Naval Research Laboratory
Washington, DC 20375-5320

NRL/6003/MR—2022/3

Surrogate Fluid Dynamics

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June 30, 2022

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
30-06-2022	NRL Memorandum Report	01-01-2022 – 05-31-2022

4. TITLE AND SUBTITLE

Surrogate Fluid Dynamics

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Jay Boris, PA

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER
1V28

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, DC 20375-5320

8. PERFORMING ORGANIZATION REPORT NUMBER

NRL/6003/MR--2022/3

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, DC 20375-5320

10. SPONSOR / MONITOR'S ACRONYM(S)

11. SPONSOR / MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

DISTRIBUTION STATEMENT A: Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

This is the fifth NRL Memorandum Report in a series. There will be several more. This paper is an explanation, justification,and discussion of the radical new Surrogate Fluid Dynamics (SFD) model introduced in the CSD#2, CSD#3, and CSD#4 memo reports (NRL/6003/MR—2021/1, NRL/6003/MR–2022/1 and NRL/IR-6003-22-3-U). SFD is designed to estimate and study turbulent mixing at higher resolution than previously practical and without the numerical diffusion usually degrading convective flow.

14. ABSTRACT

Fluid dynamic behavior stems from fundamental physical principles that may be approximated by nonlinear partial-differential equations. The present goal is to study turbulent mixing of initially separate fluids over a range of space scales that is broader than practical with current Computational Fluid Dynamics (CFD) models. This paper introduces a surrogate model for this fluid dynamic behavior that is based more directly on algorithms enacting these fundamental physical principles. Surrogate Fluid Dynamics (SFD) is more efficiently computable than present CFD approaches based on the Navier-Stokes equations and their varied numerical representations. As a result, SFD makes it possible to explore parameter regimes and interactions that are difficult to simulate using CFD. Most of the degrees of freedom in current turbulence simulations represent the small scales of motion that have only a small fraction of the total kinetic energy. SFD addresses this issue by employing a logarithmic k-space grid for the turbulent spectrum and a diffusion-free Lagrangian algorithm for the flow. This paper presents a composite model driving SFD with the Coherent Structure Dynamics (CSD) non-equilibrium turbulence model and discusses the pros and cons of this new approach.

15. SUBJECT TERMS

Computational fluid dynamics
Surrogate fluid dynamics
Coherent structure dynamics
High-speed mixing for combustion
Non-equilibrium Turbulence

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					Jay Boris
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	U	22	**19b. TELEPHONE NUMBER** *(include area code)*
U	U	U			(202) 767-3055

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1. Fundamental Physical Principles for Turbulence

Fluid dynamic behavior depends on a set of fundamental physical principles. Respecting these principles can lead to useful models for some important situations without the restrictions or high cost of current continuum fluid simulations. To the extent that a mathematical model adequately describes a fluid-dynamic situation, it must embody these principles. This paper treats these fundamental principles in the context of a new method, based on Coherent Structure Dynamics (CSD) and called Surrogate Fluid Dynamics (SFD), with properties that current Navier-Stokes models have difficulty approximating. CSD and SFD are described in a series of four Naval Research Laboratory Memorandum reports by Boris and Obenschain (2018 – 2022) and indicated in the following text and references as CSD#1 (Boris, 2018), CSD#2 (Boris, 2021), and CSD#3 and CSD#4 (Boris and Obenschain, 2022a, 2022b). These reports are available from the author.

The fundamental physical principles embedded in the CSD model, which computes a time-dependent non-equilibrium turbulence spectrum spanning six orders of magnitude in scale, are:

- Energy Conservation
- Scale Invariance in Inviscid Fluid Dynamics
- Positivity in Turbulent Cascade

The fundamental physical principles embedded in the 3D SFD model, which is driven by the CSD turbulent spectrum, are:

- Continuous Convection
- Positivity in Convection
- Mass Conservation in Convection
- Convection without Numerical Diffusion
- Momentum Conservation

The main components of the combined model, CSD-SFD are treated below in Section 2 on CSD and Section 3 on SFD. Following brief synopses of CSD and SFD, the embedded physical principles listed above are explained and discussed. Section 4 presents the "Discussion and Conclusions." An appendix, "Models, Representations, and Simulations," is given that considers more general modelling issues and provides additional modelling context including short discussions of "Consistent Realizable Boundary and Source Conditions" and "Causality."

2. The Coherent Structure Dynamics Model

The CSD model for simulating an evolving non-equilibrium turbulence spectrum cannot be derived from the Navier-Stokes equations. CSD stitches together the relevant fundamental physical principals using a representation chosen for its computational efficiency and simplicity. The combined model CSD-SFD produces multiple realizations of turbulent 3D surrogate flows useful for studying turbulent mixing and chemical reaction of species. In these realizations, the turbulence may be far from equilibrium and the inviscid fluid dynamics is free of numerical diffusion. The anisotropy attending detailed fluid turbulence still occurs with CSD-SFD in the current 3D geometry with periodic boundary conditions. The model's separation of the evolving turbulence from its convection is quite unusual, prompting questions about the accuracy of these surrogate flows. However, the key principles controlling the physics are embedded in the models, representations, and algorithms.

Manuscript approved June 28, 2022.

2.1 Synopsis of the Coherent Structure Dynamics Model

CSD Dynamics is based on computing the interactions of vortex-like filamentary coherent structures, as they evolve in time. The CSD model takes its name from the 1974 paper by Garry Brown and Anatol Roshko (1974) which concluded that "the mixing layer is dominated by large coherent structures." CSD was originally introduced (Boris et al., 1982) without the coherent-structure number-density added more recently in CSD#1. The number-density at each scale describes non-equilibrium spectra where different turbulence scales can have different coherent-structure packing fractions. The current success of CSD also awaited an improved stiff equation integrator (Mott and Oran, 2001). Figure 2.1 below is a schematic that shows a portion of the logarithmic k-space grid and indicates the two kinds of coherent-structure interactions considered.

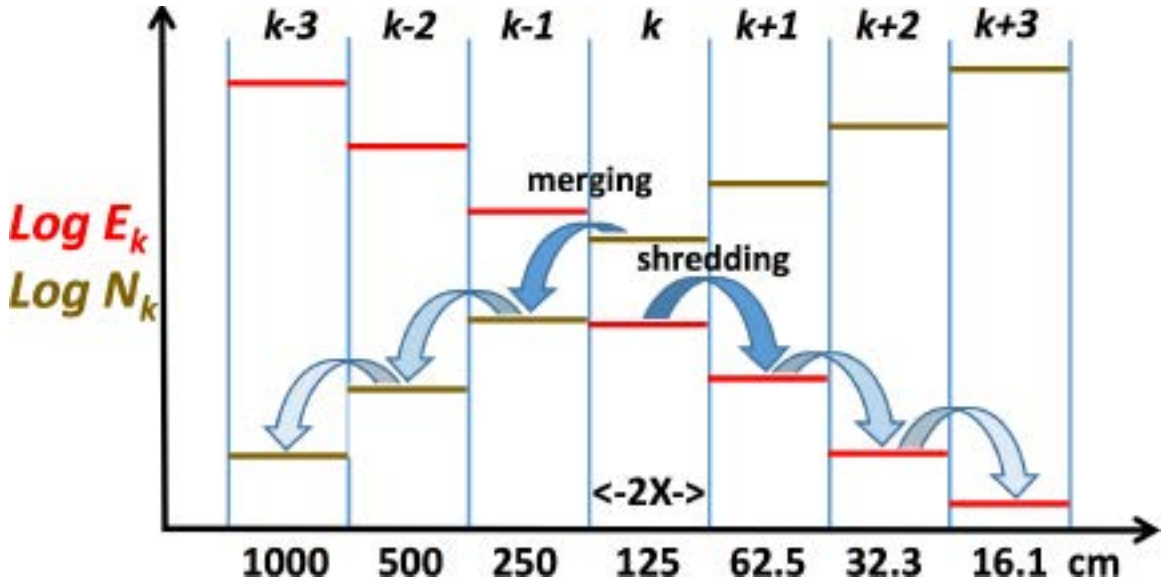

Figure 2.1 Schematic of the logarithmic k-space grid used by the Coherent Structure Dynamics model. The wavenumber increases and the corresponding turbulent scale size decreases to the right. The turbulent energy density (red) decreases from bin to bin with k, the bin index, while the coherent-structure number density (brown) increases. The local effects of coherent-structure merging and shredding interactions are shown.

