{B^2}{2} - \frac{\rho v^2}{2} \right) \quad (26)$$

which can be interpreted as the kinetic and magnetic energy density hidden in the SFSs. Note that, if such SFS contributions (usually positive-definite) are neglected in the variable inversion, this will cause a local artificial rise of the evaluated internal energy, $\bar{e}$.

Similarly, we can define the pressure as a function of all the other evolved variables $\bar{p} = p(\bar{\rho}, \bar{\rho} v^k, \bar{B}^k, E)$. Its expression depends on the EoS, as we will explain below.
C. Filtered momentum and induction equations

On the other hand, the filtered momentum and induction equations become, respectively

\[
\partial_t (\rho \mathbf{v}) + \partial_i \left[ \rho \mathbf{v} \mathbf{v}^i - \mathbf{B}^k \mathbf{B}_k^i + \delta^{ki} \left( \rho + \frac{1}{2} \mathbf{B}^2 \right) \right] = 0
\]

\[
\partial_i \mathbf{B}^i = \partial_k \left[ \mathbf{v} \mathbf{B}^k - \mathbf{B}^k \mathbf{B}_k^i + \delta^{ki} \left( \rho + \frac{1}{2} \mathbf{B}^2 \right) \right]
\]

where \( \tau_{kin}^i \), \( \tau_{mag}^i \) and \( \tau_{ind}^i \) indicate the tensors arising from the differences in the non linear products \( \mathbf{v}^i \mathbf{v}^i \), \( \mathbf{B}^i \mathbf{B}_k^i \) and \( \mathbf{v}^i \mathbf{B}_k^i \), respectively, when the filtering is considered.[1]

\[
\tau_{kin}^i = \rho \mathbf{v}^i \mathbf{v}^i - \rho \mathbf{v}^i \mathbf{v}^i
\]

\[
\tau_{mag}^i = \mathbf{B}^i \mathbf{B}_k^i - \mathbf{B}^i \mathbf{B}_k^i
\]

\[
\tau_{ind}^i = (\mathbf{v}^i \mathbf{B}_k^i - \mathbf{v}^i \mathbf{B}_k^i) - (\mathbf{v}^i \mathbf{B}_k^i - \mathbf{v}^i \mathbf{B}_k^i)
\]

\[
\tau_{pres}^i = \left( \rho - \rho + \frac{1}{2} \tau_{mag}^i \delta_{jm} \right) \delta^{ki}
\]

Notice that, by construction, \( \tau_{kin} \) and \( \tau_{mag} \) are symmetric tensors, while \( \tau_{ind} \) is anti-symmetric and its inclusion is equivalent to having a SFS electric field with components given by \( \varepsilon_{ijk} \tau_{ind}^j \). Note that the SFS kinetic and magnetic energies defined in eq. (13) are related to \( \tau_{kin} \) and \( \tau_{mag} \) by

\[
-\frac{1}{2} \left( \rho \mathbf{v}^2 - \rho \mathbf{v}^2 \right) = -\frac{1}{2} \tau_{kin}^i \delta_{jm}
\]

\[
-\frac{1}{2} \left( \mathbf{B}^2 - \mathbf{B}^2 \right) = -\frac{1}{2} \tau_{mag}^i \delta_{jm}
\]

In the literature, sometimes the functional forms of the traces of \( \tau_{kin} \) and \( \tau_{mag} \) are defined separately from the off-diagonal components (related to the strain). This is useful as a tight analogy with the standard bulk and strain viscosity, but, since our formulation is general and does not rely on the underlying physics, we prefer to avoid this distinction.

The term associated to pressure \( \tau_{pres} \) is instead purely diagonal and has been only partially considered before. If isothermal EoS or incompressibility are assumed, pressure does not depend on the evolved variables, and the only surviving term is the magnetic pressure, given by half the trace of \( \tau_{mag} \). However, in the general case, the pressure depends non-linearly on the evolved fields, so that SFS residuals implicitly appear and \( \rho - \rho \) is generally not zero. In the case of the ideal EoS, such term is proportional to eq. (13), so that:

\[
\tau_{pres,ideal} = \left[ \frac{1}{2} \gamma \tau_{kin}^i \delta_{jm} + \frac{1}{2} \gamma \tau_{mag}^i \delta_{jm} \right] \delta^{ki}
\]

Note that an ideal quasi-isothermal gas (\( \gamma \to 1^- \)) can be taken as a shortcut to minimize the spurious increase of pressure.

D. Filtered energy equation

While the momentum and induction equations have been explored in many different works, the energy evolution has usually been neglected (for incompressible and isothermal cases), or only partially considered. In particular, some authors have focused on the SFS kinetic and magnetic energy, studying in detail the inter-scale transfers between resolved and SFS.[9,10,12] Those works aim at analyzing the energy transfer, but not to perform a detailed modeling of the SFS tensors appearing in the evolution equations. Hereafter, we propose two approaches. The first is a conservative one, similar to the previous equations, where only flux terms appear, and is apt for the implementations of SGS models in a LES. In the second one, we considered the already studied inter-scale energy transfers, appearing as source/sink terms.

Conservative approach (for SGS modeling in LES). By following a similar approach as for the momentum and induction equations, we can write the energy evolution equation as

\[
\partial_t E + \partial_k \left[ \mathbf{E} \cdot \mathbf{v} + \frac{1}{2} \mathbf{B}^2 \right] = \partial_k \left[ \left( \tau_{advp}^k + \tau_{conv}^k \right) - \eta_{j} \mathbf{v}_{jk} \mathbf{B}^k \right]
\]

where the additional vectorial SFS terms on the right-hand side arise from the different non-linear terms in the original equation, as follows:

\[
\tau_{advp}^k = \rho \mathbf{v}^k - \rho \mathbf{v}^k
\]

\[
\tau_{conv} = \mathbf{v} \mathbf{v}^k - \mathbf{v} \mathbf{v}^k
\]

\[
\tau_{advkin} = \frac{\rho \mathbf{v}^k \mathbf{v}^k}{2} - \frac{\rho \mathbf{v}^k \mathbf{v}^k}{2}
\]

\[
\tau_{advmag} = \mathbf{B}^k \mathbf{v}^k - \mathbf{B}^k \mathbf{v}^k
\]

\[
\tau_{hel} = -(\mathbf{v}_j \mathbf{B}_k) \mathbf{B}_k - (\mathbf{v}_j \mathbf{B}_k) \mathbf{B}_k
\]

We distinguish three fundamental contributions. The first one is given by the SFS pressure advection term (\( \tau_{advp} \)), and the SFS convective term (\( \tau_{conv} \)). Combined, they represent the advection of the SFS enthalpy:

\[
\tau_{ent,ideal} = \tau_{advp} + \tau_{conv} = \eta \mathbf{v}^k - \eta \mathbf{v}^k
\]

where we have exploited the identity \( \rho \mathbf{v}^k = \rho \mathbf{v}^k \) to introduce the enthalpy density \( h = \rho + e + p \). In the case of an ideal EoS, this relation is reduced to

\[
\tau_{ent,ideal} = \gamma \left( \mathbf{v}^k - \mathbf{v}^k \right) \mathbf{v}^k - \frac{\gamma}{\gamma - 1} (p \mathbf{v}^k - \rho \mathbf{v}^k)
\]

where the internal energy \( \gamma \) and pressure \( \rho \) as functions of the filtered evolved quantities are given by eq. (13).

The second group of SFS terms in the right hand side of eq. (33) is given by the SFS advection of kinetic (\( \tau_{advkin} \) and

---

[1] In literature, different sign conventions are used. We use the same sign convention as Grete’s papers[3,10,11] For instance, in Kessar’s work[12], \( \tau_{kin} \), \( \tau_{mag} \) are definite with an opposite sign, while \( \tau_{ind} \) has the same sign.
magnetic energy (τ^{k}_{\text{advmag}}) densities. Note that, strictly speaking, the latter actually comes for one half from the magnetic energy advection, and for the other half from the magnetic pressure advection, similarly to τ^{k}_{\text{advmag}}. In order to keep the elegance of the enthalpy term described above, we prefer to keep the magnetic pressure inside this term.

The last term in the right hand side of eq. (44) is the cross-helicity term, which is partially related to the induced equation tensor, \(\tau_{\text{ind}}\), but cannot be written only as a function of it (or a simple contraction with another filtered quantity).

The main disadvantage of this approach is the presence of triple products of three or four conserved fields in the residual terms. This second approach is useful as an analysis tool, in the a-priori fitting tests, as in this paper.

Inter-scale approach (for analysis and fitting).

