SPH Physically Reconsidered - The Relation to Explicit LES and the Issue of Particle Duality

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In this work we will identify a novel relation between Smoothed Particle Hydrodynamics (SPH) and explicit Large Eddy Simulation (LES) using a coarse-graining method from Non-Equilibrium Molecular Dynamics (NEMD). While the current literature points at the conclusion that characteristic SPH issues become restrictive for subsonic turbulent flows, we see the potential to mitigate these SPH issues by explicit subfilter stress (SFS) modelling. We verify our theory by various simulations of homogeneous, isotropic turbulence (HIT) at $Re = 10^5$ and compare the results to a DNS solution reported in Ref.\cite{19}. Although the simulations substantiate our theory, we see another issue arising, which is conceptually rooted in the particle itself, termed as Particle Duality. Finally, we conclude our work by acknowledging SPH as coarse-graining method for turbulent flows, highlighting its capabilities and limitations.

I. INTRODUCTION

Since its first introduction for astrophysical flow problems by Lucy and Gingold & Monaghan in 1977\cite{1}, the success of SPH as a viable Lagrangian method in the Computational Fluid Dynamics (CFD) community is undeniable. In the last decades there was a considerable research effort to increase the fundamental maturity of the method, summarized in several reviews\cite{2,3}, which was in parallel accompanied by progress regarding applications of higher complexity, e.g. Ref.\cite{10,11}.

One of the most fundamental problems of classical Lagrangian SPH is that it suffers from zeroth order errors, which result in a substantial amount of noise compared to grid based Eulerian methods.\cite{12,13} Physically, this noise causes excessive dissipation by numerically induced small-scale vorticity.\cite{14} Although it could already be hypothesized based on the work of Ellero et al.\cite{15} that this might become a severe issue for subsonic turbulence, a rigorous and detailed analysis proving this fact for forced homogeneous, isotropic turbulence (HIT) was presented in the seminal work of Bauer & Springel\cite{16}. Up to date, the shortcomings of SPH for subsonic turbulence as discussed by the authors persist, namely that large scale turbulent structures can be qualitatively captured but at comparably high computational cost taking alternative CFD methods into account. This is quite unsatisfactory given that turbulence is a key aspect of most fluid flows.

However, it might be argued that the results obtained by Bauer & Springel\cite{16} are the consequence of a missing turbulence model and that they are only valid for underresolved Direct Numerical Simulations (uDNS). There were several publications on turbulence modelling in SPH\cite{17,18}, but most of them either show a marginal improvement or are rather inconclusive for three dimensional subsonic turbulence. The latter can be attributed to the fact that the models are tested only with scarce validation runs, on setups which contain complex boundaries adding other SPH specific uncertainties on top of the actual turbulent flow\cite{19} or are validated for two dimensional turbulence, which behaves qualitatively different\cite{20} and where the use of usual turbulence closure models is unjustified, e.g. Ref.\cite{21,22}. In our opinion, the most promising approach so far was presented in the pioneering work of Di Mascio et al.\cite{23} and only recently extended by Antuono et al.\cite{24}. In these works the authors explore SPH from a Large Eddy Simulation (LES) perspective, which represents a natural option as already noticed three decades ago.\cite{25} Despite the fact that the derived SPH-LES approach with its various additional terms is an important step for SPH towards turbulent flows, both works do not evaluate the foundations of the classical LES subfilter stress (SFS) in a SPH framework, which is the central quantity in LES. In our opinion, the latter objective is vital, because the classical Lagrangian SPH features a turbulent kinetic energy deficit, which questions the intention of introducing mostly dissipative SFS models from the beginning.

The work presented in this paper focuses on connecting explicit LES and SPH with a coarse-graining method from Non-Equilibrium Molecular Dynamics (NEMD). Hence, this study can be viewed as a sequel of our recent publications.\cite{26,27} We will demonstrate that the only additional term emerging from our theory is the SFS term as it is known from Eulerian LES methods. This is contrary to the statement of Di Mascio et al., concluding that a proper LES interpretation of SPH necessitates the consideration of additional SPH exclusive terms, though the authors ascertain that these terms play a minor role.\cite{23,28} Consequently, we will be able to discuss the rationality of SFS models for the SPH simulation of subsonic turbulent flows. We are not considering further heuristic noise-mitigating techniques. Most importantly, our work is motivated by the following central question: Can resolved large scale structures profit from the reduction of SPH typical small-scale noise by explicit use of SFS models?

In order to elaborate this hypothesis, this paper is structured as follows: We start with a short review of the main characteristics of subsonic HIT and how the large scale dynamics of such turbulent flows can entirely be described by coarse-graining regularization of the fluid dynamic balance equation.\cite{29} This technique is most commonly known as LES. Then, we will relate this coarse-grained picture of
subsonic turbulence to SPH. We constitute that SPH can be viewed as a Lagrangian quadrature technique for the governing equations of explicit LES and discuss the significant implications of this approach. To verify our theory, we will subsequently present various results of subsonic HIT simulations at $Re = 10^3$ and compare the results to a DNS solution reported in Ref.\cite{1}. Finally, we will draw a conclusion on the rationality of SFS models in SPH.

II. LES: COARSE-GRAINED DYNAMICS OF SUBSONIC TURBULENT FLOWS

Despite the omnipresence and extraordinary beauty of turbulent flows, a comprehensive theory is still missing. However, it is agreed by the fluid dynamics community that the concept of the energy cascade is an important cornerstone of turbulence theory\cite{33}. The cascade process was metaphorically described by Richardson\cite{33} in 1922 for the first time, before it was quantified for incompressible HIT by Kolmogorov\cite{34}, Obukhov\cite{35}, Onsager\cite{36} and Heisenberg\cite{37} about 20 years later. For fully developed turbulence it was already demonstrated back then that, in a statistically averaged sense, a range of large scales exists in which the kinetic energy of velocity fluctuations of a specific wavenumber, namely $E(k)$, is transferred from larger to smaller scales in the absence of viscous dissipation effects. This range is known as inertial range\cite{38} and its scaling characteristics of

$$E(k) \sim k^{-5/3}$$

serves as an important benchmark for CFD solvers to prove their capability to reproduce large scale dynamics of strongly subsonic turbulent flows, e.g. Refs\cite{11,13}. In contrast, latest research activities on strongly subsonic HIT focus on the smallest scales of the cascade process, namely the dissipation range and beyond\cite{19,25}. Among others, it has been rigorously argued by Sreenivasan & Yakhout\cite{40} with the aid of a novel anomalous scaling theory, that the actual smallest turbulent length scale with wavenumber $k_{\eta}$ falls below the Kolmogorov scale with $k_{\eta}$. Another example is the importance of thermal fluctuations beyond the classical dissipation range, i.e. $k_{\eta} < k < k_{mfp}$ with $k_{mfp}$ denoting the wavenumber of the mean free path, eventually leading to a $E(k) \sim k^2$ scaling\cite{41,43}. Overall, all these insights can be vividly condensed in the turbulent kinetic energy spectrum as depicted in FIG. 1 highlighting the different turbulent regimes.

Although all scales are of significant importance for a holistic view of HIT, based on the work of Bauer & Springel\cite{13} we can already conclude that classical Lagrangian SPH struggles to directly resolve turbulent small scale dynamics. Hence, it seems more convenient to combine SPH with a coarse-grained model, which intrinsically focuses on the turbulent large scales with its inertial range characteristics (Eq. $1$). This approach is more likely to be compatible, as the feedback of the smallest scales only has to be modelled and not resolved. A coarse-grained model of that kind can be derived by means of a technique from the Non-Equilibrium Molecular Dynamics (NEMD) community\cite{31} which was introduced by Hardy in 1982\cite{44}. We will abbreviate it in the following as Hardy theory. The key aspect of this theory is that it transfers arbitrary Lagrangian particles into coarse-grained particles by appropriate averaging, satisfying axiomatic conservation properties scale independently\cite{11}. The averaging is mathematically accomplished by the introduction of a normalized, symmetrical, positive, and monotonously decaying function $W_h$ with compact support $supp\{W_h\} \subset \mathbb{R}^3$, in short kernel. It is assumed that the latter is spherical and its spatial extent is quantified by the scalar index $h \in \mathbb{R}^+$. Originally, as depicted in FIG. 2 the Hardy theory was used to link the dynamics of discrete molecules and individual fluid elements governed by their continuum balance equations, e.g. Navier-Stokes for Newtonian flows. Even more important for this work is the fact that the Hardy theory can be generalized to a continuous set of Lagrangian particles as well, i.e. fluid elements (FIG. 2). This generalization leads to the governing equations of coarse-grained super fluid elements, which for $h = const$ are completely equivalent to the governing equations of LES\cite{11}. The latter represent a deterministic fluid flow model, which inherently focuses on scales above the kernel size and is able to capture the turbulence cascade\cite{24}. Thus, we interpret it as a physical description, which matches well with the SPH image for subsonic turbulence provided by Bauer & Springel\cite{13}.