The CSD representation divides the full 3D wavenumber space into one-dimensional k-space velocity magnitude bins or 'shells.' The 'shell' models are time-dependent and have been studied for some time (e.g. Gledzer, 1973; Yamada & Ohkitani, 1987; Biferale, 2003). They are sets of coupled Ordinary Differential Equations that can be quite stiff, like CSD, but they are very different equations and are solved in a different way by stable implicit integration techniques. There is one main line of effort in the literature with the Kolmogorov solution effectively incorporated in a scale similar fashion. These variants of the shell model do not consider coherent structures (vortex filaments) interacting and they do not treat the density of structures as central to CSD. The fractal nature of the solution space and intermittency in turbulence shell models seem to be related issues (Jensen, et al., 1991; Benzi, et al., 1993; Pissarenko, et al., 1993). Stiffness is sometimes solved by backward differentiation where it is extreme (L'vov, et al., 1998).

Treating the density of coherent structures, included in the CSD framework (reference CSD#1) seems to be important to predicting the 'bottleneck,' sometimes called the 'pre-

dissipation bump,' in the spectrum. The bottleneck is indicated by a gold halo in Fig. 2.2 below. The bottleneck has been found in both experimental geophysical research and in detailed simulations at high resolution but was originally thought to be a numerical artifact. CSD treats interactions representing the merging and shredding of vortex filaments based on their strength, size, and distance of separation as needed in the physical Biot-Savart law. The nonlinear effects of the coherent-structure separation distance on the merging and shredding rates are not possible in other current shell models. Including this physical dependence on separation distance doubles the number of independent variables in CSD but appears to increase the fidelity possible.

The CSD grid is shown schematically in Figure 2.1 above. The coupling of energy between adjacent k-space bins is treated by computing energy-conserving interactions for the *merging* and *shredding* of pairs of nearby filamentary coherent structures, as indicated in the figure. These interactions are not treated deterministically, as in vortex dynamics, but the energy transfer between coherent structures in adjacent scale-size bins is computed by integrating a set of coupled stiff ordinary differential equations for the summed energy density and average number density of the structures at each separate scale. These coherent structure 'k-space' bins are distributed logarithmically by factors of two so turbulent cascade can be approximated over many orders of magnitude. As a consequence, the equations are very stiff at small scales, requiring the use of an asymptotic, stiff-equation integrator originally developed for integrating extended sets of chemical reactions (Mott and Oran, 2001).

This CSD grid represents the spectrum to scales below the dissipation scale with only a few tens of bins and independent variables. It also allows a simple representation of the filamentary coherent-structure interactions. The red lines in each bin of the figure show a decreasing energy density E_k on a log-log scale and the brown lines show an increasing coherent-structure number density N_k. This compact representation permits a fast evaluation of the time-dependent, non-equilibrium turbulence spectrum. This speed will permit estimating the high-resolution turbulence, for example, in many spatial regions within a large CFD computation. The result is a prediction of the non-equilibrium turbulence evolution at spatial scales well below those that can be resolved by a 3D CFD model.

Figure 2.2 below shows the equilibrated spectrum at 10 milliseconds (ms) after the baseline runs of CSD#3 and CSD#4 began. A well-developed dissipation range forms to the right of the vertical yellow bar near 6×10^{-4} centimeters (cm). This range extends for several bins to the right where the bin energy density E_k (cyan changes to black in the dissipation zone), the spectral energy density ε_k (red to purple), and characteristic velocity V_k drop off the bottom of the plot scale. The pre-dissipative bump ('bottleneck'), circled by the gold ellipse, forms quickly, before the spectrum equilibrates. The packing fraction, a non-dimensional variable, not driven by the same dimensional arguments that constrain the spectral energy density and velocity, takes much longer than V_k and ε_k to relax to equilibrium. The packing fraction, which reaches equilibrium by the end of the run, is hard to compute beyond the dissipation region and has been relaxed to a fixed value of approximately 0.09, a factor of 10 below the initial value. The pre-dissipative bump is well formed by 2.5 ms seconds. It arises because the viscous energy dissipation in the small scales reduces its effect on shredding the coherent-structure energy at smaller scales and thus the energy piles up. The CSD model has shown that the pre-dissipative bump is absent when the coherent-structure number densities are removed from the set of equations being solved in the inviscid part of the spectrum.