Alternatively, we can consider the evolution in time of the different components of the total energy density, \(\partial_t E = \partial_t (\bar{e}) + \partial_t (\bar{\rho} \bar{v}^k \bar{v}^j) + \partial_t \left( \bar{B}^i \bar{B}^j \right) / 2\). After some algebra, one can write the final expression

\[
\partial_t E + \partial_k \left[ \left( \bar{E} + \bar{\rho} + \frac{\bar{B}^2}{2} \right) \bar{v}^k - (\bar{\nu}^i \bar{B}^j) \bar{B}^j \right] = \]

\[
= \partial_k \tau^{k}_{\text{enh}} - \phi^{\text{press}} \partial_j \partial_k \delta^{kj} + \bar{\nu}^k \partial_k \left( \tau^{kj}_{\text{ind}} - \tau^{kj}_{\text{mag}} + \frac{1}{2} \tau^{jm}_{\text{mag}} \delta_{mj} \delta^{kj} \right) \]

where \(\phi^{\text{press}} = \bar{\nu} \partial_j \partial_k \bar{\rho} - \bar{\nu} \partial_k \partial_j \bar{\rho} \).

This second approach is useful as an analysis tool, in the a-priori fitting tests, as in this paper.

E. Final filtered equations

With these considerations, we can summarize the final set of equations to be evolved for the filtered fields as are:

\[
\partial_t \bar{\rho} + \partial_k \left[ \bar{\rho} \bar{v}^k \right] = 0 \]

\[
\partial_t (\bar{\rho} \bar{v}^k) + \partial_k \left[ \bar{\rho} \bar{v}^k \bar{v}^j - \bar{B}^j \bar{B}^k \delta^{kj} + \delta^{kj} \left( \bar{\rho} + \frac{1}{2} \bar{B}^2 \right) \right] = \]

\[
= \partial_k \tau^{k}_{\text{mom}} \]

\[
\partial_t \bar{B}^k + \partial_k \left[ \bar{v}^k \bar{v}^j - \bar{\nu}^j \bar{B}^j \delta^{kj} \right] = \partial_k \tau^{k}_{\text{ind}} \]

\[
\partial_t \bar{E} + \partial_k \left[ \left( \bar{E} + \bar{\rho} + \frac{\bar{B}^2}{2} \right) \bar{v}^k - (\bar{\nu}^j \bar{B}^j) \bar{B}^j \right] = \]

\[
= \partial_k \tau^{k}_{\text{energy}} - \Sigma^{\text{energy}} \]

where

\[
\tau^{kj}_{\text{mom}} \equiv \tau^{kj}_{\text{kin}} - \tau^{kj}_{\text{mag}} + \delta^{kj} \partial_{jm} \tau^{jm}_{\text{pres}} \]

\[
\tau^{kj}_{\text{energy}} \equiv \tau^{kj}_{\text{enh}} + \bar{\nu}^j \tau^{kj}_{\text{mom}} + \bar{B}^j \tau^{kj}_{\text{ind}} \]

In the energy equation, we have reorganized the SFS source terms. Due to the (anti-)symmetric nature of the SFS tensors, we have that the integration by parts leaves a part of the terms as flux divergences, and another part which is the contraction of only the symmetric part of \(\partial_t \bar{\nu}^j\) (i.e., the resolved fluid strain tensor \(\bar{S}_{kj}\)), and the anti-symmetric part of \(\partial_t \bar{B}_j\) (i.e., the resolved current tensor \(\bar{J}_{kj}\)). The sink term is composed by the transfers of advected pressure, kinetic and magnetic energy from the resolved scales to the SFS, respectively:

\[
\Sigma^{\text{energy}} \equiv \Sigma^{\text{press}} + \Sigma^{\text{mom}} + \Sigma^{\text{ind}} \]

\[
\Sigma^{\text{press}} = \bar{\nu} \partial_j \partial_k \bar{\rho} - \bar{\nu} \partial_k \partial_j \bar{\rho} \]

\[
\Sigma^{\text{mom}} = \bar{S}_{kj} \tau^{kj}_{\text{mom}}, \quad \bar{S}_{kj} = \frac{1}{2} \left( \partial_k \bar{\nu}^j + \partial_j \bar{\nu}^k \right) \]

\[
\Sigma^{\text{ind}} = \bar{J}_{kj} \tau^{kj}_{\text{ind}}, \quad \bar{J}_{kj} = \frac{1}{2} \left( \partial_k \bar{B}_j - \partial_j \bar{B}_k \right) \]

In analogy with the viscous and resistive terms in non-ideal MHD (proportional to the strain and current tensors, respectively), at each point of the dominion \(\Sigma\) represents the transfer of energy from the resolved scales into the SFSs (positive values) or vice versa (negative).

Note that, with this compact formulation, we need to give the prescriptions for four tensors, eqs. (48)-(51) and two scalars, related with pressure, i.e. eq. (54) and the term \((\bar{\rho} - \bar{\tau})\) in eq. (52). The latter is automatically determined by \(\tau^{kj}_{\text{kin}}\) and \(\tau^{kj}_{\text{mag}}\) in the case of an ideal EoS. Once these six SFS tensors (having a total of 20 independent components in 3D) are prescribed, the sources \(\Sigma^{\text{mom}}\) and \(\Sigma^{\text{ind}}\) are as well, since they do not contain additional degrees of freedom.

Hereafter, to avoid confusion, we will indicate with an overline the SFS residuals tensors \(\bar{\tau}\) resulting from either the formal analysis or the post-process filtering of a numerical solution, and with a simple \(\tau\) the analytical models of the SGS tensors that can be implemented in LES, which is the subject of the next section.

IV. SGS MODELS

The explicit expression of the SGS tensors represents the closure of the system of equations in a LES. By definition, in a LES it is impossible to know the exact numerical values or the functional forms of the SFS tensors and sources above, \(\bar{\tau}\) and \(\Sigma\). The SGS models considered here are local, i.e. depend only on the derivatives of the fields at the smallest resolved scales: we do not consider the multi-scale (or self-similar) models, where a second filter is performed in order to evaluate the SGS
model. We also neglect the structure models, based on different possible combinations of mutual contractions of the four first-derivative tensors (fluid strain, magnetic strain, current, vorticity), maintaining the parity needed by SGS models in the equations. In general, they do not provide a good fit (a-priori tests) and are also known to be numerically less stable when implemented in a LES. Below we list the ones we explicitly compare in this work.

A. Gradient model (extended formulation)

One can consider the analytical Taylor expansion of the SFS terms appearing in the MHD equations, under the hypothesis of having a filter with a Gaussian kernel. To apply the presented derivation self-consistently to the compressible SFS stresses, one has to take into account the compressibility effects from the mass-weighted filtering operator (i.e., the Favre filtering), which is given by

$$
\bar{f} \equiv \frac{\rho \tilde{f}}{\rho} = \frac{G\ast(\rho f)}{G\ast\rho}
$$

Using the previous relations one can write

$$
\bar{f} = f + 2a \partial_k \bar{g} \partial^k \tilde{f} + O(a^2)
$$

One can solve for $\tilde{f}$, derive this expression and use the recurrence relation to obtain, at linear order in $a$,

$$
\tilde{f} \approx \bar{f} - 2a \partial_k (\ln \rho) \partial^k \bar{f}
$$

so that the following expression, function of $\bar{f}$ instead of $\tilde{f}$, holds

$$
\bar{f} \approx \tilde{f} + 2a (\partial_k \tilde{f} \partial^k \tilde{g} - \tilde{g} \partial_k (\ln \rho) \partial^k \bar{f}) + O(a^2)
$$

The correction, $2a \tilde{g} \partial_k (\ln \rho) \partial^k \bar{f}$ is zero in the incompressible case. Using the rules described before, for the expansions of the SFS terms [48]-[50] give, at leading order in $a$:

$$
\tau_{ki}^{\text{kin}} = -2 \bar{g} \partial_k \bar{v} \partial^i \bar{v}^j
$$

$$
\tau_{ki}^{\text{mag}} = -2a \partial_k \bar{B}^i \partial^i \bar{B}^j
$$

$$
\tau_{ki}^{\text{ind}} = -2a \partial_i \bar{v} \partial^j \bar{B}^i - \partial^i (\ln \rho) \bar{B}^i \partial^j \tilde{f}
$$

This formulation, with $2a = \Delta_f^2/12$ as in eq. (6), is known as the gradient model [3] (sometimes called generically non-linear) for MHD.

