High-resolution SPH simulations of a 2D dam-break flow against a vertical wall. Commentary to the collection of datasets

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Abstract

This collection of datasets may appeal to those interested in computer simulations of water flows with a free-surface using Smoothed Particle Hydrodynamics. Weakly compressible SPH is a computationally intensive and computationally demanding technique. Obtaining high resolution datasets can be either difficult, impractical or unaffordable for many scholars and practitioners.

The datasets are simulations at four spatial resolutions of the benchmark solution of a 2D dam break impinging on a vertical wall used by D.D. Meringolo, S. Marrone, A. Colagrossi and Y. Liu. See "A dynamic δ-SPH model: how to get rid of diffusive parameter tuning" in *Computers and Fluids*, 2019, 179:334-355, https://doi.org/10.1016/j.compfluid.20183.11.012.

The resolution of the initial water column with 800, 1600, 3200 and 6400 particles led to a total fluid-particle count between 1M and 82M. The simulations have been run with the open-source solver DualSPHysics 5.0 on a GPU device with a nominal peak throughput of 5300 Gflops in double precision. In line with the policy of the Delft University of Technology to produce FAIR research output — 'fair' for findable, accessible, interoperable, reusable —, the 4TU Centre for Research Data archives these SPH simulations in a dataset collection retrievable from https://doi.org/10.4121/c.5353691 under a CC-BY 4.0 license.

Possible uses are severalfold. This collection provides data on an established benchmark usable, for example, for education and dissemination, the in-depth visualisation and analysis of results, the execution of refined or extended simulations, the comparison of behaviours and results against changes of parameter settings and across different solvers, convergence and sensitivity studies.

Keywords: Smoothed Particle Hydrodynamics, dam-break flow, GPU computing, DualSPHysics solver, numerical experiment, benchmark datasets

Contents

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1 Generalities

1.1 Briefly on physics

Broadly speaking, the property of fluidity consists in the fact that small portions of a body of liquid easily move with different velocities to their neighbours; at least, this variability in time and space is distinctive of fluidity. Computer simulations of this behaviour use two major approaches; intermediate approaches do exist, but are not essential here.

1. The Eulerian approach first divides the space occupied by the body of liquid in a large number of small volumes fixed in space; and then, as time unfolds, tracks the properties of the liquid flowing across these fixed conceptual volumes.
2. The Lagrangian approach first divides the body of liquid itself into a large number of small masses that are not fixed; and then tracks the flow of each of these masses as they travel around. Lagrangian approaches are most suited to water flows with fragmented free surfaces. These are often associated to rapid and violent dynamics, such as wave breaking and impacts.

The Smoothed Particle Hydrodynamics (SPH) methodology does use a Lagrangian approach and is suitable for modelling rapid and violent flows.

1.2 Briefly on modelling

SPH has originally been developed in astrophysics as a modelling methodology for truly compressible matter. However, in most engineering and almost all environmental applications, water is very nearly incompressible. A substantial strand of SPH research has then adapted the original SPH formulation by modelling water as a weakly compressible fluid.

Even more precisely, the compressibility in weakly compressible SPH takes artificial values defined by the modellers. This artificial tweak does not impair the correct simulation of a genuine nearly incompressible fluid greatly; the proviso is not to draw specific conclusions on processes crucially dependent on compressibility, such as the propagation of sound.

This document does not expose the tenets of SPH. As an entry point see the review paper of [Monaghan, 2012]. It is important for the sequel to recall that an SPH particle's state at a time instant consists of:

- position, after the Lagrangian formulation;
- velocity, after the fundamental focus in fluid flow simulation;
- density, after the weakly-compressible formulation.

1.3 Briefly on the solver

DualSPHysics:

1. is an SPH solver with a wide range of modelling capabilities for engineering and environmental applications, implementing an artificial weak compressibility. The code can compile and run on CPU and GPU devices.
2. has been developed by a team of developers and contributors from academic and research institutions, among others the Environmental Physics Laboratory of the Universidade de Vigo in Spain and the School of Mechanical, Aerospace and Civil Engineering of the University of Manchester in the United Kingdom.