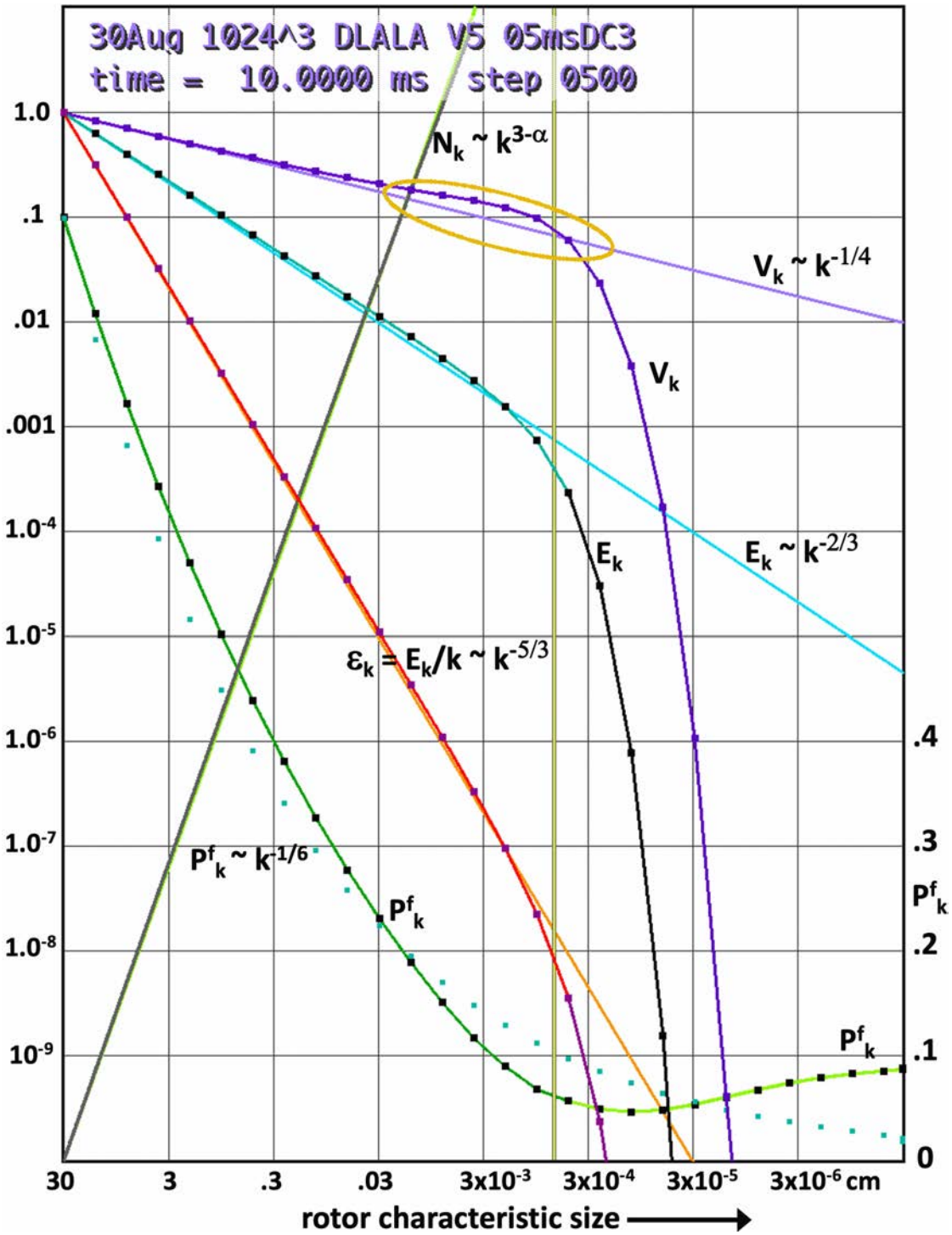

Figure 2.2 Spin-up of a stirred laminar flow to equilibrium turbulence in less than 10 milliseconds for the parameters of papers CSD#3 and CSD#4. The stirring velocity, at the longest scale, 30 cm, was 500 m/s. 30 CSD bins were used for the coherent-structure energy and number density, representing coherent-structure sizes spaced logarithmically by a factor of 2.

When viewed as a movie, the equilibrated spectrum, shown as a snapshot in Fig. 2.2, fluctuates below the dissipation scale by a couple of percent. This is the action of the stiff equation integrator, working with a finite error tolerance, to treat the extremely stiff equations

near the right edge of each of the plots. At the 10^{-4} cm scale, the characteristically stiff time scales are 10^{6} to 10^{7} times shorter than the timestep.

2.2 Fundamental Principles in Coherent Structure Dynamics

This CSD model cannot be derived mathematically from the Navier-Stokes equations. It is constructed by stitching together a number of fundamental physical principals chosen for their computational efficiency and simplicity. CSD-SFD produces multiple realizations of surrogate flows. The anisotropy possible in detailed fluid turbulence is ignored for the present, and the distinction between the evolving turbulence and the convection is unusual, allowing questions about the accuracy of these surrogate flows. However, the key principles of the physics are embedded in the model. CSD has successfully solved the high-Reynolds number Taylor-Green Vortex problem, predicted the observed 'pre-dissipative bump' in the turbulence spectrum, and demonstrated that the bump involves the variation of the coherent structure number density with scale size. Energy conservation is enforced in detail and the required scale-invariance in the behavior of the coherent-structure interactions at different scales is maintained. Both the coherent-structure energy density and the number density must be and are maintained as positive numbers in each bin. Three principles are now discussed:

- Energy Conservation
- Scale Invariance in Inviscid Fluid Dynamics
- Positivity in Turbulent Cascade

Energy Conservation:

The turbulent kinetic energy is conserved during each timestep by ensuring that energy removed from one scale-size bin in the CSD spectrum is necessarily added to an adjacent bin. That said, the stiff equation integrator used to solve the CSD equations (Mott and Oran, 2001) introduces truncation errors from the asymptotic formulae that are used when the equations are very stiff at small scales. Fortunately, these errors are also very small because the bin energies where the stiffness becomes large are within the roundoff error of the total turbulence kinetic energy. In CSD, viscosity dissipates kinetic energy throughout the spectrum according the usual heating term (last term in Eq. 4.2 of CSD#1). Since temperature is not a variable in SFD at present, the viscous heating energy is simply being extracted.

Scale Invariance in Inviscid Fluid Dynamics:

The scale invariance of the inviscid vortex shredding and merging interactions, leading to forward and inverse turbulent cascade, is built into the CSD equations for the evolution of the spectrum. The interaction of two coherent structures is scaled by their size, separation distance, and rotation speed, based on the energy of the individual structures. Therefore, a single parameter, the number of precessions of two structures around each other to interact, characterizes the rate of merging to the next larger bin and a second single parameter, the number of precessions to interact, characterizes the rate of shredding to the next smaller bin, regardless of which bin is being treated. Thus these interactions are identical non-dimensionally at each scale, meaning that they are scale invariant. However, they are not scale similar since the relative density of the structures, the 'packing fraction,' can be different from scale to scale.

Positivity in Turbulent Cascade:

The energy density in each bin and the number density in each bin must physically be non-negative numbers. Therefore, the equations of CSD, that is Eqs. 4.1 through 4.5 in CSD#1, are written to guarantee that E_k and N_k for every scale-size bin will remain positive during the forward and the inverse turbulent cascade. The negative terms in the time derivatives for each bin are proportional to the values E_k and N_k in that bin. Therefore, these values can, at most, go to zero when the bin energy density and number density approach zero.

3. The Surrogate Fluid Dynamics Model

The Surrogate Fluid Dynamics (SFD) model is considerably more complicated than the Coherent Structure Dynamics (CSD) turbulence model because SFD must provide a time-dependent, 3D velocity field that realizes the instantaneous CSD turbulence spectrum that is providing the strengths (speeds) of the coherent structures in each bin. As with the CSD component, SFD cannot be derived mathematically from the Navier-Stokes equations. Instead, it is constructed by joining together a number of fundamental physical principals and algorithms chosen for their computational efficiency and simplicity. CSD-SFD together produce multiple surrogate flow realizations. As noted above, the anisotropy present in fluid turbulence can also appear in the SFD model. The numerical separation caused by first solving for the evolving turbulence spectrum and then computing a flow field that this spectrum subsequently drives is unusual and may invite questions about the accuracy of these surrogate flows even though the key physics principles are embedded in the composite model.

3.1 Synopsis of the Surrogate Fluid Dynamics Model

SFD was developed to provide a way to study mixing of initially separate chemical species under the action of non-equilibrium time-dependent turbulence. A model fast enough the follow a macroscopic quantity of fluid as the interface separating the species becomes more and more stretched and corrugated was needed. Further, the flow on all scales has to satisfy the desired spectrum of turbulence. Exactly where each parcel of fluid goes, for this problem, is not as important as ensuring that the stretching fuel-oxidizer interface brings the fuel and oxidizer close together at about the correct rate. Decades of work with high resolution CFD methods show that this can only occur when the small scales of motion increase the interface area without the dissipative effects of numerical diffusion. Tests comparing the SFD rate of interface area increase with that of Direct Numerical Simulation (DNS) runs at the highest practical resolution is a way to calibrate/validate SFD.

To this end, convection in SFD is a 3D algorithm using axis-aligned cyclic shifts of the species densities across the entire grid. This constrained convection is entirely Lagrangian. The shift matrices contain contribitions from all scales that can be resolved on the grid and the magnitude of the contributions in the three directions sums to the energy in each energy bin at each timestep. Although limited, this approach produces reasonablely useful flow realizations that are driven by the time-dependent turbulent velocities specified in each energy-range bin of the CSD spectrum. The SFD representation begins with a uniform triply periodic grid of 16-bit integer density values for fuel and oxidizer species. These density values can go to zero but they cannot go negative. The algorithms for convection, reaction, and diffusion used in SFD guarantee this.