Although this LES perspective based on Lagrangian particles requires an additional mathematical effort compared to the common commutable filtering operation\cite{45}, it reveals a striking similarity between LES and SPH. A relation between the latter was already noticed 30 years ago by Bicknell\cite{28}, but we take the view that our perspective on LES vividly strengthens this point. As common feature, both methods perform a coarse-graining of Lagrangian particles by means of a kernel and we will use this property in Sec. III to argue that SPH can be reinterpreted as a Lagrangian quadrature technique of the governing equations of LES.

However, before we proceed with this objective, we will first concentrate on a fluid flow model, which is in general capable to describe isothermal, strongly subsonic HIT. Therefore, we select a Newtonian, barotropic fluid flow completely
Molecule Fluid Element Super Fluid Element
Kernel Averaging Molecular Dynamics Navier-Stokes Equation Large Eddy Simulation
Towards larger scales

FIG. 2. Schematic of consecutive application of Hardy theory to different particle groups. Using a spherical kernel with size ~ h, smaller particles can be transferred into coarse-grained particles by appropriate averaging. As a consequence, axiomatic conservation properties, e.g. mass, momentum, energy, are scale-independently satisfied.

specified by its density, pressure and velocity field, namely \( \rho, p \) and \( \mathbf{v} \), and apply the Hardy theory to it as detailed in Ref. \[31\]. With \( \mathbf{x} \in \mathbb{R}^3 \), we denote an individual kernel center position and its corresponding support is abbreviated as \( V_t := \text{supp}(W_h) \). Positions of specific Lagrangian particles are represented by \( y \in \mathbb{R}^3 \). Further, we assume a constant kinematic viscosity \( \nu = \text{const} \) and Mach number \( Ma < 0.3 \). The latter implies that we can simplify the viscous stress term to \( \text{div} \{ \tau_{\text{visc}} \} = \text{div} \{ 2\nu p \mathbf{D} \} \) as \( \nabla \cdot \mathbf{v} \approx 0 \) \[46,47\] with \( \mathbf{D} \) denoting the symmetric strain rate tensor. Finally, the considered LES model in its Lagrangian form reads

\[
\bar{\rho}(\mathbf{x}, t) = \int_{V_t} \rho(y, t) W_h(\mathbf{x} - y) \, dy ,
\]

\[
\dot{\bar{\rho}}(\mathbf{x}, t) = - \int_{V_t} \nabla_y p(y, t) W_h(\mathbf{x} - y) \, dy + \int_{V_t} \text{div}_y [2\nu p \mathbf{D}] (y, t) W_h(\mathbf{x} - y) \, dy - \text{div}_x \{ \tau_{\text{SFS}} \} (\mathbf{x}, t) ,
\]

\[
\begin{aligned}
\bar{\rho} &= \rho_{\text{ref}} + K \left( \frac{\rho}{\rho_{\text{ref}}} - 1 \right), \\
\rho_{\text{ref}}, \rho_{\text{ref}}, K &\in \mathbb{R}^+.
\end{aligned}
\]

The equations Eqs. \[2a\], \[2b\] & \[2c\] represent the averaged continuity equation, the averaged momentum transport equation and a linear barotropic equation of state (EOS) with \( \rho_{\text{ref}}, \rho_{\text{ref}} \) & \( K \) as constants. These describe the reference density of the strongly subsonic flow, the reference pressure and a stiffness constant, which are highly dependent on the problem. Their choice will be specified in Sec. \[IV\]. Furthermore, from Eq. \[2a\], the meaning of the overline notation for an arbitrary field \( f \) can be deduced. It describes a spatial average over a superfluid element \( V_t \) of size \( \sim h \), namely

\[
\bar{f}(\mathbf{x}, t) := \int_{V_t} f(y, t) W_h(\mathbf{x} - y) \, dy
\]

with \( dy \) as volume differential of a Lagrangian fluid element. Moreover, the momentum transport equation Eq. \[2b\] employs a density-weighted averaged velocity \( \bar{\mathbf{v}} \) over \( V_t \) as indicated by the tilde notation. Generally, this density-weighted average for a field \( f \) is termed Favre average \[21,49\], although it was already suggested by Reynolds \[50\] in 1895. It is defined as

\[
\bar{f}(\mathbf{x}, t) := \frac{\bar{\rho} f(\mathbf{x}, t)}{\bar{\rho}(\mathbf{x}, t)} .
\]

The use of Favre averages is not mandatory but handy, as it circumvents correlation terms related to the density field \[51\]. It is important to distinguish between quantities according to Eq. \[3\] & Eq. \[4\], which refer to super fluid elements in the LES framework, and fluid element quantities, which are simply noted without an overline or tilde. Additionally, as a consequence of the coarse-graining regularization of the balance equations by Eq. \[3\], an extra term \( \text{div}_x \{ \tau_{\text{SFS}} \} (\mathbf{x}, t) \) appears in Eq. \[2b\] \[31,32\]. It is the contribution from scales below \( V_t \) to the momentum transport of super fluid elements. The SFS tensor \( \tau_{\text{SFS}} \) can be written as covariance tensor of the velocity field \[31\]
which is an interesting representation as the discretized version of \( E_{3} \) localizes flow subdomains, where SPH struggles with accurate approximations.\( ^{39} \) Due to its relevance for this study, we will elaborate on this in more detail in Sec. \( \text{III B} \).

Finally, it might be surprising that the averages on the right hand side of the transport equations in Eq. \( (2) \) are explicitly noted for each \( V_{i} \) and not abbreviated by Eq. \( (3) \). By that we intend to emphasize that we follow the philosophy of explicit LES methods, e.g. Refs.\( ^{51,52} \). Contrary to the usual procedure in explicit LES, where the nonlinear convective term is explicitly filtered, the filter is explicitly applied to the right hand side of the transport equations. This is due to the Lagrangian perspective we take, in which the convective term is not directly considered but rather a consequence of the individual forces on the right hand side of Eq. \( (2b) \).

### III. SPH AS A LAGRANGIAN QUADRATURE OF EXPLICIT LES

As explained in the last section, the governing equations of LES can generally be derived by coarse-graining of Lagrangian fluid elements using the Hardy theory from NEMD. This explains the conceptual similarity of LES and SPH, which becomes also evident from FIG. 2 being a reminder of how SPH is often vividly introduced, e.g. in the work of Price.\( ^{30} \)

The objective of this section is to argue that SPH should be generally viewed as a Lagrangian quadrature technique for the governing equations of explicit LES. This general fluid dynamic framework includes the kernel concept from the beginning. In the following, we will present the resulting SPH model and discuss the implications of the explicit LES perspective.

#### A. The SPH-LES Model and its Implications

Decomposing the fluid domain into a finite number of Lagrangian SPH particles \( i \in \{1, ..., N\} \) that are connected to the kernel center positions, i.e. \( \forall i \in \{1, ..., N\} : x_{i} = y_{i} \), one can derive the final SPH model. The discretization procedure of Eq. \( (2) \) is detailed in the Appendix \( \text{(Eqs. A.10) \& (A.16)} \). It is important to highlight that the SPH particles only have to be Lagrangian representatives of super fluid elements \( V_{i} \) with the arbitrary length scale \( h \) instead of fluid elements. This is a significant difference to the usual SPH approach because traditionally SPH particles suffer from pseudo-Lagrangian behaviour at finite resolution.\( ^{40,41} \) For an individual particle \( i \) with \( j \in \{1, ..., N_{\text{ngb}}\} \) neighbors the model reads

\[
\bar{p}_{i} = M_{i} \sum_{j=1}^{N_{\text{ngb}}} W_{h,ij} = \frac{M_{i}}{V_{i}} \quad \text{&} \quad V_{i} := \frac{1}{\sum_{j=1}^{N_{\text{ngb}}} W_{h,ij}},
\]

\[
\bar{p}_{i} \frac{d\vec{v}_{i}}{dt} = -\sum_{j=1}^{N_{\text{ngb}}} (\bar{p}_{j} + \rho_{i}) \nabla W_{h,ij} V_{j} + 2(2+n) \eta \sum_{j=1}^{N_{\text{ngb}}} \rho_{i} \left(x_{i} - y_{j}\right) \cdot (x_{j} - y_{j}) \nabla W_{h,ij} V_{j} - \text{div}[\tau_{\text{SFS}}]_{i},
\]

\[
\bar{p}_{i} = \rho_{\text{ref}} + K \left( \frac{\bar{p}_{i}}{\rho_{\text{ref}}} - 1 \right), \quad \rho_{\text{ref}}, \rho_{\text{ref}}, K \in \mathbb{R}^{+},
\]

and the particle trajectories follow from the kinematic condition

\[
\frac{dx_{i}}{dt} = \vec{v}_{i}.
\]