If we consider the dependencies of the total (fluid plus magnetic) pressure for an ideal gas with index $\gamma$, as given by eqs. (23 and 32), then eqs. (51)-(52) are expressed by:

$$
\tau_{\text{enth,ideal}} = -2a \frac{\gamma}{\gamma - 1} \left[ \partial_j \bar{p} - \bar{p} \partial_j (\ln \rho) \right] \partial^i \bar{v}^j
$$

$$
\tau_{\text{pres,ideal}} = a \left[ \bar{p} (\gamma - 1) \partial_j \bar{v}^m \partial^i \bar{v}_m + (\gamma - 2) \partial_j \bar{B}^m \partial^i \bar{B}_m \right] \delta^{ij} = \left[ 1 - \frac{1}{2} \partial_{\text{kin}}^{\text{enth}} \delta_{lm} + \frac{2 - \gamma}{2} \delta_{lm} \right] \delta^{ij}
$$

Besides the well-known magnetic pressure contribution $-a \partial_j \bar{B}^i \partial^j \bar{B}_i$, there is an additional term, related to the fluid pressure $p$, proportional to $(\gamma - 1)$ times the SFS kinetic and magnetic energy. Note again that for an isothermal EoS $(\gamma \rightarrow 1)$, the fluid contribution vanishes and the only term left is the one related to the magnetic pressure, in agreement with previous formalism [7]. The proper modeling of $\tau_{\text{pres}}$ includes a much more complicated expression. Since in a LES we will use only conservative terms (i.e., no source terms $\Sigma$ will be modeled), we will avoid to model and study this term in detail.

While the induction and momentum equations obtained had already been explored in depth [20], the pressure- and enthalpy-related terms in the momentum and energy equations are a novelty, as far as we know.

The gradient model, despite its relative simplicity, strongly differs from the linear models, explained below and largely employed in literature, because there is no a-priori dissipative nature. Moreover, since they reproduce the dynamics seen as the smallest resolved scales where the inter-energy transfers are more effective, they allow a strong coupling between velocity and magnetic fields.

B. Dissipative model (Smagorinsky)

The basic purely HD model (Smagorinsky model [3]) accounts for the viscosity at small scales, introducing an effective viscosity tensor given by

$$
\tau_{ki}^{\text{kin}} = \nu \delta^{ki} = (c_s \Delta_f)^2 \sqrt{2} |S| S^{ki}
$$

where $c_s \sim O(1)$ is a factor to be determined, and the proportionality to $|S|$ is taken for dimensional reasons. For the isotropic HD turbulent cases, where the universal laws apply, the value of $c_s$ numerically in spectral methods, being around $c_s \sim 0.1 - 0.4$ [13,21], depending also on the problem. The coefficient $c_s$ can be determined with a dynamical procedure, instead of being fixed, as done for a channel flow [15,22].

A subsequent work [23] extended the Newtonian Smagorinsky model to the MHD, introducing the analogous turbulent magnetic diffusivity in the induction equation, proportional to the current density tensor. We will test then the following tensors:

$$
\tau_{ki}^{\text{kin}} = \Delta_f^2 \bar{B} \delta^{ki} \bar{S}
$$

$$
\tau_{ki}^{\text{mag}} = \Delta_f^2 |M| \delta^{ki}
$$

$$
\tau_{ki}^{\text{ind}} = \Delta_f^2 \bar{J} \delta^{ki}
$$

which are the ones commonly used in the literature, properly adapted (factors with $\bar{p}$ introduced on dimensional basis) and extended with the magnetic tensor $\tau_{\text{mag}}^{\text{ent}}$, that has been introduced only by analogy to the fluid strain, but do not correspond to any dissipative mechanism. In literature, different normalizations are present, taking trace and off-diagonal components separately, or considering different dependencies with $\Delta_f$. However, they do not show in general a substantial, systematic improvement [5] and we only test the expression above.
Note also some authors consider a mixed model, given by a superposition of the Smagorinsky model with the gradient model, basically in order to improve the numerical stability, compared to the gradient model alone.

By definition, the contractions of eq. (67) with the fluid strain tensor and of eq. (69) with the current tensors provide positive values of $\Sigma_{\text{mom}}$ (as long as the magnetic term $\tau_{\text{mag}}^{ki}$ is not dominant) and $\Sigma_{\text{ind}}$ respectively: this shows their dissipative nature.

C. Cross-helicity model

This model considers the dissipation of cross-helicity, which is given by two contributions, proportional to the fluid and magnetic strain rate tensors, $|\mathcal{S} : \mathcal{M}|^{1/2}$, and to the product of current and vorticity $|\tilde{\mathcal{J}} : \tilde{\Omega}|^{1/2}$, so that

$$
\tau_{\text{mom}}^{ki} = \Delta f^2 \, |\mathcal{S}| \, \tilde{\mathcal{S}} : \mathcal{M}^{1/2} \tilde{\mathcal{S}}^{ki}
$$

$$
\tau_{\text{ind}}^{ki} = \Delta f^2 \, \text{sgn}(\tilde{\mathcal{J}} : \tilde{\Omega}) \, |\tilde{\mathcal{J}} : \tilde{\Omega}|^{1/2} / \rho^{1/4} \, \tilde{J}^{ki} . \tag{70}
$$

As for the previous model, $\Sigma_{\text{mom}} > 0$ by definition: this model also transfers kinetic energy from resolved to SGS. On the other hand, in the induction equation the signum function allows for a back-scatter of magnetic helicity and magnetic energy (extraction of energy) in case $\text{sgn}(\tilde{\mathcal{J}} : \tilde{\Omega}) < 0$. Note also that, contrarily to the gradient and dissipative models where $\tau_{\text{kin}}$ and $\tau_{\text{mag}}$ are separately modeled, in this case there is only one functional form for the momentum residuals, $\tau_{\text{mom}}$.

D. Vorticity and Alfvén velocity models (for induction only)

Finally, we propose two new further models for the induction equation only. The first one is the vorticity model, an analogy of the Smagorinsky models for symmetry arguments:

$$
\tau_{\text{ind}}^{ki} = \Delta f^2 \, \rho^{1/2} \, |\tilde{\mathcal{S}}| \, \tilde{\mathcal{S}}^{ki} \tag{71}
$$

Qualitatively, similar models (in their co-variant version) have been proposed in general relativity for neutron star mergers, as extra-terms in the induction equation. They are based on the vorticity, assumed to be a physical tracer of the dynamo mechanism, but they consist in an arbitrary functional form. Moreover, to avoid a run-away need to be switched-off above some critical value of the vorticity.

Finally, we test a new model based on the current, proportional to the Alfvén velocity:

$$
\tau_{\text{ind}}^{ki} = \Delta f \, |\tilde{\mathcal{B}}| / \rho^{3/2} \, \tilde{J}^{ki} . \tag{72}
$$

Based on dimensional grounds only, the tensor is proportional to $\Delta f$, instead of $\Delta f^2$.

We will see that these models do not fit at all the residuals, thus not representing any visible physics at resolved scales.

V. NUMERICAL METHODS

A. Platform and numerical schemes

The code presented here has been generated by using Simflow, to run under the SAMRAI infrastructure which provides efficient parallelization and adaptive mesh refinement (not used in this work). Simflow is an open-source and user-friendly platform developed by the IAC3 group since 2008 to facilitate the use of HPC infrastructures to non-specialist scientists. It allows to easily implement scientific dynamical models, by means of a Domain Specific Language, based on MathML and SimML, and a web-based integrated development environment, which automatically generates efficient parallel code for simulation frameworks. Simflow splits the physical models and problems from the numerical techniques. The automatic generation of the simulating code allows to properly include the parallelization features, which in this case rely on the SAMRAI infrastructure. The combination of these two platforms provides a final code with a good balance of speed, accuracy, scalability, ability to switch physical models (flexibility), and the capacity to run in different infrastructures (portability).

Since the final aim of our studies is to run LES in astrophysical scenarios like binary neutron star mergers, we employ the same high-order accurate finite difference schemes used for the MHD equations in General Relativity simulations. The MHD system of equations, given by eq. (17), can be written formally in conservation law form, namely

$$
\partial_t \tilde{U} + \partial_k \mathcal{F}^k(\tilde{U}) = 0 \tag{73}
$$

where $\tilde{U} = \{ \rho, \rho \tilde{v}, \tilde{B}, \Phi, E \}$ is the list of evolved conserved fields and $\mathcal{F}^k(\tilde{U})$ their corresponding fluxes which might be non-linear but depend only on the fields and not on their derivatives. Here $\Phi$ is a scalar field introduced to dynamically control the divergence of the magnetic field by means of a divergence cleaning scheme [30]. The discretization of the continuum equations is performed by using the Method of Lines, which allows to address separately the time and the space discretization. We employ High-Resolution-Shock-Capturing (HRSC) methods [31] to deal with the possible appearance of shocks and to take advantage of the existence of weak solutions in the equations. The fluxes at the cell interfaces are calculated by combining the Lax-Friedrichs splitting with high-order non-oscillatory reconstruction schemes [32]. The time integration of the resulting semi-discrete equations is performed by using a 4th-order Runge-Kutta scheme, which ensures the stability and convergence of the solution for a small enough time step $\Delta t \leq 0.4 \, \Delta$.

