The document reported in the following pages “Sec.1.1 Code citation, Copyright, authorship and acknowledgments” is extracted from:

Amicarelli A., CFD-OUT-sweePDF v.1.0.0: documentation file, pp.1-133, 2024.

1. FORMALITIES AND SYNTHESIS

1.1. Code citation, Copyright, authorship and acknowledgments

CFD-OUT-sweePDF v.1.0.0 (Amicarelli et al.) is a Lagrangian RANS CFD-SPH code for turbulent flows around buildings or obstacles with pollutant transport. The following air-quality applications have been investigated: Outdoor Air Quality (OAQ), Indoor Air Quality (IAQ), treatment processes for duct air quality. They include ordinary stack emissions and accidental releases. The code reproduces any useful spatial resolution within any maximum domain of 2km×2km×0.5km. The information on the code citation, Copyright, authorship and acknowledgments are reported in the following sub-sections.

1.1.1. Citation of CFD-OUT-sweePDF v.1.0.0

The citation of the code described by the current documentation file is "CFD-OUT-sweePDF v.1.0.0 (Amicarelli et al.)".

1.1.1. Synthetic Copyright notice of CFD-OUT-sweePDF v.1.0.0

The synthetic Copyright notice of CFD-OUT-sweePDF v.1.0.0 is "Copyright 2002-2024 (Amicarelli et al.)".

1.1.2. Detailed Copyright notice of CFD-OUT-sweePDF v.1.0.0

The detailed Copyright notice of CFD-OUT-sweePDF v.1.0.0 is "CFD-OUT-sweePDF v.1.0.0, Copyright 2002-2024 (Andrea Amicarelli, RSE SpA, Marc van der Sluys)".
Andrea Amicarelli is the majority owner of the Copyright of CFD-OUT-sweePDF v.1.0.0.
The writing of the subset of the new contributions in CFD-OUT-sweePDF v.1.0.0 received no public funding and was carried out as a freelance activity.

1.1.3. Copyright notices of the subsets of CFD-OUT-sweePDF v.1.0.0

The Copyright notices of the subsets of CFD-OUT-sweePDF v.1.0.0 are listed hereafter:

a) New source-code parts in CFD-OUT-sweePDF v.1.0.0:
   Copyright 2023-2024 (Andrea Amicarelli). This subset represents the majority of CFD-OUT-sweePDF v.1.0.0.
b) Source-code parts imported from SPHERA v.10.0.0 in CFD-OUT-sweePDF v.1.0.0:
   Copyright 2005-2022 (RSE SpA). This subset represents a minority of SPHERA v.10.0.0 and a minority of CFD-OUT-sweePDF v.1.0.0. SPHERA v.10.0.0 is released under the GNU-GPL v3 license.
c) Source-code parts imported from LMM Library v.1.0 in CFD-OUT-sweePDF v.1.0.0:
   Copyright 2008-2015 (Andrea Amicarelli). This subset represents a minority of LMM Library v.1.0 (2015, [2]) and a minority of CFD-OUT-sweePDF v.1.0.0.
d) Source-code parts imported from libSUFR v.0.7.0 (2020, [3]):
   Copyright 2002-2020 (Marc van der Sluys). This subset represents a minority of libSUFR v.0.7.0 and a minority of CFD-OUT-sweePDF v.1.0.0. libSUFR v.0.7.0 is released under the GNU-GPL v3 license.

1.1.4. Synthetic author list of CFD-OUT-sweePDF v.1.0.0

The synthetic list of authors of CFD-OUT-sweePDF v.1.0.0 is "Amicarelli et al.".

1.1.5. Detailed author lists of the subsets of CFD-OUT-sweePDF v.1.0.0

The author lists of the subsets of CFD-OUT-sweePDF v.1.0.0 are described hereafter:

a) Subset of the new contributions in CFD-OUT-sweePDF v.1.0.0:
   Andrea Amicarelli.
b) Subset of the contributions from SPHERA v.10.0.0 :

A unique author list for this subset is not available. Instead, the list of authors of the whole code SPHERA v.10.0.0 is reported: Andrea Amicarelli, Antonio Di Monaco, Sauro Manenti, Elia Giuseppe Bon, Daria Gatti, Giordano Agate, Stefano Falappi, Barbara Flamini, Roberto Guandalini, David Zuccalà, Emanuela Abbate, Qiao Cheng.

c) Subset of the contributions from LMM Library v.1.0 (2015, [2]):
Andrea Amicarelli.

d) Subset of the contributions from libSUFR v.0.7.0 (2020, [3]):
Marc van der Sluys.