Formally, the emerging system of Eqs. \( (6) \) \& \( (7) \) is identical to the SPH discretization of the weakly-compressible Navier-Stokes equations (WCSPH) except for the SFS term \( \text{div}[\tau_{\text{SFS}}] \) in Eq. \( (6b) \). The latter is a direct consequence of the coarse-graining at the arbitrary kernel scale \( h \), compensating for subkernel effects. Contrary, in traditional SPH, the choice of the scale \( h \) is merely a matter of convergence. We understand this as a physically convincing argument, going beyond empty formalities, to state that SPH should be understood as a Lagrangian quadrature technique intrinsically connected to explicit LES. Then, from this LES perspective, deficits introduced at the kernel scale for a specific choice of \( h \) could potentially be compensated by a proper modelling of the SFS tensor \( \tau_{\text{SFS}} \) in Eq. \( (2b) \). We believe that empirical evidence for this reconsideration is also given by the fact that already in the pioneering SPH works of Lucy and Gingold & Monaghan\( ^{42} \) artificial damping terms were used. These can be interpreted as the first SFS models accounting for subkernel deficiencies. Eventually, the reinterpretation of SPH as an intrinsic Lagrangian quadrature of explicit LES comes with two significant implications:

1. Implication: Ideally, the physical resolution of SPH is limited by the kernel scale of \( V_{c} \) or more precisely the kernel diameter \( D_{K} \). Thus, SPH is unsuited as a DNS method.

2. Implication: Deficits introduced below the kernel scale of \( V_{c} \) might be resolved by explicit consideration of the SFS term, from which structures above the kernel scale of \( V_{c} \) could profit.

While the first implication can be easily understood and there is already empirical evidence proving it, e.g. the work...
of Bauer & Springel\cite{Bauer2013} the second implication should be interpreted as a working hypothesis, which we will test by numerical experiments in Sec.\textit{V}. However, before this, the importance of the SFS in SPH has to be explained, which will be the objective of the next section.

B. The Role of the Subfilter Stress (SFS)

In order to understand the central role of the SFS for SPH, again the Hardy theory proved to be a suitable tool. This is detailed in our former work\textsuperscript{30}. We want to mention that we termed the resulting SFS tensor as molecular stress at this time since we were not aware of its connection to explicit LES. In this paragraph, we shortly sketch how the SFS tensor is related to the local dissipation dynamics in SPH. Therefore, a SPH solution of the forced two dimensional turbulent Kolmogorov flow of Rivera \emph{et al.}\textsuperscript{33}\textsuperscript{34} in DNS fashion is examined. It was performed following the description in Ref\textsuperscript{30}. The most important metrics for this simulation are depicted in FIG.\textsuperscript{3} and non-dimensionalized with the absolute maximum value of the viewed snapshot.

Although the turbulent flow can be generally reproduced by particle discretization methods in terms of the energy characteristics, it is hallmarkled by excessive dissipation. This dissipation is rooted in increasing local particle disorder at higher Reynolds number introducing artificial vorticity fluctuations\textsuperscript{15,16}. Exemplary evidence is given by the noisy vorticity field in FIG.\textsuperscript{3}(a). For homogeneous turbulence it can even be analytically argued that the averaged dissipation rate $\epsilon$ is quadratically connected to vorticity fluctuations $\omega'$ according to\textsuperscript{56}

\[ \epsilon = \langle \omega'^2 \rangle_V = 2\nu \int_0^{k_D^2} E(k) \, dk , \]  

with $\langle \cdot \rangle_V$ denoting a volume average. Additionally, the analytical relation of Eq.\textsuperscript{3} links the vorticity field with the kinetic energy spectrum $E(k)$. Hence, the excessive dissipation caused by artificial vorticity should also create a specific spectral signature in the SPH solution, which is depicted in FIG.\textsuperscript{3}(b). Since the experimental scalings of the inverse and direct cascades known from the experiment can be matched above the kernel scale ($k < 2\pi/D_K$)\textsuperscript{65}, and it is known that dissipation takes place at small scales due to the $k^2$ weighting of $E(k)$ in Eq.\textsuperscript{4}, it seems likely that the saturation of $E(k)$ below the kernel scale ($k > 2\pi/D_K$) represents the signature of excessive dissipation. In accordance with FIG.\textsuperscript{11} we will term this bottleneck as artificial thermal range or artificial thermalization. It should be emphasized that this spectral signature was also observed in other works, e.g. Refs\textsuperscript{13,22,23}.

Interestingly, the SFS tensor perfectly fits into this dissipation characteristics according to FIG.\textsuperscript{3}(c) & \textsuperscript{3}(d). Considering the fact that two different spatial resolution scales exist in SPH and other kernel-based particle methods, namely the kernel diameter $D_K$ and the particle size $\Delta x < D_K$, the SFS tensor in Eq.\textsuperscript{3} can always be estimated by means of an Lagrangian quadrature, which gives

\[ \tau_{SFS,i} \approx \sum_{j=1}^{N_{nbh}} \overline{p}_i (\overline{v}_j - \overline{v}_i) (\overline{v}_j - \overline{v}_i)^T W_{h,i} V_j , \]  

even if no LES perspective is employed. Such an argument was heuristically put forward by ourselves in order to localize pseudo-Lagrangian behavior using Hardy theory\textsuperscript{30}. For the considered problem the Frobenius norm of the SFS tensor is illustrated in FIG.\textsuperscript{3} (c). A correlation between the vorticity (FIG.\textsuperscript{3}(a)) and the SFS tensor (FIG.\textsuperscript{3}(c)) is evident\textsuperscript{50} and also quantitatively supported by the corresponding bivariate probability density function in FIG.\textsuperscript{3}(d). The latter describes a cone like structure indicating that high levels of absolute vorticity and SFS are connected\textsuperscript{50}, as well as that the variance of the absolute vorticity increases with the SFS norm up to $\tau_{SFS} \lesssim 0.4$.

From these coherencies, the role of the SFS term $\text{div} [\tau_{SFS}]_i$ in the discretized explicit LES equations (Eq.\textsuperscript{6}) becomes apparent. Since the SFS term behaves diffusive regarding the velocity field in a statistically averaged sense\textsuperscript{55,57}, an explicit consideration of this term will have the effect to locally homogenize the velocity field. Consequently, this will lead to a mitigation of the SFS norm according to Eq.\textsuperscript{5} and the vorticity variance according to FIG.\textsuperscript{3}(d). Then, based on Eq.\textsuperscript{6}, the artificial thermalization of the kinetic energy spectrum should be likewise reduced. This could potentially enable an overall reduction of the effective dissipation from which large scale structures might profit.

To verify these expectations, we deem the eddy viscosity concept in connection with Boussinesq’s hypothesis\textsuperscript{6\textsuperscript{9}–6\textsuperscript{11}} for the modelling of the SFS term $\text{div} [\tau_{SFS}]_i$ in Eq.\textsuperscript{6b} as adequate. The following approaches will be utilized:

- **SMAG**: This represents the classical Smagorinsky model discretized according to Eqs.\textsuperscript{A.20}, \textsuperscript{A.21} and \textsuperscript{A.24}. It is angular momentum conserving in the continuum limit\textsuperscript{60}.

- **SIGMA**: This represents the superior $\sigma$-model of Nicoud \emph{et al.}\textsuperscript{6\textsuperscript{1}–6\textsuperscript{3}} discretized according to Eqs.\textsuperscript{A.20}, \textsuperscript{A.21} and \textsuperscript{A.25}. It is also angular momentum conserving in the continuum limit\textsuperscript{60} but should overcome severe drawbacks of the Smagorinsky model, e.g. non-vanishing subfilter dissipation in laminar regions\textsuperscript{39,6\textsuperscript{1}}.