   The website https://dual.sphysics.org/ is the entry point for the full list of developers; features, documentation and references; downloads and user interface; FAQ, forum and news; training and tutorials; animations and visualization.
3. is a suite of programs in which:
   (a) DualSPHysics proper is free software distributed under a GNU General Public License v2.1 and BSD license. It uses other pieces of free software adding functionalities to it;
   (b) other closed-source utilities are provided for the pre-processing and post-processing operations wrapped around the open-source DualSPHysics proper — more in § 3.2.

The two pathways for accessing the software suite are not entirely equivalent:

1. The GitHub repository at https://github.com/DualSPHysics/DualSPHysics.

   This features branches up-to-date with the continuous code development. However, the documentation contains only two example cases and no detailed users' guides.
2. A zipped archive from https://dual.sphysics.org/index.php/downloads/.

   That archive contains the code frozen at the latest tagged version with the complete documentation and set of examples.

Note that the versions available to the general public are not necessarily those used to produce scientific advances published elsewhere.

Resources guiding the users through the workflow of DualSPHysics are:

1. The GitHub wiki page: https://github.com/DualSPHysics/DualSPHysics/wiki. This is the principal source of the information on DualSPHysics reported in this document;

2. The help documentation of the software utilities (in repository and archive);
3. The templates for the XML input files (in repository and archive);
4. The users' guides in PDF format (in archive only).

1.3.1 Disclaimers

- Please always double check the original sources of DualSPHysics as a safeguard against possible errors and omissions in this document, beside as a source of updates and releases.
- Please take note that the Delft Institute of Applied Mathematics is not a member of the development team of DualSPHysics.

  In fulfilment of the licensing terms, the information provided with this collection of datasets and with this accompanying document implies neither endorsement nor promotion of DualSPHysics. Likewise, citation of the names of DualSPHysics contributors implies neither their endorsement nor their promotion of this collection of datasets and its accompanying document.

2 The dam-break flow impinging on a vertical wall

2.1 As an experiment

In a dam-break flow a boxful of water is released inside a tank upon removing one side of the box. The water runs against the opposite side of the tank, hits the end wall and splashes up and back again. This flow is traditionally called 'dam break' because releasing suddenly a mass of still water associates with the failure of a dam.

Broadly speaking, the flow evolution consists of four stages:

1. As the water box collapses and the leading edge advances over the box floor, the flow is gradually varied;
2. Then, follows the impact of water against the wall, hence an instance of fluid-structure interaction;
3. Then, the water raising at the wall plunges back on the upstream water, and water-water impacts cause intense fragmentation of the free surface, droplets and bubbles, and vortical motions in the bulk of the fluid;
4. Finally, the much-agitated water begins to slosh and settle into a quiescent state thanks to action of viscosity.

The physics of the last two stages is highly nonlinear and is amenable to an SPH-based solving approach.

A dam-break experiment can be material or numerical. The collection contains reproductions of dam-break flow impinging at a vertical wall provided as benchmark numerical solution by D.D. Meringolo, S. Marrone, A. Colagrossi and Y. Liu. See "A dynamic δ-SPH model: how to get rid of diffusive parameter tuning" in Computers and Fluids, 2019, 179:334-355 [Meringolo et al., 2019] — this is a long-standing and widely used benchmark, and the paper itself show past research developed with it.

In this numerical experiment, air is not modelled and the flow is two-dimensional. The problem is solved in dimensionless form, with a few noteworthy consequences:

- The problem variables describing the geometry, kinematics and dynamics express ratios of dimensional quantities with respect with a reference height of the water box (H, whose value may remain unstated), the acceleration of gravity g, and the reference fluid density, ρ_0;

- The computed time and velocity express ratios with respect to time and velocity scales derived from those reference values. The scales for time and velocity, $\sqrt{H/g}$ and $\sqrt{gH}$, are formally identical to the parameters of the forward propagation of the leading edge of the collapsing water column. Note, in passing, that the free-fall velocity, $\sqrt{2gH}$, relates with the motion of individual water droplets more closely;
- All simulation parameters with a physical dimension, for example the artificial speed of sound, are expressed in dimensionless form as well.

Please refer to Meringolo *et al.*, 2019 for more information about the problem geometry.

2.2 As a simulation

DualSPHysics, described in § 1.3, is a different SPH solver to that used by Meringolo *et al.*, 2019. This section outlines the main aspects of the general formulations and specific settings used to produce the datasets; differences of detail between the two source-code implementations are not commented upon. Dr Andrea Colagrossi of CNR-INM (National Research Council, Institute of Marine Engineering, Italy) has kindly shared the original simulation settings.

