

One-dimensional turbulence (ODT): computationally efficient modeling and simulation of turbulent flows

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Abstract

Write this last. About 100 words.

Keywords: turbulence, reacting flows, one-dimensional turbulence

Code Metadata

Nr.	Code metadata description	Please fill in this column
C1	Current code version	1.0
C2	Permanent link to code/repository used for this code version	<i>github.com/BYUignite/ODT</i>
C3	Code Ocean compute capsule	N/A
C4	Legal Code License	MIT
C5	Code versioning system used	Git
C6	Software code languages, tools, and services used	C++, Python 3.x, Yaml,
C7	Compilation requirements, operating environments & dependencies	CMake 3.12+, Cantera, Git, Doxygen (optional)
C8	If available Link to developer documentation/manual	N/A
C9	Support email for questions	davidlignellbyu.edu

Table 1: Code metadata (mandatory)

1. Motivation and significance

Turbulent flows characterize the vast majority of fluid flows in practical engineering applications, and simulations of turbulent flows provide re-

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4 searchers with valuable insights into complex systems, particularly reacting
5 turbulent flows such as combustion processes. Turbulence is a complex phe-
6 nomenon that affects the full range of a flow’s length and time scales. As a
7 result, resolving the entire flow field by numerically solving the Navier-Stokes
8 equations of fluid flow, as is done in direct numerical simulations (DNS), re-
9 quires substantial computational resources. DNS is a powerful research tool,
10 but its high computational cost makes it intractable for simulating most
11 practical engineering flows. In order to achieve numerical solutions to prac-
12 tical flow problems, researchers can use alternative frameworks that model
13 turbulence rather than resolving it directly.

14 Large-eddy simulations (LES) address the problem of wide-ranging length
15 and time scales by combining direct resolution of grid-scale quantities, as in
16 DNS, with subgrid modeling of smaller turbulence structures. The more
17 complex the flow, the more modeling is required; for example, a jet flame
18 simulation might require subgrid modeling for the combustion chemistry, ra-
19 diative heat transfer, or soot chemistry in addition to turbulence structures,
20 all of which form a tightly coupled system in which each model interacts
21 heavily with the others. While subgrid modeling makes LES more computa-
22 tionally affordable than DNS, it can introduce empiricism into simulations,
23 which can lead to inaccurate results. Additionally, unresolved quantities are
24 often parameterized in state space with empirical relationships or assumed
25 distributions that lack universal applicability. LES is a valuable simulation
26 tool, but its approach to turbulence modeling can introduce unwanted em-
27 piricism and make errors difficult to isolate and quantify.

28 The one-dimensional turbulence model (ODT) functionally reverses the
29 LES approach, modeling large-scale turbulent advection and directly resolv-
30 ing small-scale flow structures, simulating the full range of length and time
31 scales in a single dimension. Because large-scale structures are much easier
32 to study and model than small-scale structures, ODT mitigates or sidesteps
33 many of the subgrid modeling issues that complicate LES. Previous stud-
34 ies show that ODT can attain accuracy comparable to DNS at a fraction
35 of the computational cost [1, 2], making it an attractive tool for simulating
36 turbulent flows. Because the ODT model is one-dimensional, it is limited to
37 homogeneous or boundary-layer flows, such as jets, wakes, and mixing layers;
38 these types of flows, however, are common in nature and central to turbu-
39 lence research. ODT’s computational efficiency and resolution of a full range
40 of scales make it a valuable tool that complements experimental studies and
41 other simulation tools like DNS and LES.

42 Early applications of ODT focused on homogenous turbulence, wakes, and
43 mixing layers [3, 4, 5]. Later extension to variable-density flows and a spatial
44 downstream coordinate system facilitated its growth and application to more

complex flows, including combustion in jet flames [6, 7, 8, 9, 10, 11, 12, 13], counterflow flames [14], wall fires [15], and sooting flames [1, 16, 17, 18, 19], as well as other particle flows [20, 21, 22, 23]. ODT has also served to complement LES through subgrid modeling studies [24, 25, 26] and has been applied to various other flow configurations such as double-diffusive interfaces [27], Rayleigh-Taylor mixing [28], and stratified turbulence [29]. Most recently, the ODT code was extended to include cylindrical and spherical coordinate systems [30, 31, 32].