1.1.6. Content information on the subsets of CFD-OUT-sweePDF v.1.0.0

The information on the content of the subsets of CFD-OUT-sweePDF v.1.0.0 is reported in the following:

a) Subset of the new contributions in CFD-OUT-sweePDF v.1.0.0:

- Major features:

1.RANS SPH Momentum Equation (SPH RANS-ME): SPH quadrature formulae (C_0- and C_1-consistency) for the inner terms, ME stabilization term, RANS Trajectory Equation, semi-implicit Euler's scheme; convergence criteria;
2.RANS SPH Continuity Equation (SPH RANS-CE): SPH quadrature formulae (C_0- and C_1-consistency) for the inner terms, smoothing coefficient, forward-backward Euler's scheme with linear filter; convergence criteria;
3.RANS SPH Balance Equation for the mean Turbulent Kinetic Energy (SPH TKE-BE): SPH quadrature formulae (C_0- and C_1-consistency) for the inner terms, Kat&Lau-k-eps and k-eps formulations, shell SPH filter, SPH TKE-BE forward-backward Euler's scheme; convergence criteria;
4.RANS SPH Balance Equation for the dissipation rate of the mean Turbulent Kinetic Energy (SPH eps-BE): SPH quadrature formulae (C_0- and C_1-consistency) for the inner terms, Kat&Lau-k-eps and k-eps formulations, SPH eps-BE forward-backward Euler's scheme; convergence criteria;
5.RANS SPH Balance Equation for the ensemble mean concentration (SPH Cm-BE): SPH quadrature formulae for the inner terms (C_0- and C_1-consistency), SPH Cm-BE forward-backward Euler's scheme; convergence criteria;
6.Volume/mass-conservative Balance Equation for the particle Control Volume (CV-BE);
7.SPH Time-Space Ensemble (SPH-TSE) filter: Lagrangian integral time scale of turbulence, peak value of the compensated velocity Lagrangian structure function, ensemble statistics under post processing, convergence criteria to stationary conditions, ensemble statistics for Computational Solid Dynamics, quadrature formulae over monitors and positioning-grid points, C1-consistent SPH quadrature formula for functions (inner terms);
8.Fixed walls (partial feature, part 1 of 2): SPH quadrature formulae (C_0- and C_1-consistency) over the set of neighbouring fixed-wall elements for the fixed-wall Boundary terms in the Balance Equations and in the SPH-TSE filter, C_1-consistency mean pressure for fixed walls, C_1-consistency mean TKE for fixed walls, Boundary mean velocity, RANS Wall Functions, fluid-wall reactions for fixed-wall faces;
9.Solid-body terms for the CFD Balance Equations (partial feature, part 1 of 2): SPH quadrature formulae (C_0- and C_1-consistency) for the solid-body Boundary terms in the Balance Equations and in the SPH-TSE filter, C1-consistency mean TKE for body particles, major contribution to C_1-consistency mean pressure for body particles, minor contribution to body-particle Boundary velocity and proxy variables.

Minor features: tools of probability calculus; full transition from RANS-SPH to NS-SPH Balance Equations; free-surface monitor; ILES-SPH ensemble means, higher-order ensemble moments, ensemble probability density functions and ensemble cumulative density functions; ILES-SPH

higher-order LES-filtered moments; fine-grained pdf and cdf under ILES-SPH; multi-linear interpolations; numerical concentration at the Pollutant Source; freezing conditions at inlet and outlet sections; equation for hydrostatic mean pressure under Weakly-Compressible linear barotropic fluids; RANS height-dependent inlet section; particle-count balance; tensor product; heap profiler; optimization of the subset imported from SPHERA v.10.0.0 (see below both major and minor features) following best practices regarding procedure rationalization, RAM management, memory-caching techniques and OMP; conditional ensemble means. Major contributions to the following minor features: flow-rate monitoring; liquid-front monitoring; time series of the fluid-domain variables; fluid-depth Boundary Conditions; restart procedures (I/O modularized for large simulations); ILES Wall Functions; full transition from NS-SPH to ILES-SPH Balance Equations; writing of the log file. Minor contributions to the following minor features: positioning pre-conditioned dynamic vectors; 2D synthetic output fields; etc.