- **SMAG–MCG**: This represents the classical Smagorinsky model, however, discretized in the Monaghan-Cleyrat-Gingold (MCG) form\textsuperscript{6\textsuperscript{2}–6\textsuperscript{3}}. It is angular momentum conserving on the particle level as well.

It is of paramount importance that the SFS dissipation is merely introduced on subkernel scales in order to guarantee a successful application of the explicit SFS model, eventually reducing the artificial thermalization. However, the SPH discretization requires non-local approximations, which might jeopardize this goal a priori. This can be vividly illustrated by the concept of \textit{Particle Duality}, which results from the coarse-graining perspective.
FIG. 3. Metrics of a SPH solution for a two dimensional turbulent Kolmogorov flow according to Rivera et al.54,55 (a) Snapshot of the nondimensional, noisy vorticity field, (b) Kinetic energy spectrum, (c) Snapshot of the nondimensional Frobenius norm of the SFS tensor and (d) Nondimensional bivariate probability density of the Frobenius norm of the SFS tensor (abscissa) and vorticity (ordinate).

C. Particle Duality

In order to understand the concept of Particle Duality, it is necessary to precisely define the terminology of explicit LES. According to Sec. II of this work, explicit LES is introduced as a general fluid dynamic framework, in which fluid elements are coarse-grained by an explicit kernel to so called super fluid elements. This is illustrated in the left part of the schematic in FIG. 4. From the schematic, an averaging over a fluid element collective (grey particles) exactly determines the properties of a single super fluid element (red particle) with its specific kernel support. This corresponds to a truly explicit LES. However, in a SPH model the fluid element properties are unknown, which is synonymous to the closure problem of turbulence. This issue is resolved in a SPH framework by a direct substitution of the fluid elements (grey particles) by super fluid elements (red particles). Only then an averaging is performed to estimate the properties of a single super fluid element itself. As a consequence the SPH particles must represent super fluid element approximants and fluid element surrogates at the same time, which is what we term as Particle Duality. Practically, this implies that super fluid element approximants interact with each other, which are not direct neighbors but rather separated by some particles in between. This occurs as long as a the particles share the same kernel support and implicitly causes an increase of the effective interaction distance. Physically, however, the considered interaction is inadequate as the governing LES equations are a local model in terms of the super fluid element quantities. Thus, the Particle Duality as a manifestation of the non-locality introduced by the SPH discretization gives a picturesque description why the consideration of an explicit dissipative SFS...
model might fail to result in an improvement as anticipated in Sec. III B. Conceivably, the SFS model will not solely remove kinetic energy from the problematic artificial thermal range but also affect resolved scales larger than the kernel.

Having laid the foundations of SPH as a discretization intrinsically connected to explicit LES, it is now indispensable to answer our central question: Can resolved large scale structures profit from the reduction of SPH typical small-scale noise by explicit use of SFS models? Therefore, a thorough investigation of the influence of explicit SFS models for a well-defined HIT problem are vital, which is why we proceed with the description of such in the next section.

IV. THE HIT PROBLEM

The HIT problem that will be subsequently investigated is the Taylor-Green flow at \( Re = 10^5 \) presented in the work of Dairay et al.\(^\text{[1]}\). Their DNS solution will also serve as reference for our study. The initial velocity field in the tri-periodic domain \( \Omega := [0, 2\pi]^3 \) of the freely decaying flow is specified as

\[
\begin{align*}
    v_{0,x}(x, y, z) &= \sin(x)\cos(y)\cos(z) \\
    v_{0,y}(x, y, z) &= -\cos(x)\sin(y)\cos(z) \\
    v_{0,z}(x, y, z) &= 0
\end{align*}
\]

(10)

and the corresponding pressure field follows from the solution of the pressure Poisson equation in the incompressible limit\(^\text{[66]}\)

\[
p_0(x, y, z) = p_{\text{ref}} + \frac{\rho_{\text{ref}} c_a^2}{16} (2 + \cos(2z))(\cos(2x) + \cos(2y)) .
\]

(11)

The SPH cases that will be presented in the following are summarized in TABLE 1. Generally, four different particle counts were considered, namely \( N \in \{128^3, 192^3, 256^3, 512^3\} \), ranging from \( \sim 2 \) Mio. particles to \( \sim 130 \) Mio. particles.

| Case | Particles | SFS Model |
|------|-----------|-----------|
| 1    | \(128^3\) | \(\times\) | SMAG SIGMA SMAG-MCG |
| 2    | \(192^3\) | \(\times\) |
| 3    | \(256^3\) | \(\times\) |
| 4    | \(512^3\) | \(\times\) |
| 5    | \(128^3\) | \(\times\) |
| 6    | \(192^3\) | \(\times\) |
| 7    | \(256^3\) | \(\times\) |
| 8    | \(512^3\) | \(\times\) |
| 9    | \(\times\) |

TABLE 1. SPH cases for the considered Taylor-Green flow.

The basis of the given particle powers define the averaged particle distance \( \Delta l \), which exemplary for Case 1 results in

\[
\Delta l = 2\pi/128 \approx 0.0491 \text{ m}.
\]

Starting from a Cartesian lattice arrangement, the particles were regularized into a stable configuration in corresponding pre-runs following the particle packing scheme of Colagrossi et al.\(^\text{[87]}\). Only then, the fields given by Eqs. (10) & (11) were mapped onto the particles. The initial velocity field magnitude for a \( N = 192^3 \) Case is depicted in FIG. 5 (a) highlighting two shear flow planes at \( z = \pi/2 \) & \( z = 3\pi/2 \) and the rotational direction at the plane \( z = 2\pi \). In order to match the pressure field in the initial time step and avoid artificial dynamical effects beyond the one resulting from the initial particle configuration, a consistent mass distribution \( M_{0,i} = \rho_{0,i}\Delta l^3 \) was imposed. It is illustrated in FIG. 5 (b). The density field \( \rho_{0,i} \) is given by the combination of the initial pressure field in Eq. (11) and the EOS in Eq. (6c).

For the latter a reference density of \( \rho_{\text{ref}} = 1 \text{ kg/m}^3 \), a stiffness constant \( K = p_{\text{ref}} c_a^2 = 25 \text{ Pa} \) and a reference pressure \( p_{\text{ref}} = K/4 = 6.25 \text{ Pa} \) were chosen. The stiffness constant implies an artificial speed of sound of \( c_a = 5 \text{ m/s} \), which corresponds to an initial Mach number \( M_{0,i} = 0.2 \) and justifies to neglect \( \nabla \cdot \mathbf{v} \) based force\(^\text{[42]}\). We want to emphasize that different values of \( p_{\text{ref}} \) were tested, namely \( p_{\text{ref}} \in \{K/10, K/4, K/2, K\} \), however, the value \( p_{\text{ref}} = K/4 \) yielded the best trade-off between stability and numerical dissipation.

The results in the following were all computed using a Wendland C4 kernel and a kernel diameter of \( D_K = 8\Delta l \) resulting in \( N_{\text{ref}} \approx 250 \). Other comparative simulations were conducted with \( D_K \in \{4, 6, 8\} \Delta l \) and a quintic B-spline kernel but only the chosen configuration was capable to provide reasonable numerical convergence with increasing \( N \) avoiding pairing instabilities at the same time\(^\text{[68,69]}\).

To facilitate the discussion of explicit SFS models for the SPH method, the results in Sec. V will follow the subsequent argumentation sequence: First, we will demonstrate that the system of Eqs. (6) & (7), shows a convergent tendency in the numerical sense (TABLE 1 Case 1-4). These runs correspond to usual WCSPH simulations or, from our coarse-graining perspective in Sec. III, to a Lagrangian quadrature of the explicit LES equations (Eq. (2)) without an explicit...
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[0x0] in accordance with Rennehen

\[ \Delta = \frac{D}{2} = R_k \] these eddy viscosity runs were performed with a filter width Case 9), demonstrating the robustness of our observations. All ing MCG form in Eq. (A.26) called SMAG-MCG additionally combined with the angular momentum conserv-

The Cases 5-9 will represent runs in which the SFS is deddy viscosity approaches, not only the standard Smagorinsky SMAG (TABLE I: Case 5-7) model will be evaluated but also the \( \sigma \)-model SIGMA (TABLE I: Case 8), which should ensure vanishing subfilter dissipation in the initial laminar phase of the HIT problem. Moreover, the Smagorinsky model will be additionally combined with the angular momentum conserving MCG form in Eq. (A.26) called SMAG-MCG (TABLE I: Case 9), demonstrating the robustness of our observations. All these eddy viscosity runs were performed with a filter width \( \Delta = D_k/2 = R_k \) being equivalent to the kernel radius \( R_k \) and in accordance with Rennehen. From our explicit LES perspective in Sec. III the most consistent choice would correspond to \( \Delta = D_k \) but some tests led to the conclusion that only the overall dissipation is enhanced without any further physical improvements. Interestingly, for the problem considered, the choice \( \Delta = \Delta_l \) had a nearly negligible effect on our solutions. We interpret this as evidence in favor of the intrinsic connection between explicit LES and SPH, in which the particles should approximate LES super fluid elements and not fluid elements itself.