During the recent implementation of the cylindrical and spherical model formulations, the ODT code was drastically overhauled and reorganized, resulting in its current configuration. The ODT code presented here is a pared down version of the development code, representing the fundamental aspects of the ODT model and its most reliable functions. The example cases in Section 3 are a representative sample of the ODT code’s capabilities as it is presented here. Future releases will expand this code’s functionality with additional features currently in development.

2. Software description

2.1. Model description

The ODT model is described in detail in the literature [3, 5, 33, 30, 34]; only a brief explanation will be given here. In ODT, turbulent advection is modeled with stochastic processes called eddy events, which punctuate the solution of unsteady, one-dimensional transport equations for mass, momentum, and enthalpy. The ODT code uses a Lagrangian finite-volume formulation for diffusive advancement in which mass stays constant within each grid cell while cell volumes increase or decrease according to cell dilation via an adaptive mesh refinement [34].

Transport equations for mass, momentum, and enthalpy in the temporal formulation of ODT take the following generic form, derived from the Reynolds Transport Theorem [35] for a given scalar quantity per unit mass β :

$$\frac{d\beta}{dt} = -\frac{j_{\beta,e}A_{x,e} - j_{\beta,w}A_{x,w}}{\rho V} + \frac{S_{\beta}}{\rho V}. \quad (1)$$

Here, j_{β} is the diffusion flux of scalar β across the cell face area A_x where the subscripts e and w refer to the "east" and "west" faces of the grid cell, respectively. S_{β} is the Lagrangian source term derived from the conservation law for β , ρ represents mass density, and V represents cell volume. In practice, we refer to the left hand term on the right side of Equation 1 as the "mixing term" and the right hand term on the right side of Equation 1 as the "source term". The generic transport equation differs slightly in the spatial

82 formulation of ODT, but its form is the same, so we omit it here for brevity.
83 The system of ordinary differential equations (ODEs) that results is well be-
84 haved at all grid points and in all geometries in their finite-volume forms.
85 For details on transport equation derivation and use in both the temporal
86 and spatial formulations of ODT, see Lignell et al. [30].

87 Eddy events occur as a Poisson process in accordance with their eddy
88 rates, where a given eddy event of size l and location x_0 has an eddy timescale
89 t and an associated eddy rate $1/t$. Three user-defined ODT parameters
90 control the eddy event process: the eddy rate parameter C scales the rate of
91 occurrence of the eddies; the viscous penalty parameter Z suppresses small
92 eddies; and the large eddy suppression parameter β constrains eddies such
93 that they do not reach over the elapsed simulation time. Sampled eddies
94 that do not fit the defined parameters are rejected and not applied to the
95 domain.

96 Eddy events modify domain variables using triplet maps, as illustrated
97 for a cylindrical domain in Figure 1. For a region of eddy size l , the do-
98 main is copied to create three map images; the three images are then placed
99 back to back with the middle image inverted to maintain continuity, and
100 the composite is reapplied to the domain. This process applies to all trans-
101 ported variables on the domain. Applied properly, the triplet map increases
102 scalar gradients and decreases length scales consistent with the application
103 of turbulent eddies in real flows, conserves all quantities and their statistical
104 moments, and maintains continuity in property profiles. Subsequent eddies
105 in the same region will result in a cascade of scales, and eddy rates depend
106 on eddy size and the local kinetic energy such that they follow turbulent
107 cascade scaling laws.

108 Eddy events occur concurrently with diffusive advancement via solution
109 of the system of unsteady one-dimensional transport equations. In this way,
110 the ODT code marches in time or space until it reaches its end point. Due to
111 the stochastic nature of eddy events, each ODT simulation, or realization, is
112 different, even when it is provided with the same input parameters. In order
113 to obtain statistically stable data for a given set of parameters, we run many
114 realizations with the same input parameters and time-average them. This is
115 done via post-processing tools, which are provided in the ODT package.