In Appendix A we show in detail the validation of the code through benchmark tests in 2D, comparing different reconstruction schemes, of third and fifth order: FDOC3, WENO3YC, FDOC5, MP5, and WENOSZ. The latter is our final choice for all the results here presented. We defer the reader to the appendix and to our previous works [33] for further details on these numerical schemes and an extensive analysis of the performance with different discretization schemes for different problems, including MHD.
B. Spectra

Besides local densities and volume-integrated quantities, we calculate the radially-averaged spectrum. For a given field \( f \) defined in a periodic box \([0, L]^3\), we use common python functions to calculate its discrete fast Fourier transform \( \hat{f}(\vec{k}) = \sum f(\vec{x}) e^{-i\vec{k}\cdot\vec{x}} \), where the sum is performed over the \( N^3 \) spatial points \( x_i \in [0: L] \) equally spaced in each direction, with \( k_j = n \Delta k \), where \( \Delta k = \frac{2\pi}{L} \) and \( n \in [0,N/2] \) is integer.

We consider the radial coordinates of the Fourier space, describing it with \( \Delta k \)-wide radial bins also centered on \( k_r = (n \Delta k) \). Then, we calculate the spectra \( \sigma(k) \) as averages \( \langle \cdot \rangle_{k_r} \) over the annular bins of the power density per unit of radial wavenumber in 3D:

\[
\sigma_k(k_r) = \frac{L^3 4\pi}{(2\pi)^2 N^6} < |\vec{k}|^2 |\hat{f}(\vec{k})|^2 >_{k_r},
\]

\[
\sigma_m(k_m) = \frac{L^3 4\pi}{(2\pi)^2 N^6} < \hat{f}(\vec{k})^2 >_{k_r}
\]

(74)

where \( k^2 = k_x^2 + k_y^2 + k_z^2 \). The normalization comes from the Parseval identity, so that \( \int_0^{N/2} \sigma^2(k) dk_r = \int_0^L \hat{f}(\vec{x})^2 dV \) where \( f^2 = \rho v^2 / 2, \dot{B}^2 / 2 \) are the local energy densities in the real space. Note that this identity, expressed in terms of the integral in \( k_r \), strictly holds if the fluid is isotropic, so that the average over the annular bin does not lose statistically relevant information (for instance, a strong dependence on power on the direction of \( \vec{k} \)). For further technical considerations about normalizations, caveats (e.g. the systematic noise introduced by the conversion to radial coordinates in the Fourier space) and possible corrective factors, we refer to a recent dedicated paper.\[55\] Note that simulations with a large number of points \((N \geq 1000^3)\) need a parallelization, due to the large memory required. A parallelization by parallel slabs, with a dedicated python package, has been recently provided.\[56\]

C. A-priori fitting

We run simulations with a certain grid step \( \Delta = L/N \). Then, we consider a snapshot at a given time, and spatially filter all the evolved fields. The simplest recipe is to use a simple average groups of \( S_f^3 \) cells, where we define \( S_f \) as the filter factor. This corresponds to apply a filter in the real space, with a box kernel of size

\[
\Delta_f = S_f \Delta,
\]

(75)

obtaining filtered fields evaluated over \( N_f^3 = (N/S_f)^3 \) points. The information lost in the filtering process is the field variation contained between the scales represented by \( N_f \) and \( N \). The solution in these SFS can be quantitatively evaluated by the explicit formal definitions of \( \tau \), since we can evaluate the discretized version of eqs. \( \tau \)(48)-(52). Considering that a general SFS tensor is formally defined as \( \tau(\vec{x}_f) = \hat{f}(\vec{x}_f)\hat{g}(\vec{x}_f) - \hat{f}(\vec{x}_f)\hat{g}(\vec{x}_f) \), we can evaluate it at each of the \( N_f^3 \) positions of the filtered mesh \( \{\vec{x}_f\} \), as

\[
\bar{\tau}(\vec{x}_f) = \frac{1}{S_f^3} \left[ \Sigma_i \hat{f}_i(\vec{x}_i)\Sigma_i \hat{g}_i(\vec{x}_i) - \Sigma_i \hat{f}_i(\vec{x}_i)\hat{g}_i(\vec{x}_i) \right]
\]

(76)

where \( i \) indicates each of the \( S_f^3 \) discrete positions considered inside the cell centered in \( \vec{x}_f \). Note that this extension is not an exact evaluation of the loss information, since, by construction, it can only include the range of scales \( [\Delta, S_f \Delta] \). The information for scales \( \Delta \leq \Delta \) cannot be evaluated.

Once built each component of each SFS tensor, one can consider a given SGS model \( \tau \). A measurement of the linear correlation between the numerical data and the different models can be estimated with the Pearson correlation coefficient,

\[
\mathcal{P} = \text{Corr}\{\tau^{\text{best}}(\vec{x}), \tau^{\text{best}}(\vec{x})\}
\]

(77)

We will see that the Pearson correlation coefficients vary a lot between different models. We cannot set a threshold value that objectively defines when the fit is acceptable. As a matter of fact, due to the usually very large of degrees of freedom \((N_f^3)\), the associated \( p \)-value is almost always very small, and will not be taken into account as a useful indicator. Moreover, all the tested SGS models somehow depend on the derivatives of the field, which tend to correlate with the larger SFS residuals. Therefore, a certain statistically significant correlation can be expected in most cases, by construction. However, we need to identify the best-fitting model, and, in this sense, we will use the Pearson coefficients in a comparative way.

While the Pearson coefficient tests the functional form, one can also consider each SGS component with a pre-coefficient \( C \) to be adjusted. Its best-fit value can be calculated by the minimizing the L2-norm, \( \sum [\tau^{\text{best}}(\vec{x}) - C\tau^{\text{best}}(\vec{x})]^2 \), where the sum is performed over all the positions \( \{\vec{x}_f\} \). The minimization gives simply:

\[
C^{\text{best}} = \frac{\sum \tau^{\text{best}}(\vec{x}_f) \tau^{\text{best}}(\vec{x}_f)}{\sum \tau^{\text{best}}(\vec{x}_f)^2}
\]

(78)

This procedure can be repeated independently for each SGS component, for each tensor \( \tau \). Furthermore, we also look at the same correlations between the SFS interscale energy flows, \( \Sigma \), eqs. \[55\]-\[56\], and the corresponding SGS ones, being the latter defined as \( \Sigma^{\text{mom}} = S_{ki} \Sigma^{\text{best}}_{ki} \) and \( \Sigma^{\text{ind}} = J_{ki} \Sigma^{\text{best}}_{ki} \).

We repeat the same procedure for each SGS models and different times, for different simulations, varying resolutions, filter size, dimensionality, and initial conditions. Below, we report the main findings.

VI. RESULTS

We come to the main focus of the paper: the simulation and analysis of the 3D decaying (i.e., without forcing) turbulence triggered by the KHI. We choose to study the KHI because it provides different stages of the turbulent flow: the initial development at small scales, the transfer of kinetic to magnetic
energy, the saturation and mixing, and the final slow decay. Moreover, the KHI is thought to take place in binary neutron star mergers, and will be the natural mechanism to be studied in the forthcoming general relativistic simulations. The 2D setup and results are described in the Appendix. Below, we focus on the 3D case.

A. Setup

We employ a setup similar to what found in literature, consisting in a periodic cubic 3D box, with side length \( L = 1 \), with two mixing layers parallel at the \( y = \pm y_l \) planes, and given by:

\[
\rho = \rho_0 + \rho_1 \text{sgn}(y) \tanh \left( \frac{|y| - y_l}{a_l} \right) \tag{79}
\]

\[
v_x = v_{x0} \text{sgn}(y) \tanh \left( \frac{|y| - y_l}{a_l} \right) + \delta v_x \tag{80}
\]

\[
v_y = \delta v_y \text{sgn}(y) \exp \left( \frac{-(|y| - y_l)^2}{\sigma_y^2} \right) \tag{81}
\]

\[
v_z = v_{z0} \text{sgn}(y) \exp \left( \frac{-(|y| - y_l)^2}{\sigma_z^2} \right) + \delta v_z \tag{82}
\]

\[
B_x = B_{x0} \tag{83}
\]

\[
B_y = B_{y0} \tag{84}
\]

\[
B_z = B_{z0} \tag{85}
\]

\[
p = p_0 \tag{86}
\]

where \( a_l \) is the mixing layer scale, \( y_l \) is the distance of the shear layers to the plane \( y = 0 \), \( \sigma_y \) and \( \sigma_z \) are the extension scale of the initial perturbation in the \( y \)-direction and the profile of \( v_z \), respectively. The main flow is initially given by \( v_{x0} \).