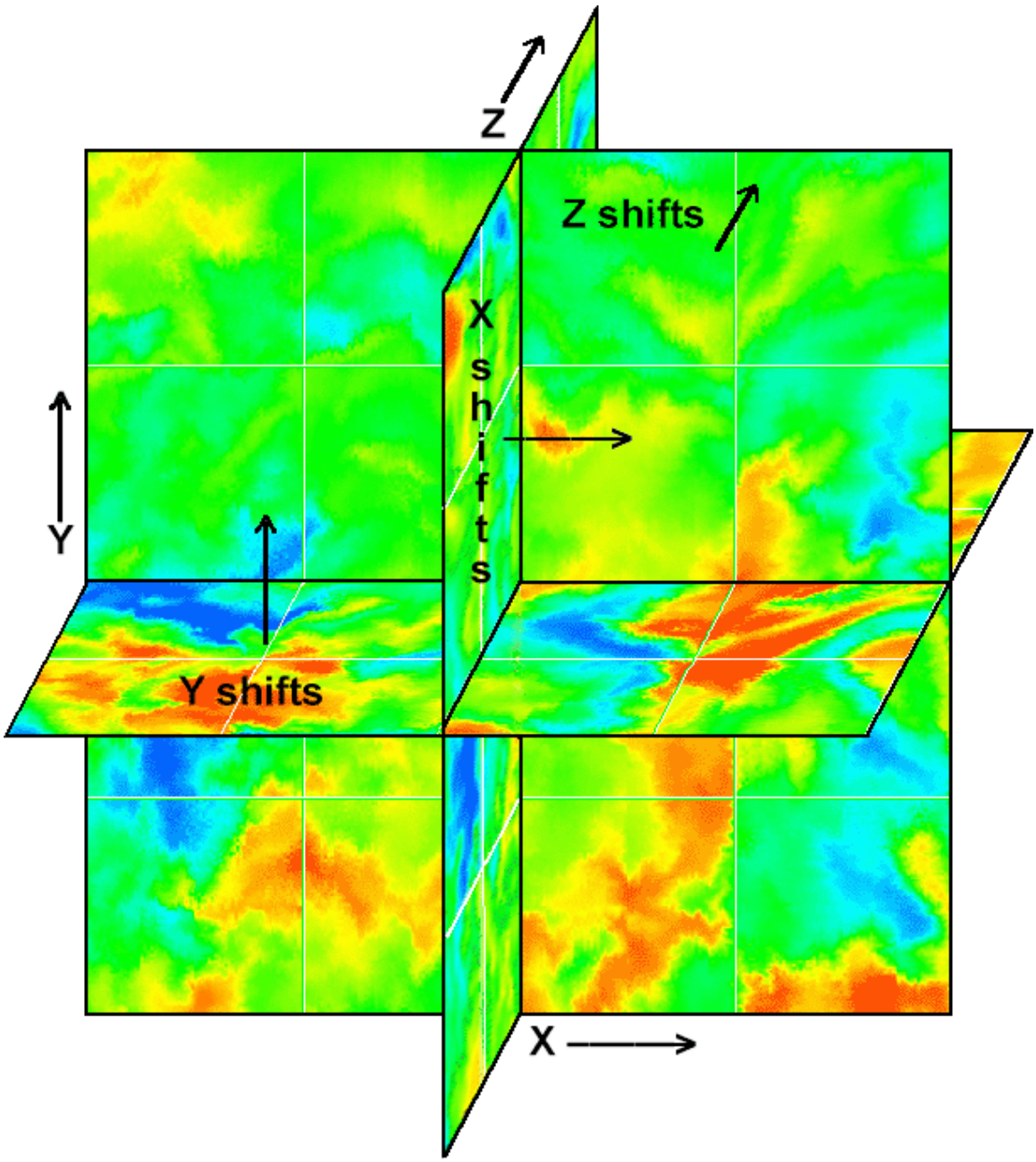

Figure 3.1: Three SFD shift planes are computed every timestep. Z shifts are along each of the N_{xyz} by N_{xyz} 1D lines of cells ('pencils') through the cube in the Z direction. Y shifts are shifts through the entire grid in the Y direction and X shifts are through the entire grid in the X direction. The shifts can all be different but must each be an integral number of cells to prevent numerical diffusion. Fractional cell shifts are accumulated for each pencil until at least an integral-cell shift is required.

Figure 3.1 above shows three orthogonal planes of shift velocities plotted as if they are defined at the center of the triply period cube. The plane labelled 'Z shifts' is a scaled version of the velocity component $V_z(x, y, t)$. Similarly, 'Y shifts' is $V_y(z, x, t)$ scaled and 'X shifts' is $V_x(y, z, t)$ scaled. Each of these velociy components is constant across the grid in the ignored direction, allowing the 2D representation. The shift velocities are real numbers re-computed every timestep from the CSD spectrum bin energies based on time- and space-correlated random numbers that can be changed to vary physical realizations for a specified spectrum. The vector

velocity field defined by the three shift arrays is 3D and has a 3D vorticity field guaranteed to be divergence free.

$$\xi_x \equiv \frac{V_z}{\partial y} - \frac{V_y}{\partial z}\,, \quad \xi_y \equiv \frac{V_x}{\partial z} - \frac{V_z}{\partial y}\,, \text{ and } \quad \xi_z \equiv \frac{V_y}{\partial x} - \frac{V_x}{\partial y}\,. \qquad \text{Eq. 3.1}$$

These density array shifts are restricted to be an integral number of cells along each axis, removing numerical diffusion entirely from SFD. The fuel and oxidizer are both packed into a single 32-bit integer so that a single cyclic shift constitutes the convection calculation for both species. This is at least a 60- to 100-fold reduction in work compared to a typical CFD algorithm. Since no Courant condition limits the timestep, the combined speed-up may be upwards of 1000.

The shift velocities are real numbers but fractional cell shifts along any of the axes are not enacted. The residual fractional shifts are accumulated each timestep and applied on timesteps whenever the integral shift threshold has been reached for a single particular line of cells, often called a 'pencil', in a given timestep. Thus, interpolation of densities back onto the grid is unnecessary. These shifts are direction-split and cycled through the three dimensions. The length of the shift on each line is determined by the coherent-structure velocities in each bin at the time the shift is made. In 3D, the relative shear of different shifts on adjacent lines of cells (i.e. 'pencils') generates density gradients. The term 'fine-graining' is often used to describe how a density becomes highly variegated by the action of relatively smooth flow components.

Turbulence continually convolutes and stretches the geometric interface separating two species. Actual molecular mixing, however, can only occur within a few mean-free paths of this evolving interface. Therefore, only a small fraction of the volume should become well mixed for a relatively long time – until the interface has moved close to most locations in the volume. To provide molecular mixing in the absence of numerical diffusion, SFD adds a small amount of grid-scale diffusion every other timestep. See Section 9 of CSD#2 for some details. Fig. 9.1 there shows that the 'molecular mixing' diffusion, varied over a factor of 8 to 1, has little effect on the macroscopic mixing as long as the diffusion coefficient is small enough. Eulerian grid-based convection would require very high resolution to keep the species physically separated for as long as they should be. Unless the computational cells are smaller than the density gradients that would contribute most heavily to molecular mixing, resolution-based numerical errors in Eulerian CFD will give the appearance of mixing prematurely two species that are entirely unmixed initially.