2.2.1 SPH governing equations

- For both solvers the kernel function is a Wendland C2 formulation: its smoothing length, h, is half the radius of the support. The radius of the support is also referred to as kernel size or cut-off length. In simulations the smoothing length, an SPH parameter, is expressed as a multiple of the interparticle distance in the initial conditions, Δp, a discretisation parameter: commonly $h/\Delta p$=2.
- As for the equation of state, both solvers implement a linear relationship between density and pressure; the pressure is relative to the total pressure for which the density takes the reference value ρ_0. The artificial speed of sound has the value of 10 units; since the dam-break celerity is 1 unit, the Mach number of the simulation is 0.1, thus well in the range of weakly compressible behaviour. Density can be converted into pressure with this artificial equation of state.
- As for the mass-conservation statement and the SPH-characteristic density-diffusion term, the DualSPHysics simulation uses a formulation by [Molteni and Colagrossi, 2009], while the simulation by Meringolo *et al.*, 2019 does a δ-SPH formulation using [Randles and Libersky, 1996].
- As for the momentum-conservation statement, in both simulations the viscous term is expressed with the artificial-viscosity formulation:

$$\alpha h c_0 \frac{\rho_0}{\rho_i} \sum_j \Pi_{ij} \nabla_i W_{ij} V_j$$

  The source code of DualSPHysics has been modified in order to substitute the formulation of the function Π_{ij} by [Monaghan and Gingold, 1983] — devised to alleviate specific astrophysical problems such as collapsing gas clouds — with the same formulation as Meringolo *et al.*, 2019:

$$\Pi_{ij} = \frac{(\vec{u}_j - \vec{u}_i)(\vec{r}_j - \vec{r}_i)}{(\vec{r}_i - \vec{r}_j)^2}.$$

  See § 3.2.1 for the handling of this modification.

  Meringolo *et al.*, 2019 resolved a dam-break problem with a range of artificial viscosity parameters; in this dataset, $\alpha = 0.01$ only.
- Finally, the boundary conditions prescribe free slip at solid-fluid interface. In DualSPHysics this has been implemented by the so-called 'dynamic boundary conditions': gauged repulsive forces exerted by the in-boundary particles keep the free-flowing particles 1.5 smoothing

lengths away from the boundary surface [Crespo et al., 2007]. Meringolo *et al.*, 2019 use the established technique of 'ghost particles' whereby the fluid particles can approach the boundary surface freely.

2.2.2 Numerical parameters

- In both simulations, the smoothing length is twice the initial interparticle distance, $h/\Delta p = 2$.
- The $H/\Delta p$ ratios discussed in Meringolo *et al.*, 2019 vary between 480 and 1600. The present datasets contain four reproductions of that benchmark with spatial-resolution ratios of 800, 1600, 3200 and 6400.

  For the given geometry, the counts of fluid particles in the simulations are 1,280, 5,120, 20,480 and 81,920 thousands respectively.
- The time integration method is a Runge-Kutta formulation with a frozen diffusive approach in Meringolo *et al.*, 2019; and a single-stage, two-step, 'kick-drift' Verlet scheme in DualSPHysics.

  Both methods march in time explicitly and are subject to a stability constraint: in both cases the Courant number is 0.125. Note that the time step for the entire cloud of particles is reduced based on the stability of the particle with the highest velocity of all.
- The simulated time is 20 units: at that point in time, the energy dissipated by the system is estimated at around 88% of the initial energy – see Meringolo *et al.*, 2019, Fig. 16. This is the early stage 4 mentioned in § 2.1.

Note that higher resolution in SPH simulations entails a considerable compute workload. A higher number of particles increases the operations at each time instant; owing to the stability of explicit time-marching methods, the time steps are smaller and the temporal resolution increases accordingly. Finer spatial and temporal scales cause a wider range of velocities to be resolved, thus further occasions for reductions of the time step. Also, the ratio of the smoothing length to the artificial speed of sound, h/c, is a scale for the initial time step. Therefore, simulations at an increased spatial resolution do take longer to complete. Table 1 summarises these trends for the datasets.