116 2.2. Software Architecture

117 The ODT package consists primarily of an object-oriented C++ code re-
118 sponsible for running flow simulation cases and generating data. The package
119 also contains auxiliary data processing and visualization tools, written mostly
120 in Python. Within the main download package, several directories organize
121 the code:

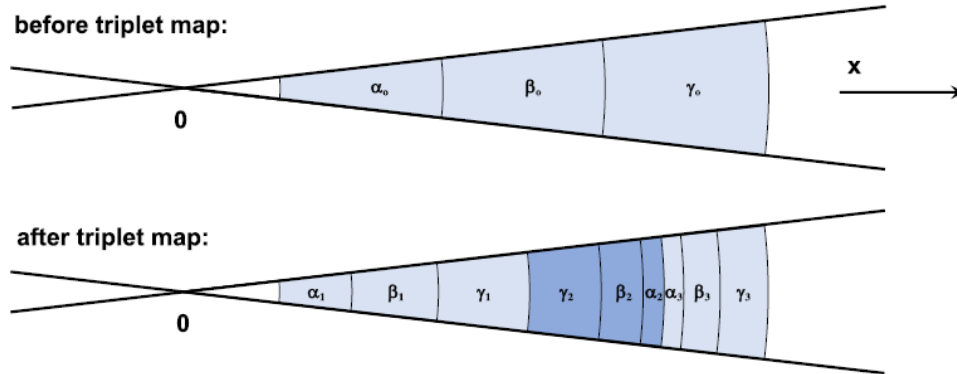


Figure 1: Schematic diagram of a cylindrical triplet map, adapted from [30]. Before the triplet map, the domain contains three grid cells of equal volume, while after the triplet map has been applied, the domain contains nine cells. The nine final cells are labeled according to the cells from which they originated and shaded to indicate that three map images were combined to create the final composite.

- 122 • **source:** ODT source code
- 123 • **build:** compiles and builds source code via CMake
- 124 • **run:** ODT executable and run scripts
- 125 • **data:** data generated by source code
- 126 • **input:** input files used to specify case variables
- 127 • **post:** data post-processing and visualization scripts
- 128 • **doc:** code documentation generated by Doxygen

129 In an individual simulation, variables live within in the `domain` class;
 130 wherever these variables are used within the code, pointers refer back to these
 131 locations. Key quantities are referred to as line variables, and their individual
 132 properties and functions exist within child classes of the `domainvariables`
 133 parent class.

134 The system of nonlinear ODEs is solved using CVODE [36] and user
 135 input files are processed with YAML [37], both of which are installed locally
 136 during the ODT build process. For reacting flow cases, chemical kinetics and
 137 transport are handled by Cantera [38], which must be previously installed
 138 by the user.

139 3. Example Cases

140 3.1. Pipe Flow

141 First, we present an incompressible pipe flow simulation using the tempo-
142 ral, cylindrical ODT formulation. Results for three different friction Reynolds
143 numbers ($Re_\tau = 550, 1000, 2000$) are compared to DNS results from El
144 Khoury et al. [39] ($Re_\tau = 550, 1000$) and Chin et al. [40] ($Re_\tau = 2000$) for a
145 pipe diameter of $D = 2.0$ m and flow density of $1.0 \text{ kg}\cdot\text{m}^{-3}$. Friction velocity
146 values of $1 \text{ m}\cdot\text{s}^{-1}$ ($Re_\tau = 550, 1000$) and $2 \text{ m}\cdot\text{s}^{-1}$ ($Re_\tau = 2000$) were assumed
147 and used to calculate the mean pressure gradient driving the flow. Using
148 initial conditions with uniform velocity profiles, simulations were run until a
149 state of developed flow was achieved, at which point data were gathered until
150 statistical convergence for the root mean square (RMS) velocity difference
151 from the mean profiles occurred.