For our initial conditions, the vorticity, \( \tilde{\omega} = \vec{\nabla} \times \vec{v} \), is concentrated around the shear layers \( y \pm y_l \), with maximum values of the order \( \omega_z \sim v_{x0}/a_l \) and \( \omega_x \sim -v_{z0}/\sigma_z \). The integrated values in the volume are \( \int_V \tilde{\omega} \cdot \vec{v} \, dV = O(\delta v) \) and \( \int_V \tilde{\omega} \, dV = O(k \delta v) \), due to the symmetry of the main flow with respect to each layer, where \( k \) is the inverse of the typical scale of the perturbation. Therefore, \( v_{z0} \) is used to primarily control the initial net kinetic helicity \( \mathcal{H}_k = \int_V \tilde{\omega} \cdot \vec{v} \, dV \). As a matter of fact, since \( v_z \) and \( \omega_z \) are aligned in both layers, the kinetic helicity has the same sign in both layers, and it is of the order \( \mathcal{H} \sim 2 v_{z0} v_{x0} L^2 \). The initial kinetic helicity is important since it is known to affect the dynamo mechanism in MHD turbulence.

The components of the initial perturbation, \( \delta v_i \), are a single-mode perturbation with a number of nodes \( n_i \in [1,N/2] \), periodic in the boundary box:
TABLE I. 3D KHI models: initial setup parameters. The others parameters are the same in all simulations: \( \rho_0 = 1 \), \( \alpha_1 = 0.01 \), \( y_l = L/4 \), \( L = 1 \), \( B_{01} = 0.001 \), \( B_{00} = B_{30} = 0 \), \( \sigma_y = 0.1 \), \( \sigma_z = 0.01 \), \( n_x = 11 \), \( n_y = 7 \), \( n_z = 5 \), \( \delta v_0 = 0.01 \), \( p_0 = 1 \), \( \gamma = 4/3 \).

| Model  | \( N^3 \) | \( v_{x0} \) | \( v_{y0} \) | \( \rho_1 \) |
|--------|-----------|-------------|-------------|-----------|
| KH3D250 | 250\(^3\) | 0.50 | 0 | 0.5 |
| KH3D500 | 500\(^3\) | 0.50 | 0 | 0.5 |
| KH3D500h | 500\(^3\) | 0.50 | 1 | 0.5 |
| KH3D500x | 500\(^3\) | 0.25 | 1 | 0.5 |
| KH3D500d | 500\(^3\) | 0.50 | 0 | 1.0 |
| KH3D1000 | 1000\(^3\) | 0.50 | 0 | 0.5 |
| KH3D1000h | 1000\(^3\) | 0.50 | 1 | 0.5 |
| KH3D2000 | 2000\(^3\) | 0.50 | 0 | 0.5 |

We underline that the specific form of the initial perturbation has no influence on the asymptotic turbulent behavior, as long as \( n_1 \gg 1 \) and \( \delta v_i \ll v_{0c} \).

We consider the models with input parameters given by Table I, varying the number of points between \( 256^3 \) and \( 2000^3 \). The standard values that we consider are \( \rho_0 = 1 \), \( \rho_1 = 0.5 \), \( \alpha_1 = 0.01 \), \( y_l = L/4 \), \( L = 1 \), \( v_{x0} = 0.5 \), \( B_{01} = 0.001 \), \( B_{00} = B_{30} = 0 \), \( \sigma_y = 0.1 \), \( \sigma_z = 0.01 \). For the perturbation we use \( n_x = 11 \), \( n_y = 7 \), \( n_z = 5 \), \( \delta v_i = 0.01 \). We employ \( p_0 = 1 \) and an ideal EoS with \( \gamma = 4/3 \). We use \( \Delta t = 0.4 \Delta t \) to evolve the system up to \( t = 20 \), except for the KH3D2000 model, which required over two million CPU hours to reach \( t = 10 \).

**B. General behaviour**

In Fig. [1] we show the density distribution over the slice \( z = 0 \), at \( t = 1, 5, 9 \), for the highest resolution case, KH3D2000. The following qualitative behaviour is the same in all cases. At the beginning, the instability develops as small-scale structures with modes given by the initial perturbation. The development starts at the shear layer, where the transfer of kinetic energy (dynamo effect) is fast up to \( t \approx 2 \) in all models (left panel). Then, a larger scale mixing takes place (middle and right panel), during which the effectiveness of the dynamo mechanism reduces. After about \( t \approx 10 \), the mixing is completed and the fluid looks isotropic.

In Fig. [2] we compare the evolution of the integrated kinetic and magnetic energy (left panel), for all models. The middle and right panels show the kinetic and magnetic radial-averaged spectra, as calculated with eqs. (74).

In our initially kinetic-dominated setup, the magnetic energy and the internal energies (the latter appears constant due to the small change compared to the large absolute values) keep rising during the evolution, at the expense of the kinetic budget. For this particular setup, the internal energy is quantitatively the dominant one (due to the chosen values of the initial pressure), while the magnetic energy is always quite smaller than the kinetic energy.

At the end of our simulations we do not reach yet a quasi-stationary state, and the dynamo mechanism is still acting, though at a slower pace. It is not our purpose to study in detail a putative final quasi-equilibrium/adiabatic state, or equipartition. Indeed, we are interested in exploring a variety of different states (in terms of magnetic and kinetic energy and spectra), which are well covered during the evolution of the simulations.

As well-known for an initial kinetically dominated setup, the magnetic energy grows and its spectrum is well reproduced by the Kazantsev slope (dotted thin line \( \propto k^{3/2} \)) while the kinetic spectrum is given by the Kolmogorov slope (thin solid black line \( k^{-5/3} \)). When the turbulence is developed, at small scales the magnetic energy is comparable to the kinetic energy. In this sense, at the end of our simulations the equipartition regards only the turbulent scales, since at large scale the kinetic energy is dominant over the magnetic one. For both kinetic and magnetic spectra, the results converge for the inertial range. This stresses that the dynamo mechanism is much more effective at small scales.

As well known, increasing the total kinetic helicity in the initial data enhances the dynamo mechanism, as seen if we compare the magnetic energy evolution for the cases KH3D1000 and KH3D1000h, and KH3D500, KH3D500h, KH3D500x for instance. While the growth rate is the same and originates from the shear layer, a second dynamo mechanism can be powered by an helical flow. Increasing the density jump also allows a more effective transfer to magnetic energy (compare KH3D500 with KH3D500d).

The higher effectiveness of the dynamo mechanism at small scales is reflected by the fact that the magnetic energy rises more for the higher resolution cases, as expected. This can be seen in Fig. [3] where we show the representative images for the \( B_z \) component in the \( z = 0 \) plane at \( t = 9 \), for the same model with different resolutions, KH3D500, KH3D1000, KH3D2000. It is clear how stronger small-scale structures are created in the best resolved cases. No large-scale order is seen, as confirmed also by the flat magnetic spectra.

The spectra also show that the intrinsic dissipation of the finite difference code is well visible as a change of slope (knee) in all the spectra. The spectral knee is given by the Kolmogorov slope (thin solid black line \( k^{-5/3} \)) while the kinetic spectrum is given by the Kolmogorov slope (thin solid black line \( k^{-5/3} \)). The total energy is larger (as the spectrum shows), due to the lesser numerical dissipation. This contrasts with the low-dissipative spectral schemes often used in turbulence box simulations (spectral methods especially), where indeed bottleneck effects are often seen, in terms of storing of energy in the smaller scales. Finite difference schemes suffer of the opposite problem due to numerical dissipation, but are more robust for realistic scenarios involving strong shocks, which are the ones...
FIG. 3. $B_z$ component in the $xy$-plane for different resolutions (from left to right), for the non-helical case, at $t = 9: 500^3, 1000^3, 2000^3$.

FIG. 4. Evolution of the Pearson coefficients $\mathcal{P}$ (top panels) and the best-fit coefficients $C_{\text{best}}$ (bottom) for the KH3D1000 model with $S_f = 2$, comparing different SGS models, indicated by symbols as in legends. First and second columns: diagonal and off-diagonals components of $\tau_{\text{kin}}$ ($\tau_{\text{mom}}$) for the dissipation and gradient models (cross-helicity model). Third column: $\tau_{\text{mag}}$ for the dissipation and gradient models. Fourth column: $\tau_{\text{ind}}$ for the gradient, dissipation, cross-helicity, vorticity and Alfvén model. All values here represented are the average over all the independent, non-zero tensor components ($3, 3, 6, 3$, respectively). For the sake of visibility, we employ a semi-log plot for the best-fit coefficients, where colors indicate positive (blue) or negative values (red).

we are interested. We see the same knee in 2D, for all models and for other fifth-order methods (FDOC5 and MP5), while WENO3 (see Appendix A) fails even to accurately reproduce the Kolmogorov slope at any range. Such relatively strong change of slope is quantitatively similar to what obtained from other finite-difference codes employing splitting schemes [80, 81].