To evaluate the quality of the results, different metrics will be invoked. On the one hand the assessment of the overall dissipation inside the domain will be based on the density weighted averaged kinetic energy

\[ e_v(t) := \frac{1}{2} \sum_{i=1}^{N} \mathbf{p}_i \mathbf{v}_i^2 V_i. \] (12)

This metric is in accordance with the definition of Dairay et al.\(^\text{[1]}\) except for the density weighting. It only has a minor influence as we could verify, but should be included for consistency with the weak compressibility approach. On the other hand the overall dissipation will be assessed by the corresponding averaged dissipation rate, which can be computed from a finite difference approach for sufficient temporal sampling\(^\text{[1]}\) using the relation

\[ e_v(t) = -\frac{d e_v}{d t}. \] (13)

Furthermore and most importantly, we will compute the kinetic energy spectra \( E(k) \) at time \( t = 14 \) s where HIT with the characteristic inertial range scaling of Eq. (1) should be present up to a wavenumber of \( k_{DNS} \approx 50 1/m \), see Ref.\(^\text{[1]}\). Therefore, we employ the nearest neighbor sampling technique of Bauer & Springel\(^\text{[13]}\) on a Cartesian grid with \( \Delta l/2 \) in combination with the method of Durran et al.\(^\text{[10]}\). This methodology is kinetic energy conserving or in other words satisfies the discrete Parseval relation. Due to the Nyquist criterion, spectra will only be presented up to wavenumbers corresponding to \( 2\Delta l \). The interpolation method of Shi et al.\(^\text{[1]}\) will not be considered as is unclear whether it might introduce smoothing in the artificial thermal range, which we want to avoid. Since the values \( e_v(t = 14 \) s \) in different cases in TABLE I can significantly differ, we will normalize the corresponding spectra with the product \( e_v(t = 14 \) s \) \( L_c \) and \( L_c = 1 \) m for all runs to enable a relative comparison. Observations in spectral space will further be related to physical space by means of the Frobenius norm of Eq. (3), namely \( \| \tau_{SFS} \|_{L_c} \), and the backward finite-time Lyapunov exponent (FTLE)\(^\text{[21,13]}\) in the time range \([11,14] \) s. While the first is indicative for small scale structures (see Sec. III B), the latter will be used to assess the quality of the large scale structures. Additionally, we introduce a signal to noise (SNR) metric for the kinetic energy spectra defined by the ratio of energy above the kernel scale (with kernel wavenumber \( k_{kern} \)) in relation to the overall

FIG. 5. Initialization of the Taylor-Green flow at \( Re = 10^5 \) with \( N = 192^3 \) particles. (a) Velocity magnitude field with highlighted shear flow planes and rotational direction for \( z = 2\pi \). (b) Mass distribution corresponding to the initial pressure field.

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\[ 120 \]
energy, namely

\[ SNR := \frac{\int_{k=0}^{k_{\text{max}}} E(k)\,dk}{\int_{k=0}^{k_{\text{max}}} E(k)\,dk}. \tag{14} \]

It is important to stress that the SNR metric is only indicative for the reduction of the artificial thermalization but gives no insight about the solution quality above the kernel scale.

All computations in this work were performed for a time range of \( t_f = [0; 15] \) s with the in-house SPH code turboSPH. The latter was developed for the prediction of primary atomization. For details, please refer to the work of Chaussonnet et al.\[12\] for more information.

V. RESULTS & DISCUSSION

A. Numerical Convergence of the WCSPH Scheme

We will first start with a qualitative discussion of the numerical convergence of the discretized LES equations resulting from the Lagrangian quadrature (Eq. [9]). For now the SFS model is neglected, formally leading to the standard WCSPH discretization of the Navier-Stokes equations (TABLE I Case 1-4). Hence, these results will serve as reference to evaluate the effect of explicit SFS models in SPH.

From FIG. 5(a), which illustrates the temporal evolution of the averaged kinetic energy \( \epsilon_v \) (Eq. [12]) for increasing particle counts \( N \) (darker colors), one can apparently conclude that the metric is numerically converging towards the DNS reference solution of Dairay et al.\[11\] (solid black line). However, even for \( N = 512^3 \approx 130 \) Mio. particles, a significant gap remains compared to the DNS in the interval \( t \in [2.5; 10] \) s. The reason for this gap can be understood from the averaged dissipation rate \( \xi \) (Eq. [13]) as depicted in FIG. 5(c). Especially in the initial timeframe \( t \in [0; 2.5] \) s the vanishing dissipation rate of the DNS solution is strongly overestimated by the WCSPH scheme. This is probably linked to the strong anisotropic particle rearrangement of the initially laminar vortex configuration, causing numerical dissipation effects. Interestingly, although the highest resolution contains 64 times more particles than the lowest resolution, the curves only slowly approach the vanishing DNS level. The overestimation of the dissipation rate continues until \( t \approx 7.5 \) s, where the blue WCSPH lines cross the black DNS line, and passes over to a systematic underestimation until the end of the simulation, except for the \( N = 512^3 \) case, which overestimates the dissipation rates again for \( t \geq 12.5 \) s. Nevertheless, this global dissipation characteristic leads to the consequence that the energy levels in FIG. 6(a) approach the DNS solution again for \( t \geq 7.5 \) s. Despite these qualitative deviations, it should be highlighted that the qualitative agreement of the dissipation rates \( \xi \) in FIG. 6(c) is reasonable. For all \( N \) the temporal occurrence of the dissipation peak at \( t \approx 9 \) s is matched and for increasing \( N \) the formation of the second local dissipation peak at \( t \approx 11 \) s is also evident.

Having verified that the global dynamics of the kinetic energy is reasonably well approximated by the WCSPH scheme, it remains to clarify whether HIT with the characteristic inertial range scaling in Eq. [1] develops after the dissipation peak at \( t \approx 9 \) s. Therefore, we consider the normalized kinetic energy spectra as explained in Sec. III A for \( t = 14 \) s, which is in accordance with the work of Dairay et al.\[11\]. From their work an inertial range scaling should prevail up to a wavenumber of \( k_{\text{DNS}} \approx 50 \) 1/m. The computed spectra for the Cases 1-4 (TABLE I) are visualized in FIG. 6(e). For better orientation, the latter also contains a solid black line representing the \( k^{-5/3} \) scaling and a dashed black line with a stronger \( k^{-4} \) scaling. Moreover, the diagram includes the integral scale of the HIT problem (fawn dashed line) and the kernel scale of the simulation run with the highest particle count \( N \) (fawn solid line). The corresponding SNR values (Eq. [14]) are also listed. Indeed it can be observed that the utilized WCSPH scheme without SFS model is able to recover a significant amount of the inertial range scaling for increasing \( N \). While for the lowest \( N \) the scaling is only evident in the range \( k \in [4; 7] \) 1/m, the scaling range for the highest \( N \) covers nearly an order of magnitude in wavenumber, namely \( k \in [4; 30] \) 1/m. Hence, we can infer that WCSPH without SFS model is generally able to capture subsonic HIT, though at significant expense of \( N = 512^3 \) and \( N_{\text{neb}} \approx 250 \). This is consistent with the convergence properties described by Zhu et al.\[13\]. However, even for the highest resolution run whose kernel wavenumber \( k_{\text{ker}} = 64 \) 1/m exceeds the maximum inertial range wavenumber \( k_{\text{DNS}} \approx 50 \) 1/m of the reference DNS, the HIT is much earlier damped than the actual kernel scale. This must be rooted in numerical dissipation effects. The latter cause the WCSPH method to produce coarse-grained LES solutions, which is in accordance with the 1. Implication in Sec. III A. Quantitatively this manifests in the approximate \( k^{-4} \) scaling observable in all simulations that sets in well above the kernel scale and represents the SPH characteristic kinetic energy deficit.\[13\] Following the argumentation of Sec. III B this excessive dissipation is likely to be related to the artificial thermalization of the kinetic energy spectra below the kernel scales in FIG. 6(e). Although it can be reduced with increasing \( N \), which also is confirmed by an increase of the SNR values in FIG. 6(e), even for the highest resolution the artificial thermalization persists.