152 The simulations were performed with ODT parameters $C = 5$ and $Z =$
153 350 for the temporal ODT formulation. The values of C and Z were adjusted
154 to give good agreement of the ODT results compared to the DNS. Schmidt
155 et al. [25] showed that higher Z results in the buffer-layer being located
156 further from the wall, and increasing C results in a lower slope of the mean
157 streamwise velocity in the log-layer.

158 RESULTS AND PLOTS GO HERE

159 3.2. Non-reacting Jet

160 Here, we present ODT simulation results for a non-reacting round, tur-
161 bulent jet compared to the experimental data of Hussein et al. [41]. The
162 jet consists of air issuing into air through a 1 in (0.0254 m) diameter duct
163 with a uniform exit velocity of $56.2 \text{ m}\cdot\text{s}^{-1}$ and a reported Reynolds num-
164 ber of 95,500. The ODT simulations use this diameter and velocity with a
165 kinematic viscosity of $1.534 \cdot 10^{-5} \text{ m}^2\text{s}^{-1}$, resulting in a Reynolds number
166 of 93,056. The initial velocity profile in the ODT simulations is a modified
167 top-hat profile in which a hyperbolic tangent function of width $\delta = 0.1D$ is
168 used on either side of the jet to smooth the transition between the jet and
169 the free stream. In the spatial formulation of ODT, the streamwise velocity
170 must be positive everywhere on the line, so a small minimum velocity of
171 $v_{min} = 0.1 \text{ m}\cdot\text{s}^{-1}$ is specified and added across the entire velocity profile.

172 ODT simulations were performed with parameters $C = 5.25$, $\beta_{LES} = 3.5$,
173 and $Z = 400$. The value of Z is the same as the spatial simulations in [15],
174 and the values of C and β_{LES} were adjusted to give good agreement with
175 the experimental data. Note the close agreement of the C and Z parameters
176 here to the optimal values used for the pipe flow simulations ($C = 5$ and
177 $Z = 350$). This illustrates a level of robustness in the ODT parameters

178 and suggests that intermediate values could be successfully applied in both
 179 configurations.

180 1024 independent ODT realizations were performed and results were en-
 181 semble averaged. All quantities are normalized consistent with jet similarity
 182 scaling. Downstream locations are normalized by the jet diameter D , and ra-
 183 dial locations are normalized by $(y - y_0)$, where y is the downstream location
 184 and $y_0 = 4D$ is the virtual origin used in [41].

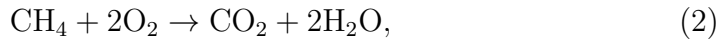
185 RESULTS AND PLOTS GO HERE

186 3.3. Jet Flame

187 ODT is uniquely suited for reacting flow simulations. Here, we present
 188 illustrative ODT simulation results of a round, turbulent jet flame based on
 189 and compared to the experimental DLR-A flame of Meier et al. [42]. This
 190 canonical flame configuration has been used extensively to study and validate
 191 turbulent combustion models [43, 44, 45, 46, 47, 48].

192 The DLR-A fuel stream is mixture of 22.1% CH_4 , 33.2% H_2 , and 44.7%
 193 N_2 (by volume) that issues into dry air via a nozzle with an inner diameter
 194 of 8 mm at a mean exit velocity of $42.2 \text{ m}\cdot\text{s}^{-1}$. The coflow air stream issues
 195 from a concentric nozzle 140 mm in diameter at a velocity of $0.3 \text{ m}\cdot\text{s}^{-1}$. The
 196 reported jet Reynolds number is 15,200.