Last, note that, since the conserved quantity in MHD is the total energy (which is exactly conserved for a periodic box), the inferred internal energy evolution inside each cell depends on the resolution-dependent estimation of the resolved kinetic and magnetic energy inside the cell volume, eq. (23). A lower resolution captures a smaller fraction of the total kinetic energy: this loss of information will represent an unphysical extra contribution to the internal energy.

After this qualitatively description, let us focus on the a-priori fitting. For more details about the dependencies of integrated quantities and spectra with initial data (like the initial magnetic field), we refer to a forthcoming paper (with LES comparisons) and to the abundant literature on turbulence.

C. A-priori fitting: representative case

As a representative example, we consider the model KH3D1000, filtered with $S_f = 2$ (thus, averaging the $N = 1000^3$ values to $N_f = 500^3$). In Fig. 4 we show the best-fit
coefficients and the related Pearson values, for $t \leq 20$, for the different SGS tensors. We consider the correlation of SFS and SGS tensors, as mentioned in § V C. To be precise, the reported values of the Pearson coefficients and the best-fit pre-coefficient are an average between the values relative to the different independent components of a given tensor. While at the beginning there is a preferential direction due to the initial conditions, as the turbulence develops we can consider the fluid isotropic and homogeneous. In any case, the values of $\mathcal{P}$ and $C_{\text{best}}$ are always very similar for all the different components. For instance, compare in Fig. 4 the averaged values for the diagonal (first column) and off-diagonal (sec-
instead of $\Delta$). The same holds for the $\tau$ differs from the dissipative model for the normalization ($\tau$ models, the dissipation and cross-helicity model for tensor components ($\tau$-models, the dissipation and cross-helicity model for

In general, the gradient model is by far the best model, since the associated Pearson coefficients are very close to one for all tensor components ($\mathcal{P} \geq 0.9$) at all times. Among the other models, the dissipation and cross-helicity model for $\tau_{\text{kin}}$ and $\tau_{\text{mag}}$ have a lower, but still non-negligible Pearson value (0.1-0.3). The same holds for the $\tau_{\text{ind}}$ Alfvén model, which only differs from the dissipative model for the normalization ($\Delta/\beta$ instead of $\Delta^2/\rho$). On the other hand, the dissipation model for $\tau_{\text{mag}}$, and both the cross-helicity and vorticity models for $\tau_{\text{ind}}$

Besides the better Pearson values, the gradient model outperforms all the others for another reason. As a matter of fact, the best-fit coefficients for the gradient model are fairly constant in time and $\sim \mathcal{O}(1)$. Instead, for the other models that fairly fit, the best-fit coefficients can change by orders of magnitude depending on the time considered (dissipation model for $\tau_{\text{kin}}$ and $\tau_{\text{ind}}$, cross-helicity model for $\tau_{\text{mom}}$, and Alfvén model for $\tau_{\text{mag}}$). The best-fit values of the dissipation and cross-helicity model (which is also known to be dissipative) are often below unity, in line with what found in literature. For models unable to fit SFS, the best-fit coefficients can even change sign (vorticity models, dissipation model $\tau_{\text{mag}}$, cross-helicity models for $\tau_{\text{ind}}$), confirming their unreliability.

A closer look to this correlation can be seen, for a given time, by looking at the 2D distribution of the $N^2$ pairs of SFS-SGS values, for a given tensor component. In Fig. 5 we show a representative case, the model KH3D500 at $t = 10$. These plots are very similar for all times, components and models, with only differences in the range of the value. We plot with colors the 2D SFS and SGS distribution frequency, showing their range of value $[\mathcal{P} \geq 0.25 \sigma]$ where $\mathcal{P}$ and $\sigma$ are the mean and standard deviation of the sample (see caption for detail). We show the correlations for three different models of $\tau_{\text{kin}}$ (top panels) and $\tau_{\text{ind}}$ (bottom) calculated with dissipation (left), gradient (center) and cross-helicity (right, for which we show $\tau_{\text{mom}}$ instead of $\tau_{\text{ind}}$) models. For these components, the distributions are quite symmetrical around zero, as expected for shear terms under isotropic conditions. A perfect correlation would be indicated by a single line with a finite slope corresponding to $1/C_{\text{best}}$. Only the gradient tensor is approaching such distribution, indicating its ability to systematically reproduce quite well the lost information on average. All the others visually show a very poor correlation, as the Pearson values quantitatively show.

The overall best performances of the gradient model are well known due to the strong mathematical basis on

### FIG. 7. Evolution of the best-fit coefficient (left panels) and the Pearson coefficients (right) for the gradient $\tau_{\text{kin}}$ (top), the $\tau_{\text{ind}}$ (middle) tensors, and the dissipative $\tau_{\text{kin}}$ (bottom) for all the models with $N = 500^2$, and different filter factors $S_f = 2, 4$. 

### FIG. 8. Evolution of the best-fit coefficient (left) and the Pearson coefficients (right) for the gradient $\tau_{\text{kin}}$ for the 2D models with $N = 500^2, 1000^2, 2000^2$, with filter factors $S_f = 2, 4, 10$ (see Appendix A2 for the description of the setup). The qualitative and quantitative behavior is the same as in 3D: the gradient model outperforms all the others, for all tensors. The best-fit values and their Pearson values are also in the same range as in 3D.
D. Dependence with initial conditions and dimensionality

By comparing all the simulations with the same resolutions but different initial conditions, we notice that the obtained Pearson and values best-fit coefficients are almost coincident with the previous case. An example is given in Fig. 7, where we show the results of the gradient models for $\tau_{\text{kin}}$ and $\tau_{\text{ind}}$ respectively, with filter factors $S_f = 2$ and $S_f = 4$. Differences with initial conditions are really minor, compared to the ones obtained by changing $S_f$, as we will see below. The same holds for the other SGS models, and other resolutions.

Moreover, we used the same approach for a 2D case, with the periodic box setup described in Appendix A2, with $N = 500^2$, $1000^2$, $2000^2$. We obtain very similar results regarding the best-fit coefficient and Pearson values, for all models and tensors. As a representative example, we show the results for $\tau_{\text{kin}}$, for the gradient model, in Fig. 8. Actually, the best-fit coefficients are even more constant than in the 3D case, and the Pearson value is slightly better. The degrading trend of the Pearson value for increasing filter factors $S_f$ (see below) is instead the same. The independence of the results on the
dimensionality is remarkable, given the qualitative differences in the kinetic cascade in the two cases.

E. Dependence with filter size and resolution

Changing the resolution (i.e., $\Delta$) or the filter size $\Delta_f$ affects the scale range of the lost information. Therefore, the best-fit coefficients and Pearson values of the SGS models can change. For all cases, the gradient model results to be the best one. However, there are some differences in the quantitative performance indicators.

First of all, in Fig. 9 we show that, for a given $S_f$ (in this case 2 or 4), the dependency on the initial resolution is mild. If we maintain the same filter factor, the results are very similar. This reflects the fact that the relative amount of information lost, for instance, between $N = 2000$ and $N_f = 500$, is similar to the one lost between $N = 500$ and $N_f = 125$. On the other hand, by increasing the filter size, instead, the relative amount of “hidden” information increases. Thus, the fit gets worse for higher filter size, as shown with more detail in Fig. 10 for the model KH3D1000 and $S_f = 2, 4, 10$. Increasing the size of the filter, the Pearson values of the gradient model decrease from $\sim 0.95$ to $\sim 0.6 - 0.7$ for $\tau_{\text{kin}}$ (top panels), and from $\gtrsim 0.9$ to $\sim 0.3 - 0.5$ for $\tau_{\text{ind}}$ (middle). In Fig. 11 we show the 2D correlations of the gradient model $\tau^{\text{GR}}_{\text{ind}}$ for the KH3D1000 simulation, comparing different size filters. It is evident how increasing the filter (i.e., the amount of information loss), the correlation degrades.

The best-fit coefficients of the gradient model increase by up of a factor of a few as the filter factor increases, deviating from the theoretical unitary value. This can be understood taking into account that the higher-order $\mathcal{O}(a^2)$ terms will become more important for larger $S_f$. The same trends (degrading of $\mathcal{O}$ and mild increasing of the best-fit coefficient, for increasing $S_f$) are seen for the dissipative model (see $\tau_{\text{kin}}$ in bottom panels of Fig. 7 and $\tau_{\text{ind}}$ in Figs. 2 and 10), and for the cross-helicity model for $\tau_{\text{kin}}$. For the Alfvén model, instead, the best coefficient scales as $\Delta_f$, as expected, since we defined it to be proportional only to $\Delta_f$, instead than $\Delta_f^2$. On the other hand, the vorticity model, the dissipative model for $\tau_{\text{mag}}$, and the cross-helicity model for $\tau_{\text{ind}}$ do not show any apparent trend with filter size and resolution, probably because of the absence of a true minimum in the least square residuals function.