Figure 3.2 below shows what an SFD fuel flow looks like. The top three rows (t = 0 through 10 sec) were computed on a 1024^3 grid in 160 timesteps. Initially only the largest scale is activated, the stirring scale, and this appears as large-scale displacements of the lavender (fuel = 1.0) and black (fuel = 0.0) regions on Z layer 24. Rapid turbulent cascade to smaller scales appears though t = 5 sec. Grid-scale 'molecular mixing' was not turned on until the 6th second beginning at step 81 so the lavender and black pixels move initially without mixing. Red through blue pixels in the bottom two rows of the figure indicate the presence of the applied mixing. Because the flow velocities are different in the planes above and below Z plane 24, the mixing into the plane between adjacent Z layers makes the grid-scale diffusion appear larger than would occur in 2D alone. The bottom row of panels in Fig. 3.2, showing Z layer 12 on a 512^3 grid using the same timestep, show close agreement (convergence) with the corresponding time panels just above, an important special feature of SFD simulations.

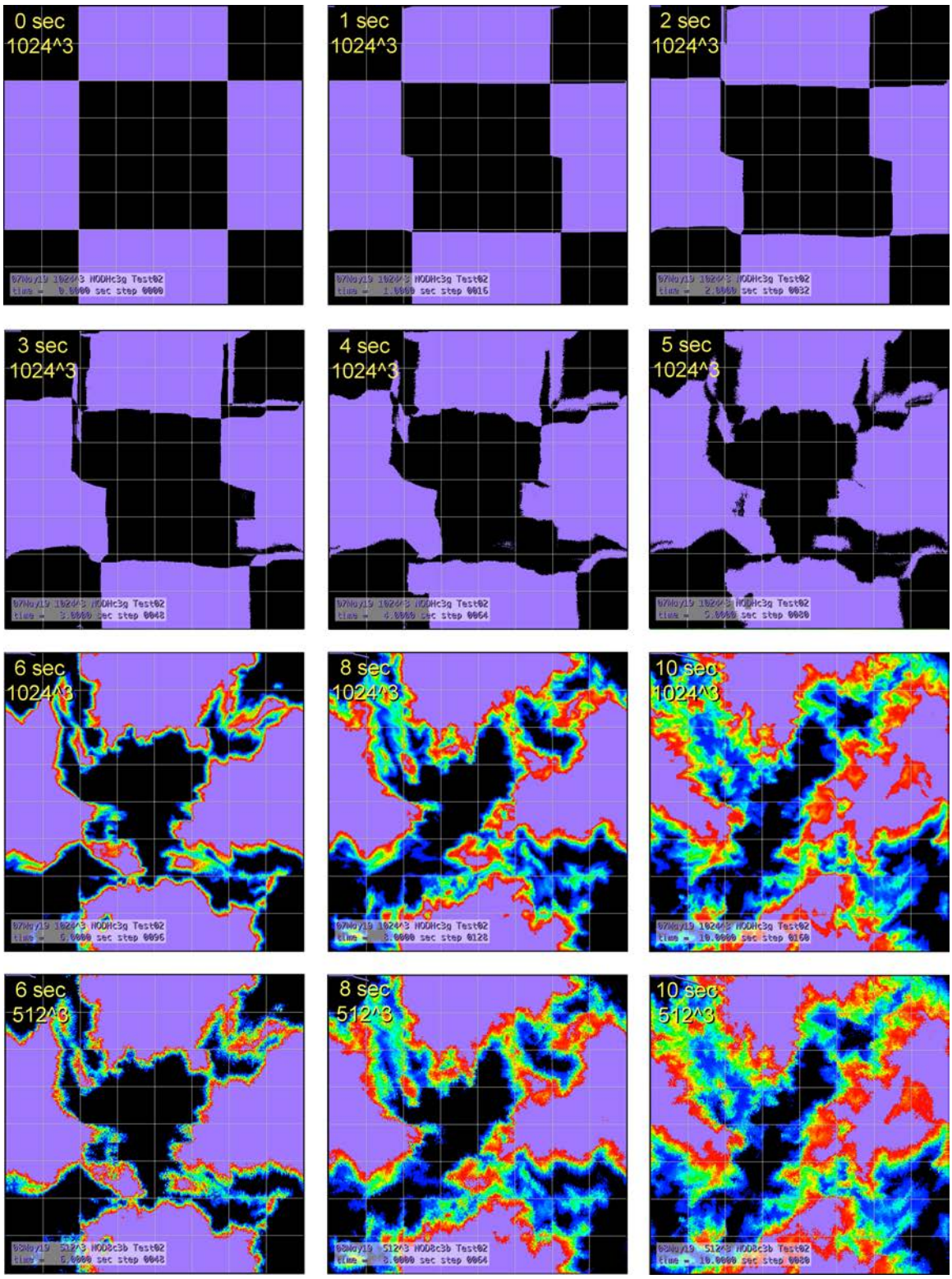

Figure 3.2: Fuel density on Z plane 24 with initial values 1.0 (lavender) and 0.0 (black). The times of each snapshot are shown in the upper left. When grid-scale diffusive mixing sets in after 5 seconds, the images show the maximum density (< 1.0) on this single plane as red and the minimum (> 0.0) as dark blue. The top three rows were computed using a 1024^3 grid. The bottom row, for comparing with the third row directly above, used Z plane 12 on a 512^3 grid.

The detailed solution of 3D continuity equations for these turbulent mixing problems is possible in principle using DNS but at prohibitively high resolution. This simple SFD mixing model is more computable and allows access to difficult parameter regimes for turbulent convective mixing. Movies of the evolution shown in Fig. 3.1 appear realistic despite the inaccuracies of the surrogate nature of the representation of convection. Different realizations of the small scales in real and detailed simulations of turbulent flows cause otherwise identical initial conditions to begin to deviate after one or two large-eddy turnover times. The phasing of even large-scale fluctuations in fluid dynamics can deviate quickly by 100% although macroscopic averages will generally track each other for longer times, even at different spatial resolutions. Because the small scales in a detailed simulation of turbulence rapidly cause deviations in the larger-scale flows, demonstrating numerical convergence of CFD solutions with increasing spatial resolution is not really possible for more than a very short time.

The panels of Fig. 3.2 suggest that mixing does not begin until the turbulence small scales have become populated. The 'molecular' diffusion, applied there after 5 seconds, is coupled to the smallest grid scale on the assumption that smaller scales down to the physical diffusive-mixing scale will become populated as soon as the smallest grid-resolved scales have become energized. The eddy turnover time for unresolved scales (Oran and Boris, 1993) is much faster than for the smallest resolved scales in the inertial range when the turbulence is in or near equilibrium. Therefore, it is safe to assume that actual mixing has occurred at and below the grid scale after the grid scale structures have become energized.

3.2 Fundamental Principles in Surrogate Fluid Dynamics

Continuous Convection and Conservation are two of the fundamental physical principles that give SFD quantitative underpinnings. The physical quantities addressed directly have units, e.g. kilograms, meters, seconds. The units are important when making predictions because they are necessary for comparisons with real-world experiments. This is particularly important when trying to debug a full simulation or to use experimental data to calibrate parameters in new models and algorithms. Further, the CSD-SFD modelling approach is trying to get at scales and phenomena where good DNS or experimental data are not easily available for calibration. However, because CSD-SFD is based on accepted fundamental principles, one should expect that any calibration data, even if not exactly where in parameter space we want to be working, will be useful.