Consequently, the aim of the next section is to investigate whether the explicit consideration of a dissipative SFS model can reduce the thermalization in favor of the resolved large scale structures. This should not only lead to an improvement in spectral space but also in physical space in terms of the global dynamics. Consequently, we will seek for evidence for the 2. Implication in Sec. III A following the argumentation line of Sec. III B. We start with the SMAG model.

B. Effect of the Smagorinsky Model

Although the usage of a consistent LES model with an explicit SFS model should lead to an overall improvement of the solution, the investigation with the static SMAG model undermines this positive expectation (TABLE I Case 5-7). Especially in terms of the global dynamics, represented by FIG. 5.
FIG. 6. Comparison of quantitative metrics for different particle counts. The first column (a), (c) & (e) represents the WCSHP solutions without SFS model and the second column (b), (d) & (f) represents the solution with SMAG SFS model. The color coding is explained in (a). (a) Temporal evolution of the density weighted averaged kinetic energy $e_v$ without additional SFS model. (b) Temporal evolution of the density weighted averaged kinetic energy $e_v$ with SMAG SFS model. (c) Temporal evolution of the averaged dissipation rate $\varepsilon_t$ without additional SFS model. (d) Temporal evolution of the averaged dissipation rate $\varepsilon_t$ with SMAG SFS model. (e) Kinetic energy spectra at $t = 14$ s without SFS model. (f) Kinetic energy spectra at $t = 14$ s with SMAG SFS model.
scales of the individual cases is mitigated by the SMAG confirmed by an increase of the SNR metric (Eq. (14)) for a specific (f) demonstrates the reduction of the artificial thermalization to HIT (FTLE) in the time range \( t < 7.5 \) s, up to the point where the blue dissipation lines cross the black DNS line, that the excessive dissipation of the WCSPH solution is significantly enhanced by the SMAG model. For the lowest particle count of \( N = 128^3 \) it even results in a noticeable qualitative shift of the first dissipation peak from \( t \approx 9 \) s to \( t \approx 6 \) s. For the two remaining particle counts the position of the first dissipation peak in FIG. 6(d) is quite robust, though a slight shift towards earlier times is perceptible. It is interesting to note that in this initial timeframe the vortex system is still in transition to HIT (FTLE), which prompts the eventuality that this deterioration of the solution might be linked to the drawbacks of the Smagorinsky model as explained in Refs. [57,59]. In order to refute this eventuality, we will also present an investigation employing the superior SIGMA model (see Sec. 4) in Sec. V.C.

From the discouraging global kinetic energy balance one might be tempted to conclude that the described link between explicit LES and SPH in Sec. III might be flawed. However, the kinetic energy spectra at \( t = 14 \) s in FIG. 8(f) reveal that the coherences presented in Sec. III are correct. Most importantly the comparison of the spectra in FIG. 6(c) & FIG. 6(d) demonstrates the reduction of the artificial thermalization for a specific \( N \). The relative energy content below the kernel energies of the first wavenumber shells (\( k \leq 7 \) /m) increases as the comparison of FIG. 7(e) & 7(f) demonstrates. Although the differences might seem extraneous, we want to emphasize that the plots are double logarithmic. Interestingly, this improved spectral signature can also be linked to physical space by means of the backward finite-time Lyapunov exponent (FTLE) in the time range \([11, 14] \) s. Slices of the resulting FTLE fields at the plane \( z = \pi \) from the \( N = 256^3 \) runs without explicit SFS model and with SMAG model are illustrated in FIG. 8(a) & FIG. 8(b). Apparently, the resulting fields are representative for the coherent large scale vortices remaining from the initialization. Generally, the FTLE fields are quite similar in their appearance, however, it is undeniable that the structures formed in the cases with the SMAG model in FIG. 8(b) are less tattered than the reference WCSPH solution in FIG. 8(a). The most positive difference between the fields is that the consideration of the SMAG model approximately restores the mirror symmetry of the vortex system at the midplanes \( x = \pi \) & \( y = \pi \). This mirror symmetry is a characteristic of the vortex system and a vivid prove that a reduction of the artificial thermalization can even positively influence the large scale coherent motion. As a sidenote, symmetry breaking of a similar kind was also observed in molecular approximations of the Taylor-Green system in the work of Gallis et al. [59] albeit caused by physical thermal fluctuations.

So far, all these observations agree with our theoretical expectation in Sec. III B and demonstrate that the dissipative...
FIG. 8. Backward FTLE at the plane \( z = \pi \) for \( N = 256^3 \) and \( t = 14 \) s in the range \([11;14]\) s. (a) Without explicit SFS model. (b) With SMAG model. (c) With SIGMA model. (d) With SMAG-MCG model.

SFS model reduces the artificial thermalization in favor of the largest resolved structures. Nevertheless, the deterioration of the global dynamics in terms of the averaged kinetic energy in FIG. 6(b) and the corresponding dissipation rate in FIG. 6(d) indicate that the negative aspects outweigh the positive ones. The spectral signature of this setback caused by the SMAG model manifests in FIG. 6(f) for \( k > 7 \) \( 1/\text{m} \) and \( k < k_{\text{ kern}} \). A comparison of FIG. 6(e) & 6(f) clearly shows that the effect of the dissipative SMAG model is affecting not only scales below but also well above the individual kernel scales. Tantalizing to this is the fact that the observed SPH \( k^{-4} \) scaling is expanded to a larger wavenumber range. Although such an effect could already be anticipated from the Particle Duality of SPH introduced in Sec. III C, it is unfortunate to find this intuition finally confirmed. Based on these observations, one must infer that the consideration of the SMAG model in SPH is eventually degrading the solution. In order to demonstrate that this conclusion holds in general for dissipative SFS models, we will discuss the influence of alternative SFS models in the next section.

C. Effects of other Dissipative SFS Models

In this part a comparison between the WCSPH solution without SFS model and with SMAG, SIGMA & SMAG-MCG model will be presented (TABLE I: Case 3 & 7-9). As the observations seem to be independent from the particle count \( N \), only the \( N = 256^3 \) runs will compared. The results are depicted in FIG. 9. All in all, the observations are very similar to those presented in Sec. V B. Neither the superior SIGMA model nor the discrete angular momentum conserving SMAG-MCG model changes the situation. In fact, both models are even worse. As depicted in FIG. 9(a), the averaged kinetic energy levels of both variants are slightly below the SMAG solution. The global dissipation rates in FIG. 9(b) confirm these results. Accordingly, this is also reflected by the spectra in FIG. 9(c). This result is surprising for different reasons.

For the SIGMA model one would expect a vanishing dissipation in the initial laminar phase by the nature of the SFS model\(^ {59,61} \). However, as depicted in FIG. 9(b), the overall
dissipation is increased from the beginning. One might be tempted to conclude that this is related to the missing zero order consistency of the SPH-LES model in Eq. (6), prohibiting the flow discrimination required for the SIGMA model. Nonetheless, similar observations were made using high-order Eulerian grid-based schemes utilizing the same SFS model for Taylor-Green flows. Consequently, this indicates that the Taylor-Green flow is a challenging problem for the SIGMA model independent of the numerical discretization scheme. The kinetic energy spectrum in FIG. 9(c) further demonstrates that the qualitative effect of the SIGMA model and the SMAG model are similar. Compared to the SMAG model, the artificial thermalization below the kernel scale is slightly reduced, from which the first wavenumber shells ($k \leq 7 \, \text{1/m}$) do profit as expected. This is also reflected by the FTLE field in FIG. 8(c), which compared to the WCSPH solution in FIG. 8(a) is less tattered and, moreover, approximately mirror symmetric at the midplanes. Most importantly the dissipative SIGMA model still suffers from the issue of Particle Duality causing a removal of kinetic energy from scales in the range $k > 7 \, 1/m$ and $k < k_{\text{kernel}}$. This leads to an intensification of the observed deficient SPH energy scaling with $E(k) \sim k^{-n}$, $n > 4$.