Table 1: Numerical parameters and problem size

$H/\Delta p$	800	1600	3200	6400
h/H	0.00125	0.000625	0.0003125	0.00015625
Fluid particles (10^3)	1,280	5,120	20,480	81,920
Time steps	1,395,921	2,863,036	5,728,950	11,743,221

3 The collection of simulation datasets

3.1 Usages of a shared dataset

Completing a high-resolution SPH simulation requires powerful compute devices such as GPUs and, of course, time. The increased workload affects the pre-processing, proper processing and post-processing stages alike. In sum, high-resolution simulations push the limits of the affordable and practical.

Sharing this collection has general aims and specific usages:

- In broad terms, sharing aims to stimulate and facilitate the informed access to general and special features of modelling rapid flows using weakly compressible SPH.

Consider also that a higher resolution for one field of application can be an entry level for another field of application. Therefore, the insights gained from a benchmark can have a wider scope than the specific subtopic where they originated from (dam break flows, here).

- In more specific terms, a dataset of pre-computed, highly-resolved results lends itself to several usages. Here, some are envisaged in a loose order of increasing complexity:
  1. preparing educational and presentational material;
  2. deriving secondary flow variables from the particles' states; for examples, the fields of pressure and vorticity;
  3. serving as initial condition for hot starts, also for refined investigations inside the intervals between the read-out frequency;
  4. serving as a yardstick to anticipate the loss of information incurred at the resolution that users can afford in their own situation;
  5. contrasting the results with practical knowledge and measurements, taking into account the modelling assumptions;
  6. comparing with the results obtained with other weakly-compressible SPH solvers;
  7. studying the sensitivity to physical parameters;
  8. quantifying the changes introduced by newly introduced submodels for special physics;
  9. studying the sensitivity to numerical parameters;
  10. quantifying the gains in accuracy and performance that numerical expedients can deliver in nonlinear conditions, where a trend of convergence metrics is not tractable;
  11. analysing the dataset in terms of frequency and distribution of nonlinear events; for example, fragmentations/collapses/impulses.

Take note that the dataset contains the information needed for replaying the simulations and reproducing the data. Post-processing is possible using the closed-source tool kit provided with DualSPHysics: among others, this tool kit enables producing files that can be read by open-source ParaView, which has own data analysis capabilities – see § 3.2.9. Both the native DualSPHysics binaries and the ParaViewfiles are part of the datasets — see § 3.2.7 and § 3.2.8.

3.2 Creation of dataset

We give file sizes in bytes and decimal prefixes. So 1 MB is 1000 B and 1 GB is 1000 MB.

3.2.1 DualSPHysics source code

- The version used is DualSPHysics v5.0.164 of 21-11-2020; the corresponding commit can be downloaded from the GitHub repository at https://github.com/DualSPHysics/DualSPHysics/archive/ec025723b947f9d3af96ead3025393681b4fd1ed.
- The collection does contain a zipped file of this commit, downloaded on 15 Dec 2020. Importantly, the zipped archive contains the license terms of DualSPHysics.
- When unzipped, the archive file expands from 307 MB to a directory tree totalling 786 MB worth of documents. The abridged directory tree is show below; in the following we indicate the root element of this tree dsph-root.
- The source code is contained in the subdirectory dsph-root/src/source and has been edited minorly in two places, namely for
  1. the implementation of the viscous terms, as explained in § 2.2.1;
  2. the number precision in the output of the 'gauges' numerical device.

The changes with respect to the DualSPHysics release are listed in a 'patch document' attached to the data set – see § 3.3.2. The patch is human-readable list of the files and lines changed; this has been produced with the Git command git diff [original code] [modified code], and the command git apply can be used to reproduce the modified code from the original code, Two entry points for the working of these Git commands are the manual pages at https://git-scm.com/docs/git-diff and https://git-scm.com/docs/git-apply.

The abridged tree of the DualSPHysics suite distributed with the zip archive is:

```
DualSPHysics-ca069033f1721c6d885d63065024fd4ce44fc0e0
├── bin
│   ├── linux
│   └── windows
├── doc
│   └── ...
├── examples
│   └── ...
└── src
    ├── lib
    │   └── ...
    ├── source
    ├── VS
    └── src_mphase
```

3.2.2 Compilation

- The operating system of the machine that the source code has been compiled in is the Linux distribution Debian GNU/Linux 10 (codename "buster").
- The compilation tools were g++ 8.3.0 for C++ and the Software Development Kit 10.1, v10.1.168 for Cuda.
- The building process has been driven by GNU Make 4.2.1; a template makefile is distributed with DualSPHysics suite.