Continuous Convection:

'Continuous convection' means that any mass density or chemical species number density that moves from point A to point B *must* pass along a continuous path through locations lying in between. This is a likely problem with some mathematically implicit algorithms because some convective transport can occur to remote cells in a single timestep. There is no 'teleportation' in the numerical SFD model. Physical convection is implemented as integral-cell shifts along the grid axes in SFD so density values cannot leapfrog their neighbors to get out of order. SFD is a Lagrangian model so numerical diffusion is zero. Transverse motions to a given pencil of density values can occur but they are enacted separately so all cell values still pass through the cells between. Convection is a quantitative phenomenon by definition because it determines how far material moves in a given time interval, both quantities with units.

In a discretely gridded model such as CFD or SFD, 'continuity' must seem to require an ambiguous interpretation because the 'computational representation' is not continuous. "Here the term *computational representation* includes:

- the particular discretization, i.e. the *mesh, grid, or expansion*, used to approximate the continuous flow variables,
- the data structures used to present this discretization to the computer, and
- the interpretation procedure used to reconstruct a numerical approximation of the continuous variable from the set of discrete quantities." (Oran and Boris, 2001, pg. 159)

Positivity in Convection:

Some density variables, mass density and kinetic energy density for example, must remain positive definite quantities. Positivity is mathematically guaranteed by the continuity equation applied to continuous variables. Before a convected quantity can pass continuously from positive to negative at a point, it must pass through zero. For this to happen, it must be a minimum at the first point reaching zero. At this location, in 1, 2, or 3D, the decrease in value also goes to zero. This fundamental principle should be required of numerical algorithms and is built into many modern discrete continuity-equation solution techniques. Unfortunately, most of the classical methods, such as Fourier spectral methods and Lax-Wendroff algorithms, do not maintain this important positivity property. Since, however, SFD convection is intrinsically Lagrangian, it maintains positivity by construction.

Mass Conservation in Convection:

Because convection is Lagrangian in SFD, species masses are guaranteed conserved during convection. Because the values are stored and convected as integers, there is not even any roundoff error. Conservation data from the baseline run 17JanE, which had the grid-scale mixing turned off until step 200, were summed for the fuel and the oxidizer every 20 timesteps. A few of the system-averaged conservation sums are listed in Table 3.1.

Table 3.1: System-Averaged Fuel and Oxidizer Conservation Sums

	step	system avg	step	system avg	step	system avg	step	system avg
fuel	**0**	**0.500000000**	**100**	**0.500000000**	**180**	**0.500000000**	**200**	**0.142766838**
oxidizer	**0**	**0.495000000**	**100**	**0.495000000**	**180**	**0.495000000**	**200**	**0.137766838**

These values have been averaged over the entire grid and are recorded as real numbers although computed from 16-bit integers. To the accuracy of numerical roundoff error, there is no change in the conservation sums until step 200 when the grid-scale 'molecular' mixing was turned on (see Fig. 4.3 in CSD#4 and Fig. 3.4 in CSD#3). Run 17JanE also had the fast reaction of fuel and oxidizer turned on wherever overlap of the two species in a cell occurred, explaining the immediate reduced system average conservation sums in Table 3.1 values as soon as the grid-scale diffusion was initiated at step 200.

Convection without Numerical Diffusion:

These tests also demonstrated the lack of numerical diffusion in the Lagrangian turbulent mixing of SFD. Because the cells at the two initial densities, 0.0 and 1.0 have been allowed to turbulently interpenetrate into adjacent cells at all resolved scales without actually mixing and reacting, nearly 75% of the fuel and oxidizer are consumed in the first timestep mixing is active, step 200, even though the mixing only occurs in adjacent cells at this step. This is a highly artificial situation chosen to illustrate this advantageous diffusion-free property of SFD. If the grid resolution were even higher than 1024^3, the result would be the same. The fuel and oxidizer would stay rigorously separated until the sub-grid-scale mixing is turned on.

When the mixing diffusion is active, adjacent fuel density (and oxidizer density) cells are averaged with a scaling parameter N_D that can be set to allow no averaging. This operation nominally causes roundoff error, particularly since the density values are integers. A special algorithm is included in this adjacent-cell mixing to ensure cancellation of the potential round-off, which can be important because SFD, in the current implementation, is working with reduced-precision 16-bit integers rather than 64-bit reals.

Momentum Conservation:

Momentum is conserved in the algorithm that converts the kinetic energy in each turbulence bin to the time- and space-correlated convective-shift arrays for computing convection and mixing on the resolved (gridded) portion of the spectrum. Each bin energy from the CSD simulation of the non-equilibrium turbulence spectrum determines the rotational speed of coherent structures in that bin but the direction of the convective shifts associated with that rotational speed is varied across the shift-array cross sections shown in Fig. 3.1 to reflect the actual scale size of the structures in that bin. These shift variations are determined from a master table of random numbers that is completely independent of the grid resolution. The shift variations are only implemented, however, down to the allowed resolution of the fuel and oxidizer density grids. The three axial convective shifts for each bin are normalized so that the bin energy is maintained while the shift directions vary continuously in a time-correlated manner determined by the precession speed of the determined coherent-structure scale.

The overall momentum is maintained at zero by making small corrections to the three shift arrays, typically a fraction of a cell. When the frame of reference is non-zero, as in the high-speed simulations, the X-shifts average about -5 or -6 while the Y- and Z-shifts applied average about +/- 1 before correction. Every timestep, the maximum and minimum shifts across the 3D grid are +/- 30 to 40, about 3% of the system. There are only a few of these large shifts but they still cannot be construed as non-continuous since there is no opportunity for density from elsewhere to be interposed between two adjacent cells for the other two directions. The direction-split nature of the convection guarantees this.

4. Discussion and Conclusions

The Coherent Structure Dynamics (CSD) turbulence model implements fundamental fluid dynamic principles, positivity of the coherent-structure kinetic energy density and number

density, conservation of turbulent kinetic energy throughout the inertial range, viscous dissipation at all scales, and scale invariance in the interaction rates between the coherent structures in the turbulence. The goal is to treat all scales from the system size down to below the viscous dissipation scale. The new Surrogate Fluid Dynamics (SFD) model embodies additional fundamental principles including continuous, positive convection without numerical diffusion but with mass and momentum conservation. These fundamental principles appear to be enough to give reasonable physical results for the surrogate fluid dynamics and turbulent flow mixing that is predicted. The CSD-SFD model has been shown to work well, stably and efficiently. This seems to say that fluid dynamics is a more robust process in our universe than necessarily defined by the Navier-Stokes equations. This, conclusion should be obvious anyway since fluids are actually vast numbers of individual atoms and molecules bumping into each other - and not at all continuous. However, CSD and SFD are also just models, imperfect representations of a 'fluid' system that will be invalid in some regimes and imprecise by some amount almost everywhere.

The CSD model was originally developed to study the rapid evolution of turbulent cascade at small scales. The CSD representation focuses on the dynamic interactions of the coherent flow structures that comprise turbulence. Its recent successes had to wait for an improvement to the model, the addition of coherent-structure number densities as primary variables, and the development of a better stiff equation integrator. As a result, the non-equilibrium evolution of the turbulent spectrum can now be simulated satisfactorily without the need to compute and post-process multiple individual 3D flow fields. The model and its representation allow the evolving spectrum of an ensemble of turbulent flow realizations to be approximated with one fast computation that sacrifices some detail about the longer-wavelength scales to obtain more accuracy and useful information at short scales.