b) Subset of the contributions from SPHERA v.10.0.0 :

- Major features (specific author lists within brackets, where available):

8.Fixed walls (partial feature, part 2 of 2): geometrical SPH quadrature formulae over the single wall element (Di Monaco), fluid-wall reactions for fixed-wall edges (Di Monaco);
9.Solid-body terms for the CFD Balance Equations (partial feature, part 2 of 2): major contribution to body-particle Boundary velocity and proxy variables (Amicarelli), minor contribution to C_1-consistency mean pressure for body particles (Amicarelli);
10.Balance Equation for the Linear Momentum of solid bodies -SLME- (Amicarelli), included reaction forces and sliding friction force;
11.Balance Equation for the Angular Momentum or Torque of solid bodies -SAME- (Amicarelli), included 3D rotations;

Minor features: fixed-wall contributions to the SPH ILES-ME sub-particle term (Di Monaco); geometrical Initial Conditions for particles (Amicarelli et al.) and fixed walls (Di Monaco et al.); inlet section for Bazin's sharp-crested weirs (Amicarelli); roughness length under CORINE Land Cover with DEM/DTM (Amicarelli); Equation of State (Amicarelli); ILES-SPH uniform inlet section; detection of particles crossing open sections; string management. Major contributions to the following minor features: geometry tools (Amicarelli et al.); allocation tools (Amicarelli); input-file template (Amicarelli); code-independent skeleton of the Makefile (Amicarelli); 2D synthetic output fields (Amicarelli); code-independent skeleton of the main procedure for the elapsed-time profiler (Agate et al.); management procedure to set hydrostatic pressure (Agate et al.); code-independent skeleton of the procedures for writing ".vtu" and ".pvd" files; writing of a ".vtk" geometry file; general reading procedures; positioning pre-conditioned dynamic vectors. Minor contributions to the following minor features: flow-rate monitoring (Amicarelli); time series of the fluid-domain variables (Amicarelli); fluid-depth Boundary Conditions (Amicarelli); ILES Wall Functions (Amicarelli); inner contribution to the SPH ILES-ME sub-particle term (Di Monaco); liquid-front monitoring; restart procedures; writing of the log file.

c) Subset of the contributions from LMM Library v.1.0 (2015, [2]):

Minor feature: stochastic inlet turbulence for ILES-SPH.

d) Subset of the contributions from libSUFR v.0.7.0 (2020, [3]):

Major contribution to the following minor feature: assessment of the confidence intervals for the time series of the fluid-domain variables.

1.1.7. Acknowledgments

Those source-code parts which were imported from SPHERA v.10.0.0 (RSE SpA, 2022, [4]) are noticed in Sec.1.1.3 and Sec.1.1.5-1.1.6. They were imported in CFD-OUT-sweePDF in compliance with the international and national Copyright laws and the specific Italian laws which apply to SPHERA. 'SPHERA v.10.0.0 is realised by RSE SpA thanks to the funding "Fondo di Ricerca per il Sistema Elettrico" within the frame of a Program Agreement between RSE SpA and the Italian Ministry of Economic Development (Ministero dello Sviluppo Economico)'. These imported parts are mentioned in Sec.4.5, Sec.5.4-5.5, Sec.5.8-5.10, Sec.7.2 and Sec.9 of the current guide, with an explicit description only if absent in the guide of SPHERA v.10.0.0, whose synthetic list of authors is "Amicarelli et al.".

Those source-code parts which were imported by libSUFR v.0.7.0 (Marc van der Sluys, 2020, [3]) are noticed in Sec.1.1.3 and Sec.1.1.5-1.1.6. They were imported in CFD-OUT-sweePDF in compliance with the international and national Copyright laws. The sole author of libSUFR v.0.7.0 is Marc van der Sluys.