Previous ODT studies of turbulent jet flames have used the temporal
 planar formulation, but the spatial cylindrical formulation developed recently
 [30] more closely matches the experimental configuration. This simulation
 uses the experimentally reported velocity profiles and jet dimensions. In
 the non-reacting case, a small minimum velocity was added uniformly to
 the velocity profile; no such addition is required here because of the slow-
 moving coflow air stream that issues alongside the reacting jet. The fuel
 was diluted with N_2 in the experimental flame to minimize radiative heat
 losses, and radiation is ignored in the simulation. This flame has a low
 Reynolds number, and the combustion chemistry proceeds quickly. The ODT
 simulation transports the chemical species O_2 , N_2 , CH_4 , H_2 , H_2O , and CO_2 .
 We assume that reactions proceed to the products of complete combustion
 and apply simple, fast reaction rates according to the following chemical
 equations:



197 These assumptions are not reasonable for the DLR-A flame, but they allow
 198 us to illustrate ODT in a reacting jet configuration with variable properties

199 and heat release, which is the primary purpose of this example case. More
200 complex combustion reaction mechanisms are available within the source
201 code and can be accessed by changing the appropriate input file parameter.

202 This simulation uses ODT parameters $C = 20$, $\beta_{LES} = 17$, and $Z = 400$.
203 The values of C and β_{LES} were adjusted to give good agreement with the
204 experimental data, and the value of Z is the same as it was for the non-
205 reacting jet in Section 3.2. 1024 independent flow realizations were performed
206 in parallel and the results ensemble averaged. Downstream distance y and
207 radial position r are normalized by the jet diameter D .

208 RESULTS AND PLOTS GO HERE

209 4. Impact

210 Questions to answer in this section (from SoftwareX template)

- 211 1. How can new research questions be pursued with this software?
 - 212 • possibility of parametric studies (much harder with DNS/LES/RANS)
 - 213 • study of late-flame soot and radiation interactions, soot emissions
214 as smoke
 - 215 • comparative radiation model studies?
- 216 2. How does the software improve pursuit of existing research questions?
 - 217 • late-flame behavior becomes easier to study
 - 218 • validation of LES subgrid models
 - 219 • soot stuff, especially late in the flame (because soot moves slowly
220 compared to gas species and therefore short simulation times like
221 in DNS aren't enough to study it effectively)
- 222 3. How does the software change the daily practice of its users?
 - 223 • cases take hours or days rather than weeks using supercomputer
224 resources
 - 225 • test cases can be run on local computers (unlike something like
226 DNS) and as background tasks without disrupting other tasks
 - 227 • ODT as a tool complements other approaches, can cover blind
228 spots and be used in validation
- 229 4. How widespread is the software? Who uses it? (Within and outside of
230 intended research area and/or group.)
 - 231 • BYU group
 - 232 • JCH at Sandia

- 233 • Chalmers group in Sweden (Marco Fistler, etc.)
- 234 • German university group (Heiko Schmidt, Juan Media, Marten
- 235 Klein, etc.)
- 236 • TO DO: find other groups who have used or currently use ODT
- 237 5. How is the software used in commercial settings (if any)? Has it led to
- 238 creation of spin-off companies?
- 239 • No commercial use (I think).

240 5. Conclusion

241 Write this part next to last

242 6. Conflict of Interest

243 We wish to confirm that there are no known conflicts of interest associated
 244 with this publication and there has been no significant financial support for
 245 this work that could have influenced its outcome.

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Current executable software version

Ancillary data table required for sub version of the executable software: (x.1, x.2 etc.) kindly replace examples in right column with the correct information about your executables, and leave the left column as it is.

Nr.	(Executable) software meta-data description	Please fill in this column
S1	Current software version	2.1
S2	Permanent link to executables of this version	For example: https://github.com/combogenomics/DuctApe/releases/tag/DuctApe-0.16.4
S3	Legal Software License	MIT
S4	Computing platforms/Operating Systems	Linux, OS X, Microsoft Windows
S5	Installation requirements & dependencies	CMake 3.12+, Cantera, Git, Doxygen (optional)
S6	If available, link to user manual - if formally published include a reference to the publication in the reference list	For example: http://mozart.github.io/documentation/
S7	Support email for questions	davidlignell@byu.edu

Table 2: Software metadata (optional)