Turbulence models for use in CFD have tended to treat the unresolved inertial range below the scale of the CFD grid as if obeying a renormalizable or scale-similar equilibrium described by the Kolmogorov spectrum with a spectral energy density that scales as $k^{-5/3}$. However, to represent small-scale effects more accurately, CSD solves not only for the kinetic energy density at each scale but also considers the number density of coherent structures at each scale to allow the relative spacing of the structures to vary from scale to scale. The spacing differences at each scale are non-dimensionalized in terms of a 'packing fraction' to describe the coherent-structure number density as a function of time (see CSD#1). The packing fraction provides additional degrees of freedom that appear to be important in describing the pre-dissipative bump in turbulent cascade. The conclusion is that the turbulence can be visibly different at different scales in the inertia range and through the dissipation zone, and thus is not necessarily scale similar even though it still satisfies the modified Kolmogorov spectrum.

In principle, the small spatial scales, generally not resolved by CFD, also control aspects of combustion that continue to evade expensive, time-dependent reacting-flow CFD simulations. Some detailed fluid dynamics is not available in the CSD-SFD representation, but the non-equilibrium evolution of turbulence can be simulated over a range of scales exceeding what CFD can do. The Taylor-Green Vortex problem was used to calibrate the free parameters in the CSD model approximately (see Fig. 7.1 in CSD#1). The resulting time-dependent system dissipation rate compares quite well quantitatively with multiple CFD computations of the problem taking orders of magnitude more memory and time to compute. The Re ~1 million CSD solution shown

in Figs. 7.1 and 7.2 of CSD#2 would take weeks or months with a 10^6 x 10^6 x 10^6 grid on an exascale computer.

The main goal of the SFD model is to study mixing of chemical species that can react once they are molecularly mixed by the action of the turbulence. The composite CSD-SFD model also addresses situations where changes in the driving fluid dynamics are fast and the resulting turbulence can be far from equilibrium as mixing occurs because the small scales will not have had time to adjust. There are a number of situations where out-of-equilibrium turbulence may be important. For example, chemical reactions can be significantly delayed until the short scales in the turbulent energy spectrum are energized. This is an ongoing concern in combustion research where non-equilibrium mixing actually empowers the turbulence at scales much smaller than the system size. For example, the CSD-SFD model was used to predict the extra time-delay in a non-equilibrium fuel-oxidizer reaction due to the finite mixing delay (see Section 6 of CSD#2). This driven turbulent mixing problem and the Taylor-Green vortex decay problem, plus other tests in CSD#1, have provided a number of checks on convergence with timestep and spectral resolution, energy conservation, and computational performance. However, CSD-SFD is a model that still needs a broader and deeper calibration with extensions to the two models that have not yet occurred.

It seems to be physically significant that the Kolmogorov cascade establishes itself quickly, in a few large-scale eddy turnover times (several seconds in a meter/second flow), but the non-dimensional packing fraction takes minutes to relax to an equilibrium, non-constant dependence on coherent-structure scale. Thus turbulence seems to 'retain' information from a non-equilibrium initial condition long after the energy cascade is well established. It is also important to remember that this reduced-order CSD model predicts a 'pre-dissipation bump,' or 'bottleneck,' in the spectrum just before and entering the dissipation zone. Though now well-established by detailed simulations and experiments, this small deviation from Kolmogorov cascade near the end of the inertial range was, at one time, attributed to numerical error in CFD.

The heat release from combustion, once it has begun, adds another mechanism that must yet be imposed on SFD: the baroclinic generation of additional turbulence that enhances mixing rates once the reactive-flow turbulence has established. These effects, both the local baroclinic turbulence generation and the nonlocal effect that modifies the entire spectrum, are currently being worked on. They may not significantly speed the onset of combustion but can likely enhance its strength once they are initiated. Surrogate models for these effects are being coded and tested in the CSD-SFD model and are the subject of a report in process of being released (CSD#4). One goal, in practical CFD applications, is information about the duration of the non-equilibrium reaction delays to be expected and data for a simple reduced-order approximation for incorporating these reaction delays in high fidelity (but more expensive) engineering models.

SFD is fundamentally Lagrangian. Lagrangian models have long been applied to complex flows for both compressible and incompressible CFD. As long as the grid motions are entirely Lagrangian and the grid does not need to be restructured to alleviate excess distortion, the convection can be diffusion free. However, numerical diffusion is not absent from practical Lagrangian methods in multidimensions because realistic flows with vortices distort Lagrangian grids so much that remapping onto a more regular grid must be done many times in a run with turbulence to keep the computation numerically stable. Interpolating the physical properties attached to each Lagrangian node onto a remapped grid introduces diffusion. Further, even

when the mass and species densities are completely Lagrangian, the energy density in a compressible flow on the same grid cannot be Lagrangian. Energy density is convected through the fluid at a different velocity from the mass and species densities and thus the energy will still have numerical diffusion.

Future improvements of SFD are worth discussing briefly. Adding closed loops of shifts to the system-wide grid-aligned shifts currently implemented could improve fluid dynamic fidelity qualitatively without adding numerical diffusion. If it can be shown that the full range of closed shift loops is a complete representation of incompressible flows, any incompressible flow could be simulated. The computational cost of developing such an extension to SFD would be extreme, however, and so is not high on the list of planned future work. Finding the Probability Density Functions of the current treatment of velocities, embodied in the system-wide grid-aligned shifts, is a research direction that could show if the current treatment deviates from the full fluid dynamics and by how much. This effort has been started but is currently on hold.

A higher priority project currently is applying metrics to the goal for which SFD was created in the first place, the efficient treatment of mixing as a precursor to reactive flow. This is an idealized research problem that could reduce anxiety about the use of SFD, at least for its primary goal. One way this could be accomplished is an investigation of how a well-resolved DNS model treats the time-dependent area increase of the interface between initially separated fuel and oxidizer species in a fully developed turbulent flow. The same initial condition could be run in SFD and multiple realizations computed by the two models could be compared. This involves writing an accurate way to track the interface between the two species in any 3D flow field and computing its area. Numerical diffusion would be a problem with the CFD solutions so its effects would have to be evaluated, and this could change unstably when the resolution is changed. An issue to be resolved is determining if a time long enough to approach molecular mixing, for a limited Reynolds number, can be predicted without the interfacial area being limited by the numerical diffusion.

SFD affords the opportunity both to study an ensemble of distinct 3D flow realizations, all satisfying exactly the same turbulence spectrum time history, and to compute the convergence of flow metrics for such an ensemble. This convergence study is left to another paper. However, the fidelity of the CSD-SFD model used here merits further discussion. The SFD simulations are clearly surrogates for high Reynolds number fluid dynamics, but they are not engineering-grade computations. The extensions and calibrations mentioned in several places above have not yet been performed. Even when these extensions and calibrations are far more complete, SFD will still be a non-quantitative surrogate model. CSD-SFD scenarios are valuable because they permit study of high-speed and non-equilibrium phenomena in parameter regimes that are not being accessed by other methods because of the computational cost and experimental difficulty.