The study of the trends for varying filter factors allows to understand that even the best SGS models are able to fit the unseen tensors only until an effective improvement of resolution of a factor of a few.

VII. CONCLUSIONS

This work generalizes and extends previous efforts of a-priori comparison of local SGS models, considering compressible MHD with a rather generic EoS $p(\rho, e)$, although we focus here on the specific case of an ideal EoS. We have extended the formalism of filtering in LES context, including also the energy evolution equation. We have reviewed the most important SGS models.

We have then numerically assessed them, using our platform Simflowy [24] endowed with HRSC finite-difference schemes commonly used in numerical relativity applications, already described in depth in our previous work [33]. We stress that we use methods that may not be optimal for periodic box turbulence, but are adequate in astrophysical simulations with the development of strong shocks. As a matter of fact, many works in turbulence use spectral methods, which are particularly suitable for studies of smooth solutions (or with weak shocks) in periodic boxes due to their intrinsic low numerical dissipation. However, in a real problem, where the domination is not periodical, and the dynamics includes strong shocks, codes employing finite-difference or finite-volume schemes are preferred due to their robustness.

We have compared different SGS models and studied in depth the best-fitting one: the gradient model, the only one with a strong mathematical foundations compared to the other models considered here, which are mainly based on physical assumptions (Smagorinsky) or on dimensional basis (vorticity, cross-helicity...). Our results are in line with what found
in literature. The gradient model outperforms all the others in terms of fitting SFS residuals and provides stable performance (the best-fitting coefficient do not deviate from unity more than a factor of 2), for a remarkable variety of: dimensionality, initial conditions, resolution, time within a simulation and filter factor. The Pearson value is excellent (\( r > 0.9 \)) for a filter factor \( S_f = 2 \), and gradually degrades, being still decent (\( r > 0.5 \)) for a filter factor 10. The degradation of the performance is understandable: if the LES resolution is too coarse compared to the dynamically interesting scales, then the inclusion of the SGS model will not be able to represent all the missing scales. For the gradient model, the deviation of the pre-coefficient from unity (up to a factor a few, but usually less than 2) is much smaller than any other SGS model. The small deviation can be interpreted as the effect of the form factor of the effective filter (a box in the position space instead of a Gaussian shape) and higher order corrections \( O(a^2) \) in terms of fitting SFS residuals and provides stable performance.

This paper casts the basis for a series of studies that have as a final aim the generalization of SGS-based LESs to the framework of General Relativity. The next step is to test the gradient model performing a-posteriori comparison for what concerns the integrated quantities and the spectra. The relativistic extension of the gradient model will be also presented soon for the first time.

Our schemes, fifth-order accurate in space, represent the state-of-the-art in binary neutron star merger simulations, where turbulence develops at very small scales. Unfortunately, the high computational cost of DNS is not currently allowing us to fully capture of the turbulent dynamics, making LES one of the few viable ways to describe these unresolved scales.

Therefore, we will present the complete formalism to generically consider a system of equations with conserved and primitive variables, as already done here partially.

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**Table II.** Table of 2D single layer models, with the theoretical and best-fit values (1 σ error typically \( \lesssim 2\% \)) of the growth phase for the simulations run with WENO5Z.

| model | N | \( v_0 \) | \( a_l \) | \( k_s \) | \( B_0 \) | \( \alpha_{an} \) | \( \alpha_{num} \) |
|-------|----|----------|-------|------|-------|--------|--------|
| grv1  | 50 | 0.645    | 0.05  | 1    | 0     | 1.73   | 1.53   |
| grv2  | 100 | 0.645   | 0.05  | 1    | 0     | 1.73   | 1.70   |
| grv3  | 200 | 0.645   | 0.05  | 1    | 0     | 1.73   | 1.75   |
| grv4  | 400 | 0.645   | 0.05  | 1    | 0     | 1.73   | 1.75   |
| grv5  | 200 | 0.645   | 0.025 | 1    | 0     | 2.4    | 2.37   |
| grv6  | 200 | 0.645   | 0.1   | 1    | 0     | 0.66   | 0.68   |
| grv7  | 200 | 0.3225  | 0.05  | 1    | 0     | 1.09   | 1.07   |
| grv8  | 200 | 0.9215  | 0.05  | 1    | 0     | 1.77   | 1.79   |
| grv9  | 200 | 0.645\^2 | 0.05 | 2    | 0     | 1.36   | 1.32   |
| grv10 | 200 | 0.645   | 0.05  | 1    | 0     | 1.29   | 1.70   |
| grv11 | 200 | 0.645   | 0.05  | 1    | 0.258 | 1.56   | 1.54   |

\( ^\circ \) this value has previously incorrectly reported\(^\circ \) to be half of this, incompatible with the corresponding growth rate.

**Appendix A: 2D tests**

1. **Open boundaries Kelvin Helmholtz test**

As a validation test for the methods employed, we run a well-known 2D KHI test set-up\(^\circ \) with open boundaries in the vertical direction. We set a rectangular domain in the \( x-y \) plane, with side length \( L_x = 1, L_y = 2 \), centered in \( (0,0) \), with a number of points \( (N,2N) \). The initial conditions consist of \( P = \rho = 1 \) everywhere, with an ideal EoS with \( \gamma = 5/3 \), with a \( a_l \)-thick shear layer along the \( x \) direction, with the following initial conditions:

\[
\begin{align*}
v_x &= \frac{v_0}{2} \tanh \frac{y}{a_l} \quad (A1) \\
v_y &= \delta v_y \exp[-(y/4a_l)^2] \sin(2\pi k_x x) \quad (A2) \\
B_x &= B_0 \quad (A3) \\
B_y &= 0 \quad (A4)
\end{align*}
\]

where \( v_0 \) is the shear velocity, and \( \delta v_y \ll v_0 \) represents the initial perturbation. We impose periodic boundaries in the \( x \)-direction, and open conditions (i.e., copying the values of the last cell to the ghost cell) in the \( y \)-direction (see a previous detailed study\(^\circ \) for the effects of changing the boundaries in the \( y \)-direction from open to reflecting, but this is not the focus of our work).

We set \( \delta v_y = 10^{-6} \) and we considered different cases, as listed in Table II, similar to Table A.1 in the reference paper\(^\circ \). We use different reconstruction methods: WENO3YC, FDOC3, FDOC5, MP5, WENOSZ (for details about the parameters of these models and further tests, see our dedicated paper\(^\circ \)). We follow the simulations well beyond the saturation time, with a time-step \( \Delta t = 0.25 \Delta \), where \( \Delta = L_x/N \) is the homogeneous resolution of the numerical grid.

As a first example, in Fig. 12 we show the plots of the density and velocity fields (white arrows), at \( t = 10 \) and \( t = 15 \).
FIG. 12. Development of KHI for the single layer problem, at $t = 10$ (left panels) and $t = 15$ (right panels). We show the density with colors and the velocity fields with white arrows for the model $\text{grw3}$ (top panels) and $\text{grw10}$ (middle panels), and the vorticity with colors and the magnetic fields with black arrows for the model $\text{grw10}$ (bottom panels). (left/right panels, respectively), for the reference model $\text{grw3}$ (top panels) and its magnetic version, $\text{grw10}$ (middle panels). For the latter, we also show in the bottom panel the plots of vorticity (with colors) and magnetic field (black arrows). After an initial phase, the instability is triggered and develops vortices, until a quasi-stationary configuration is reached.

A quantitative tracer of the degree of the turbulence developed at a given time during the development stage is the $y$-component of the kinetic energy integrated in the volume:

$$E_{ky} = \int_V \frac{1}{2} \rho v_y^2 \, dV,$$

FIG. 13. Comparison of the growth of $E_{ky}$ for the cases $\text{grw1}$ (top) and $\text{grw10}$ (bottom), with the five different reconstruction methods.

(A5)

After an initial time, $E_{ky}$ tends to grow exponentially until it saturates. We fit the exponential growth rate phase with a function $E_{\text{fit}} = E_0 e^{2 \alpha k h t}$, and compare the best-fit values of $\alpha k h$ with the numerical values obtained by the numerical simulations available in literature and the ones theoretically obtained by means of a theoretical stability analysis.

The growth rate and the saturation value of $E_{ky}$ are physically controlled by different values of $v_0$, $a_l$, $k_x$ and $B_0$, but not by the amplitude of the perturbation $\delta v_y$, which only influence the time at which the instability starts to develop. Furthermore, the numerical methods and resolution are crucial to determine the growth rate and the instability trigger time.