The SMAG-MCG model results are very similar to the SIGMA model in terms of the global dynamics. Compared to the SMAG model the overall dissipation is enhanced. This becomes evident in FIG. 9(a) & FIG. 9(b). It is surprising as one would intuitively expect a general improvement related to the restoration of the angular momentum conservation property. Instead, the considered problem demonstrates that this comes at a certain cost. The kinetic energy spectrum in FIG. 9(c) once more confirms the already noted observations. The SMAG-MCG model is characterized by the strongest reduction of the artificial thermalization, which repeatedly has a positive effect on the first wavenumber shells ($k \leq 7 \, 1/m$) in the spectra, as well as the FTLE field in FIG. 8(d). Nevertheless, the issue of Particle Duality for the SMAG-MCG model in the range $k > 7 \, 1/m$ and $k < k_{\text{kernel}}$ is yet evident. Compared to the SMAG model, the angular momentum conservation property of the MCG form intensifies the observed deficient SPH scaling $E(k) \sim k^{-n}$, $n > 4$ similar to the SIGMA model.

From all these observations it can be concluded that the Particle Duality, as vivid interpretation of the non-local discretization introduced by classical SPH, prohibits an improvement of the solution by explicit dissipative SFS models. Although the largest resolved scales can profit from the mitigation of the artificial thermalization, which most notably becomes evident in the depicted FTLE field in FIG. 8, the SFS model also removes kinetic energy from scales larger than the kernel, which are already badly resolved. Consequently, we can confirm the statement of Rennehen that dissipative SFS models overall degrade the SPH solution.

**VI. CONCLUSION**

Summarizing, the contributions of this work are numerous and especially important for SPH simulations trying to
capture subsonic turbulent flows. Our main goal was to argue in Sec. II and Sec. III that, based on the Hardy theory from NEMD, SPH should be viewed as a non-local Lagrangian quadrature procedure intrinsically related to explicit LES. This implies on the one hand that subsonic turbulence captured by SPH will be correctly represented, in the best case, up to the kernel scale but also at significant cost, taking the convergence characteristics into account. This is consistent with observations in the literature, empirically supporting our LES perspective on SPH. On the other hand, it paves a potential way to mitigate SPH characteristic shortcomings by explicit consideration of a dissipative SFS model as explained in Sec. III B. In order to test the hypothesis that a reduction of the artificial thermal range correlates with an improvement of the kinetic energy content of the resolved large scales, several simulations of freely decaying HIT at Re = 10^5 in accordance to Dairay et al. were conducted and analyzed. However, it must be stated from the results presented in Sec. V that the explicit SFS model only leads to an improvement of the largest coherent structures. This was vividly reflected by the symmetry restoration of the vortex system in the computed FTE fields. For the remaining structures larger than the kernel scale, the dissipative SFS models merely remove kinetic energy where SPH is already characterized by a spectral energy deficit. Eventually, it deteriorates the overall solution outweighing the positive effects. This is rooted in the non-local character of the Lagrangian quadrature, which can be explained by the concept of Particle Duality. The latter states that the SPH particles must simultaneously represent super fluid element approximants and fluid element surrogates at the same time, causing an non-physical increase of the effective particle interaction distance. Finally, our work allows to confirm Rennehen’s expectation that explicit SFS models in a SPH framework only degrade the quality of the approximation for subsonic turbulent flows and from our current understanding they should be disregarded. It seems to be the case that the implicit dissipation mechanisms of SPH outperform the explicit dissipative SFS models considered in this work. All in all, it can be expected that SPH simulations of subsonic turbulence without explicit SFS term provide a coarse-grained LES solution but at significant cost.

As next step it would be interesting to study whether the issue of Particle Duality can be either circumvented by higher-order schemes or by the use of the LES-SPH scheme developed by Di Mascio et al. and Antuono et al.. Their LES perspective exposes of the Favre averaging, from which a mass diffusion term emerges, and includes additional noise-mitigating techniques. Although we currently believe that the issue of Particle Duality is a conceptual problem of SPH, there may be the chance that cross-effects between different modelling terms can restore the actual goal of an explicit dissipative SFS model.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Appendix: SPH Discretization of the Explicit LES model

1. The Averaged Density

In order to approximate the averaged density of a specific particle i ∈ {1, ..., N} at position xi, the integral expression in Eq. (2a) has to be discretized. Therefore, we define a mass differential for the Lagrangian element y with dM(y) := ρdy, which allows one to rewrite Eq. (2a) into

\[ \overline{\rho}_i := \overline{\rho}(x_i,t) = \int_{V_i} W_h(x-y) \ dM(y). \]  (A.1)

Assuming that Vi after the decomposition contains j ∈ {1, ..., Nngb} neighbor (ngb) particles, a naive quadrature can be applied, in which dM(y) is replaced by a finite mass at position y = y_j, namely M_j := M(y_j). With the abbreviation \( W_{h,ij} := W_h(x_i - y_j) \), this gives

\[ \overline{\rho}_i = \sum_{j=1}^{N_{ngb}} M_j W_{h,ij} + \mathcal{O}(N_{ngb}^{-\gamma}), \quad \gamma \in [\frac{1}{2}; 1]. \]  (A.2)

The approximation in Eq. (A.2) is the standard way of density estimation in SPH and contains an error term, which vanishes with N_{ngb} → ∞ according to Ref. [56].

For a homogeneous distribution of mass corresponding to \( M_i = M_j \), Eq. (A.2) implies a definition for the particle volume

\[ \overline{V}_i \approx M_i \sum_{j=1}^{N_{ngb}} W_{h,ij} = \frac{M_i}{V_i} \quad \Rightarrow \quad V_i := \frac{1}{\sum_{j=1}^{N_{ngb}} W_{h,ij}}. \]  (A.3)

Moreover, Eq. (A.3) represents another common way of density approximation in SPH, which is often used in subsonic multiphase problems with density discontinuity even when \( M_i \neq M_j \). Hence, Eq. (A.3) is chosen as density approximation in our work due to its higher level of generality, although we utilize an inhomogeneous mass distribution (see Sec. IV). However, we tested both approximations (Eq. (A.2) & Eq. (A.3)) finding negligible influence on our results.

Contrary to the usual SPH approach, Eq. (A.1) is exact and should not be interpreted as a smoothed approximation of the true fluid density. Our goal is to approximate the density of LES super fluid elements, hence the Lagrangian quadrature applied in Eq. (A.2) is the only approximation which is introduced.
2. The Averaged Pressure Gradient

For the averaged pressure gradient in the momentum balance of \( V \) in Eq. (2b), we will first apply integration by parts

\[
- \int_{V_\ell} \nabla_y p(y,t)W_h(x - y) \, dy = 0
\]  
and vanishes. For the second term on the right hand side of Eq. (A.4), the chain rule can be used to demonstrate that \( \nabla_y W_h(x - y) = -\nabla_x W_h(x - y) \) and this results in the exact expression

\[
- \int_{V_\ell} \nabla_y p(y,t)W_h(x - y) \, dy = 0
\]

Before we apply a Lagrangian quadrature to Eq. (A.6), we add the expression \( p(x,t)\int_{V_i} \nabla_x W_h(x - y) \, dy = 0 \), considering that the kernel gradient is anti-symmetric by definition. With that, we can state

\[
- \int_{V_\ell} \nabla_y p(y,t)W_h(x - y) \, dy = 0
\]

If a Lagrangian quadrature is applied to Eq. (A.7), adapting the particle notation with index \( i \) & \( j \) like for the density above, one finds the following approximation for the averaged pressure gradient

\[
- \int_{V_\ell} \nabla_y p(y,t)W_h(x - y) \, dy \approx -\sum_{j=1}^{N_{nbg}} (p_j + p_i)\nabla_x W_{h_{jj}}V_j
\]

From this discretized form, the operation in Eq. (A.7) becomes comprehensible. It generates an anti-symmetric pressure force between particle \( i \) & \( j \) in accordance with Newton’s third law This leads to momentum conservation in the discretized transport equations and is often derived in the SPH community by a variational principle for an ideal Euler fluid, e.g. Refs. However, it is important to realize that the fluid element pressures \( p_i \) & \( p_j \) in Eq. (A.8) are unknowns for the super fluid elements in the LES framework. Hence, the only option to estimate these quantities is by a replacement

with the averaged pressures of the approximated super fluid elements itself, namely

\[
p_i \approx \overline{p_i} + \mathcal{O}(h^2) + \mathcal{O}(N_{nbg}^{-7/2}), \quad \gamma \in \left[ \frac{1}{2}; 1 \right]
\]