Appendix A. Models, Representations, and Simulations

Speaking more generally than the preceding sections, "The objective of modelling is not necessarily to produce an exact copy of a system but to reproduce certain salient features of the system. Because approximations are made to derive the model, it is understood that the model is an imperfect representation of the system. The result is that a model is invalid in some regimes and imprecise by some amount almost everywhere. A simulation, then, exercises a model or collection of models for a particular choice of physical parameters, initial conditions, and boundary conditions." (Oran and Boris, 2001, pg. 2)

Modeling, for physical systems such as fluid dynamics, has four aspects:

1. The model is the entirety of the formulae, tables, and data proposed to contain a description of a physical system of interest. This includes the desired initial and boundary conditions.
2. The computational representation includes the particular discretization (that is, the mesh, grid, or expansion used to approximate the flow variables), the data structures used to present the discretization to the computer, and the interpretation procedure used to reconstruct an approximation to continuous fluid variables from the set of numerically determined discrete values (Oran and Boris, 2001, pg. 159).
3. Algorithms are solution procedures used to implement components of the overall model on the computer. They are not models and need not be directly numerical.
4. Simulations, built from these algorithms, attempt "to imitate the dynamic behavior of a system and to predict the sequence of events that control that behavior." (Oran and Boris 2001, pg. 2)

There are many approaches to modeling fluid dynamics on a computer, all approximate in some degree and generally computationally expensive. Boltzmann methods, molecular dynamics, and even cellular automata all require a very great number of degrees of freedom. There are Eulerian methods, Lagrangian methods, and free particle methods. There are also finite-difference, finite-volume, and finite-element methods. Sometimes, even small variations of a method are given very different names. Some methods are good and some are better. Those that are not so good are often characterized as schemes.

The goal is usually to determine a solution of the Navier-Stokes equations, a theoretical/ mathematical model that applies to most engineering applications and, further, underpins intuitive understanding of fluid behavior and turbulence. Fluid dynamic behavior, as suggested in the body of the paper, actually stems from more fundamental principles than a set of 3D partial differential equations. Respecting these principles can also lead to useful models for some important applications without the restrictions and high cost of extant models. This paper has discussed these principles and a new method called Surrogate Fluid Dynamics (SFD) with properties that current Navier-Stokes models have difficulty approximating.

"As a basis for evaluating representations and the reactive-flow algorithms implemented in those representations, we list some general properties that the continuity equation algorithms should have. These algorithms should:

1. be numerically stable for all cases of interest,
2. conserve quantities that are conserved physically,
3. ensure the positivity property when appropriate,

4. be reasonably accurate,
5. be computationally efficient,
6. generalize to multidimensions, and
7. be broadly applicable, that is, not problem dependent." (Oran and Boris, 2001, pg. 162)

Consistent Realizable Boundary and Source Conditions:

Realizability usually is addressed as an issue in the context of turbulence closure models for treating the unresolved scales of fluid-dynamic systems. "The realizability requirement enunciates the rudimentary expectation that an acceptable turbulence closure expression be based on the statistics of a velocity field that is physically achievable or realizable." (Girimaji, 2004). Turbulence closures such as second-order closure methods arise from an expansion that takes moments of the nonlinear Navier-Stokes equations. This means that the usual concerns with realizability stem for the mathematics of the attempted solution method, not the actual flow physics itself. Stated more correctly, these issues stem from trying to specify an approximation to close, or limit, the number of additional terms that need to be retained and computed in the expansion. Realizability often concerns subgrid models for use with Large Eddy Simulation and other CFD methods, which are always limited by resolution (e.g., Mokhtarpoor and Heinza, 2017).

For SFD, realizability is made easier in one way because there is a lot of information about the part of the turbulence spectrum at smaller scales than are resolved on a discrete spatial grid. Doing something physical with that extra small-scale data is not automatically constrained by the necessity of cutting off a mathematical expansion. On the other hand, though the SFD approximation of axis-aligned shifts expressing the convection provides approximately the right amount of material motion at each scale, the paths that the fluid follows is arguably 'surrogate' and not physical in detail. For example, closed vortex loops below the system size are not provided for even though the interaction of the small-scale convective motions have a divergence-free curl and will provide much of the same phenomenology. The flow field itself may not be achievable or realizable in detail even though, at some level, the statistics may be (e.g. Section 7 and Fig. 7.1 of CSD#1 concerning the Taylor-Green Vortex problem).

Realizability enters SFD in yet another way. The surrogate approach revolves entirely around respecting the boundary conditions and principles of the physics and seeing what can be predicted from that. For the solutions to be useful, physical boundary conditions must be implemented faithfully and accurately. For example, if mass is being extracted at a system boundary where the flow velocity is actually into the system, a seriously non-physical situation, errors must occur and even instability can result. In the same vein, a source of a particular species should not appear first in free space interior to the system boundary. If these conditions are respected, the CSD-SFD model has the benefits of a much wider range of space scales than does CFD and a much faster computation of the scales which are gridded.

Causality:

Causality is a property of most physical interactions, at least in the classical sense, and so should be present in any fluid dynamics model. "To establish causality you need to show three things – that X came before Y, that the observed relationship between X and Y didn't happen by chance alone, and that there is nothing else that accounts for the X -> Y relationship. Absent any one of

those things, and at best you can demonstrate a correlational (covariance) relationship, hence the phrase, correlational does not imply causation" (https://info.umkc.edu/drbanderson/establishing-causality/). The last two conditions, that the 'X causes Y' relationship is not a coincidence and there isn't 'some other cause' are not really issues in fluid dynamics. The scientist is solving a known model algorithmically and so is nominally in charge of the universe of possible effects. A good simulation often is complicated enough that the results may be surprising but the surprise does not void the model's causality.

The potential issue in fluid dynamics is temporal causality, sometimes labelled 'action at a distance.' This can appear to happen when an infinite propagation speed is introduced to the physical model of the system by a simplifying assumption such as incompressibility. Fast acoustic (pressure) waves are a real physical mechanism and have a finite propagation speed, i.e. X comes before Y. However, an incompressible model, computationally faster than solving for the pressure waves, seems to say the reaction and the cause are simultaneous. In SFD, the time delay between an action, such as local energy release from combustion, and its effects appearing somewhere else is governed by a finite timestep. Thus SFD is causal by construction.

Causality is a big a concern in relativity due to the finite speed of light, but has been addressed in some detail and causality is maintained in the mathematics and physics there. Further the finite speed of light is not really a problem in SFD at this time. A more relevant problem is the leading, low-density diffusion precursor whose speed can be arbitrarily large if the discretized equations are solved implicitly (Pu, et al., 2010a, 2010b). This is an artifact of solutions of the continuum diffusion equation and is absent from the underlying particle models of the fluid and explicit numerical solutions such as employed in SFD. Thus SFD is causal on this account as well.

Acknowledgements

The initial research leading to Coherent Structure Dynamics (1982) was supported by the Basic Research Program of the U.S. Naval Research Laboratory. Subsequent research was supported by the project on “Highly Complex Fluid Dynamics” within the ONR/NRL 6.1 research program. The program on “Advanced Computational Models that Exploit Many-Core Computer Architectures” supported the optimization of the CSD-SFD models through OpenMP. The program on "Numerical Simulation of Hypersonic Scramjet Combustion with Non-Uniform Inlet Conditions" supported the preparation of report CSD#2. My NRL collaborators, Keith Obenschain, Gopal Patnaik, Gabe Goodwin, and Jesse Maxwell contributed to the progress of this work. Professor Alexei Poludnenko and Mr. Calvin Colby (University of Connecticut), Professor Elaine Oran (TAMU), Professor Forman Williams (UCSD), Dr. Fernando Grinstein (Los Alamos National Laboratory), and Professor Paul Woodward (University of Minnesota) have contributed to the underpinnings of this paper and the Coherent Structure Dynamics research during the last few years.

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