In Fig. 13 we show the $E_{ky}$ growth for two of the eleven cases analyzed and listed in Table II: $\text{grw1}$ (low resolution) and $\text{grw10}$ (magnetic case). Inspecting the first, low-resolution case, $\text{grw1}$, we underline that the third-order methods, FDOC3 and WENO3YC, are not able to capture the in-
stability in the low resolution case, while the fifth-order methods do, even though the growth rate is different. In particular, WENO5Z gives the higher value, slightly larger than MP5 and and FDOC5, and slightly smaller than the theoretical reported values. Such differences disappear already with intermediate resolutions, \( N = 200 \) (model grw3, right panel). In this case, the third-order method still show a value of \( \alpha_{kh} \) slightly inferior than the theoretical value, which is instead perfectly matched by the simulations with the three fifth-order methods. The three of them are basically indistinguishable.

We then test all the cases of the benchmark paper with the method WENO5Z, which was the one with the best behavior. For all of them, we find an excellent agreement with the theoretical expectation, as shown in Table II. One side, the trends between the growth rate and the physical parameters \( v_0 \) (compare grw3, grw7, grw8), \( a_i \) (grw3, grw5, grw6), \( B_0 \) (grw3, grw10, grw11) and \( k_x \) (grw3, grw9) are correctly recovered. On the other hand, the differences among the models grw1, grw2, grw3 and grw4 show how the resolution allows one to better capture the instability. For this particular case, having \( N > 200 \) seems to be enough to capture the instability. However, we underline that the importance of the numerical resolution is amplified if the initial perturbation mode \( (k_x) \) is larger: the smaller the scale, the more important the resolution and methods become.

As a final preliminary test with this setup, we examine the possible issue considered in literature: in presence of a uniform, Galilean boost in one direction (i.e., an additional advection velocity, constant everywhere), the development of the KHI can be numerically inhibited, due to the numerical dissipation which is enhanced by the value of the advecting velocity. Thus, we compare the same model (grw3 in this case), with and without an additional advection in the direction \( x \) with a value comparable to the difference of velocities, \( v_{\text{x,adv}} = 1 \), such that, initially, eq. (A1) becomes

\[
v_x = 1 + \frac{v_0}{2} \tanh \frac{y}{a}
\]

Fig. 15 shows the growth of the kinetic energy with and without the advection, with WENO5Z, for the problems grw1, grw3, grw10. No important differences are noticed. We repeated the test with for the cases with lower-order methods (WENO3YC, FDOC3) and/or the low-resolution problems, and in any case we found an appreciable difference.

This first test shows that the numerical implementation is correct and able to reproduce the expected growth rate of the KHI, as long as at least one among the resolution and the accuracy order is high enough.

2. Periodic 2D Kelvin Helmholtz tests

We also tested the KHI in a periodic 2D box with a double mixing layer, similar to the 3D case presented in § VI. This has allowed us to compare the literature of 2D turbulent periodic boxes. We consider a square domain with \( x, y \) both in the range \([-L/2, L/2]\] with \( N \) points in each direction. The initial positions of the mixing layers are \( y = \pm L/4 \), as the initial set-up describes:

\[
\begin{align*}
\rho &= \rho_0 \pm \delta \rho \\
v_x &= \pm 0.5 v_0 + \delta v_x \\
v_y &= \delta v_y \\
p &= p_0 \\
B_x &= B_0 \\
B_y &= 0
\end{align*}
\]

See also Athena webpage:

\url{http://www.astro.princeton.edu/~jstone/Athena/tests/}
![Image of the KHI simulation in 2D with 1000^2 points at t = \{0.5, 3, 5, 7\} from left to right, respectively. Colors indicate the density, while white and black arrows represent the velocity and magnetic fields, respectively.](image1)

![Image of the KHI simulation in 2D with N^3 = \{1000^2, 400^2, 100^2\} points from left to right, at time t = 10. Colors indicate the density, while white and black arrows represent the velocity and magnetic fields, respectively.](image2)

where the sign ± indicate the region |y| > L/4 and |y| ≤ L/4, respectively. The perturbation in each i direction is given either by an uniform random distribution within [−δv_0, δv_0], or by δv_i = δv_0 \cos(2\pi n_i/L), where n_i ∈ [0, N]/2 are integers and they can be different in the two directions.

Hereafter we set L = 1, v_0 = 1, \rho = 1, δρ = 0.5, p_0 = 2.5, and we use an ideal EoS with γ = 1.4, with a sinusoidal perturbation with δv_0 = 0.01, n_x = 4 and n_y = 7, unless specified otherwise. We impose periodic boundary conditions in all directions and we run with a time-step Δt = 0.25 Δt, in order to be sure that the numerical errors are not dominated by the time discretization. We run up to t = 10, a time long enough to reach the quasi-stationary state, and we run the same simulation with different resolutions, N ∈ [100^2, 2000^2] with WENO5Z.

We have run different values of the initial magnetic field. In general, the initially constant magnetic field partially inhibits the KHI. This feature is well known and is quantified by the Alfvén factor, defined as the ratio between hydro and Alfvén velocities, A = v_0 / \sqrt{B^2/\rho}. When A ≤ 1, the KHI is totally inhibited, as explained in detailed in previous works. In our case, we start from a value A \sim 10^3, thus the KHI takes place.

Fig. 16 shows the evolution for a N = 1000^2 simulation with WENO5Z, including magnetic field with δB_0 = 0.001. We show the density map (color scales) and the velocity and magnetic fields with arrows, at different times.

The stages of the dynamics are similar to the 3D case: at the beginning, vortical structures are formed with a pattern given by the k_i wave-numbers of the initial perturbation (t \lesssim 1 for the chosen values of δv_0). The symmetry of the patterns is broken when the structures at the two mixing layers start to interact (t \gtrsim 1). Then, the turbulence, initially concentrated around the mixing layer, tends to homogeneously spread over the entire dominion, thanks to the periodic boundary conditions. Meanwhile, the vortexes tend to merge (the well-known inverse kinetic cascade in 2D), and at late time (t \gtrsim 10 in this case) only two large vortexes of opposite vorticity sign survive. The turbulent dynamics reaches a saturated, fully developed state, dominated by these large vortexes, and, given the absence of any forcing, it decays, transforming kinetic energy into internal energy.

For our setup, when the system reaches a quasi-stationary state, the magnetic energy remains still significantly smaller than the kinetic energy, and is significantly stored in small scales. Kinetic and magnetic spectra show the same characteristics as the 3D case (main text), with the expected 2D Kolmogorov and Kazantsev slopes in the inertial range.

The timescales and the resolved structures mainly depend on the problem parameters (B_0, δv_0), and on the resolution, respectively. At this respect, Fig. 17 shows the plot of density with colors, and the velocity and magnetic fields at t = 10, for decreasing resolution N = 1000^2, 400^2, 100^2. It is evident how the the resolution affects the capability to capture the turbulent details.
We have also performed the a-priori fitting for different resolutions and filter sizes. We report a representative case in Fig. 8 briefly mentioned in the main text. Overall, for all tensors and SGS models results are really similar to the 3D ones.

We checked that the growth of $E_{gy}$, indicating the development of the turbulent state, is enhanced if high resolution or high-order methods are used, and MP5 and WENO5Z provide statistically compatible results, if the same resolution is used. The difference between two different numerical schemes are only stochastic: the particular position of the vortices can be different, but the spectra and the integrated quantities are statistically indistinguishable. In the main text, all simulations are run with WENO5Z.

The same holds if we compare the fully developed turbulence obtained with different initial perturbations: the specific time of growth can change, but at saturation the runs are statistically equivalent. In this sense, we checked that the values of $\delta_{v0}$ or the specific form of the perturbation can affect the delay of the beginning of the exponential growth, but not the growth rate and the asymptotic value of $E_{gy}$. This holds always as long as the initial values of the perturbation is random, or it is sinusoidal but at least one among $n_1$ and $n_2$ of the initial perturbation has no common integer factors with $N$. When the three numbers have a common integer factor $C$, then the initial data are effectively periodic in the $x$-direction on a scale $L/C$. Therefore, in these cases, a mode with wavenumber $C$ and its higher harmonics are maintained during the entire simulation, since the $x$-scales larger than $L/C$ are not explored, thus preventing a proper spectral cascade (the spectrum is constituted by spike corresponding to the chosen modes and its harmonics) and the related full development of the turbulence. For instance, we numerically proved that, starting with $n_x = n_y = 4$ or $n_x = n_y = 8$, and $N = 500$ (for which $C = 4$), the simulations show a periodicity in the $x$-direction given by $L/4$, being 4 the common factor between $N$, $n_1$ and $n_2$. This is a further test for the correct numerical implementation, that shows no sign of numerical break of symmetry. Note that we employ a periodic initial perturbation instead of a random one, in order to avoid numerical instabilities when run in parallel, rising from the technical SAMRAI management of the boundaries between different patches.

Summarizing, the 2D tests has allowed us to validate the capability of the code to simulate turbulent dynamics, and to identify WENO5Z as the best numerical method, that we use in the main text.

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