This is a crucial step in order to obtain an expression fully consistent with the well-known SPH formulation, but certainly introduces two errors: The first showing a non-local \( h^2 \) dependence due to the super fluid element replacement and the second showing a \( N_{nbg}^{-7/2} \) dependence with \( \gamma \in \left[ \frac{1}{2}; 1 \right] \) due to the Lagrangian quadrature. Summarizing, one finally obtains a well-known SPH approximation of the LES pressure gradient from the Lagrangian quadrature, which reads

\[
- \int_{V_\ell} \nabla_y p(y,t)W_h(x - y) \, dy \approx -\sum_{j=1}^{N_{nbg}} (p_j + p_i)\nabla_x W_{h_{jj}}V_j
\]

and comes with the usual SPH peculiarity. The formulation depends on the pressure level \( p_{ref} \) of the EOS in Eq. (A.7) and breaks its gauge invariance but simultaneously introduces an implicit particle regularization based on the local particle order.60

3. The Averaged Viscous Stress Term

For the viscous stress term in Eq. (2b), the same manipulations can be applied in order to find an expression equivalent to Eq. (A.6). It finally reads

\[
\int_{V_\ell} \nabla_y [2\nu \rho D](y,t)W_h(x - y) \, dy
\]

We could theoretically continue as in the last section for the averaged pressure gradient, which would lead to an SPH approximation for the viscous stress term similar to the one presented in Ref. However, another formulation for strongly subsonic flows is much more common in the SPH community, which is conserving angular momentum in discretized form and not only in the continuum limit. Thus, we change our strategy for the viscous stress term. Therefore, it should be recognized that the tensor \( 2\nu \rho D \) in Eq. (A.11) depends on \( y \) and the integration is performed in respect to \( y \) as well. Hence, the \( \nabla_x \) operator and integration can be interchanged. Assuming \( \nu = const \) and using the abbreviation defined in Eq. (3), it exactly yields

\[
\int_{V_\ell} \nabla y [2\nu \rho D](y,t)W_h(x - y) \, dy = 2\nu \nabla x [\rho D](x,t)
\]

Equation Eq. (A.12) can be rearranged with the Favre average in Eq. (4), resulting in

\[
\int_{V_\ell} \nabla y [2\nu \rho D](y,t)W_h(x - y) \, dy = 2\nu \nabla x [\overline{\rho D}](x,t)
\]
Since we are interested in strongly subsonic flows, the assumption of weak spatial changes in \( \rho \) is viable. Consequently, it seems likely that the spatial changes of \( \overline{\rho} \) are even weaker or negligible compared to spatial changes in \( \overline{D} \). Thus, \( \text{div}_x \overline{\rho} \) and \( \overline{\rho} \) can be interchanged and we assume that for the dynamic viscosity \( \eta := \nabla \overline{\rho} = \text{const.} \) Then, one arrives at

\[
2\text{div}_x [\overline{\rho} \overline{D}](x, t) = 2\eta \text{div}_x [\overline{D}](x, t) = \eta \Delta \overline{\nu}(x, t). \tag{A.14}
\]

So far all performed manipulations are exact, given that the assumptions made are valid. In order to discretize the Laplacian in Eq. (A.14), a technique from the SPH community is used, which was firstly introduced by Brookshaw and reduces the sensitivity of the discretization to the local particle order. The main idea is to approximate second order derivatives by a non-local integral expression\(^{[25]} \). This opens the opportunity to shift the effect of the subfilter stress term by its averaged, non-local counterpart\(^{[25]} \). It reads

\[
\text{div}_x [\tau_{\text{SFS}}](x, t) \approx \int \overline{\tau}_{\text{SFS}}(y, t) \nabla \overline{w}_h(x - y) \, dy. \tag{A.19}
\]

Applying a Lagrangian quadrature to Eq. (A.19) and using particle index notation, the approximation takes the form

\[
\text{div}_x [\tau_{\text{SFS}}](x, t) \approx \sum_{j=1}^{N_{\text{ngb}}} (\overline{\tau}_{\text{SFS}, j} + \overline{\tau}_{\text{SFS}, i}) \nabla w_{h, i,j} V_j. \tag{A.20}
\]

However, as usual for LES, the most interesting part of the subfilter stress term approximation consists in finding an estimate for the SFS tensor \( \tau_{\text{SFS}} \) itself.

The standard option is to employ the eddy viscosity concept in connection with Boussinesq’s hypothesis\(^{[45,57,59]} \). Although this class of SFS models is known to oversimplify physical effects below the subfilter scale\(^{[57,59]} \), it is compliant with the dissipative statistical property of the energy cascade\(^{[55,57]} \). This means that kinetic energy is mostly transferred from larger to smaller scales. As our goal is to eliminate numerical noise in favor of the large scales, explained in Sec. [III.B] we deem eddy viscosity models as appropriate for this study. Therefore, the SFS tensor can be approximately expressed as\(^{[25]} \)

\[
\tau_{\text{SFS}}(x, t) \approx -2\nu \overline{\rho} \overline{D}(x, t), \tag{A.21}
\]

assuming that the isotropic part of the tensor is negligible for strongly subsonic flows. In Eq. (A.21), the scalar field \( \eta \) denotes the eddy viscosity and the tensor field \( \overline{D} \) the Favre averaged strain rate. The latter is defined by

\[
\overline{D}(x, t) := \frac{1}{2}(\overline{J} + \overline{J}^T)(x, t) \tag{A.22}
\]

with \( \overline{J} \) representing the Favre averaged velocity field Jacobian. With the aid of the techniques described above, one can construct a Lagrangian quadrature approximation for the Jacobian, which is well-known in the SPH community and first order consistent in the continuum limit\(^{[15]} \), namely for a specific particle

\[
\overline{J}_i := \overline{J}(x_i, t) \approx \sum_{j=1}^{N_{\text{ngb}}} (\overline{\nu}_i - \overline{\nu}_j) \nabla w^T_{h, i,j} V_j. \tag{A.23}
\]

Hence, Eq. (A.22) is defined on the particle level as well.

For the remaining unknown field \( \nu \) in Eq. (A.21), we will explore two different models. The first model will be the standard Smagorinsky model with constant \( C_S = 0.15 \) and the filter width \( \Delta \) given by\(^{[15,48,59]} \)

\[
\nu := (C_S \Delta)^2 \sqrt{2 \text{tr}\{\overline{D}^2\}}, \tag{A.24}
\]

in which \( \overline{D} \) can be computed from Eqs. (A.22) & (A.23) and \( \text{tr}\{\cdot\} \) denotes the trace operation. The second model considered, is the \( \sigma \)-model developed by Nicoud \textit{et al.}\(^{[61]} \). It overcomes some severe drawbacks of the Smagorinsky model, e.g.
it guarantees vanishing subfilter dissipation in laminar regions and proper wall scaling.\(^{[59,61]}\) Based on the singular values \(\sigma_k, k \in \{1, 2, 3\}\), of the tensor \(J^T J\), the alternative eddy viscosity model with the model constant \(C_\sigma = 1.35\) reads\(^{[59,61]}\)

\[
V_i := (C_\sigma A)^2 \frac{\sigma_i - \sigma_j}{\sigma_i^2} (\sigma_i - \sigma_j)
\]  

(A.25)

It should be noted that the modelled subfilter stress term according to Eq. (A.20) is only angular momentum conserving in the continuum limit, but not on the discrete particle level.\(^{[60]}\) Therefore, for comparative reasons, we will additionally consider a heuristic augmentation of the averaged viscous stress term in Eq. (A.16) to variable eddy viscosity based on the ideas of Ref.\(^{[63]}\). Exemplary, it is utilized in the SPH-LES works of Di Mascio et al.\(^{[64]}\) and Antuono et al.\(^{[65]}\) The inherently angular momentum conserving alternative of Eq. (A.20) is

\[
div \left[ \tau_{\text{eff}}(x,t) \right] \approx (A.26)
\]

\[
2(2+n) \sum_{j=1}^{N_{\text{reg}}} \frac{p_i}{p_i + p_j} V_i j + V_j i - \frac{(x_i - y_j)^2}{(x_i - y_j)} \nabla W_{h,i} V_j
\]

and will be called Monaghan-Cleary-Gingold (MCG) form according to Ref.\(^{[66]}\)

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