  The configuration file of Make provided by DualSPHysics has been edited to accommodate for the CUDA version and the compute capability of the GPU device; this edited version of the Make configuration file is not part of this dataset, for compilation is machine-specific.

3.2.3 Hardware

The GPU used for the computation is a Nvidia Quadro GP100. A white paper with technical specifications is available from https://images.nvidia.com/content/pdf/tesla/whitepaper/pascal-architecture-whitepaper.pdf, last accessed 27 March 2020. The nominal peak throughputs are 5.3 GFLOPS in double precision and 10.6 GFLOPS in single precision.

Information on the device is available in the simulation output – see § 3.2.7; however, we recommend not to take the compute times as a measure of performance blindly: the runs have been performed while the machine processed varying workloads, and no analysis to disentangle confounding factors had been carried out at the time of writing this document.

3.2.4 Simulation settings (XML file)

The user states the simulation settings for DualSPHysics in a text file in XML format. The XML file format is open and platform-independent.

- The user-defined XML settings file, Meringolo_Def.xml, is in the shared dataset.

This can be used to start a fresh simulation as well as restart a simulation from an intermediate output time. It is strongly recommended to inspect this file for familiarising oneself with limitations and possibilities of the data set, as for both the physical and the numerical modelling.

Note that in the simulations the particle-spacing parameter has been assigned as a command argument in the driver script, commented next in § 3.2.5, rather than as a statement within this XML file.

- The frequency of the output data is set in this file.
  - Fields. The particle states are saved to output every 0.10 time units. Since the simulated time is 20 units, the output rounds are 201 including reading out the initial conditions. Clearly, the number of output rounds, hence files, determines the size of the dataset.
    This output is part of the dataset – see § 3.3.2.
  - Gauges. The gauges are numerical devices implemented in DualSPHysics which record the time evolution of flow quantities at points in space. These simulations implemented gauges to record the water-surface height at three locations, and the velocity in three arrays of 21 numerical probes placed at the corners and middle of the tank.
    This output is not part of the dataset.
  - Time steps. The values of all variable time steps during a simulation have also been recorded.
    This output is not part of the dataset.

3.2.5 Driver script

The dataset contains the script file launching the pre/proper/post-processing executables, meringolo.sh

- This is written for a GNU Bash shell, so specifically for a Unix-like operating system. Nonetheless, the document is shared to show the arguments passed on to the utilities of the DualSPHysics suite.

  Of particular relevance is the fact that DualSPHysics runs with the -stable flag: this option acts on the memory management procedures and produces precisely the same results as a simulation is repeated (information courtesy of https://forums.dual.sphysics.org/discussion/1537/; last accessed 20/3/2021). This option is important for replaying the simulations and obtaining the same results.
- The driver script also determines a directory tree for and the names of the output files. The directory tree below is shared for illustration, so that the users can interpret the script and adapt it to their preferred work-flow. The root element, simulation-root, is a local path designated in the driver script as well.

  Note, though, that the collection and datasets do not permit using folders and § 3.3.2 describes the data organisation after flattening.

The abridged tree of the simulations was:

```
[simulation-root]
├─ data # see § 3.2.7
├─ gencase # see § 3.2.6
└─ particles # see § 3.2.8
```

3.2.6 Pre-processing output files

The user-defined XML settings file of § 3.2.5 is fed into the closed-source pre-processing utility GenCase v5.0.197 (18-07-2020).

- GenCase is distributed in the repository subdirectory dsph-root/bin/linux of § 3.2.1; refer to the subdirectory dsph-root/doc/help for the command-line arguments and options.

- The output of GenCase consists of ParaView-readable files for the domain design, a log file, and the input XML file for DualSPHysics.

  This *second* XML file, Meringolo.xml, is generated by GenCase upon appending some pre-processing information to the user-defined one of § 3.2.4; it can be used to start a fresh simulation too. This second XML file is part of the datasets.

  The driver script of § 3.2.5 gathered the output of GenCase in the subdirectory simulation-root/gencase of the output directory tree.

3.2.7 Proper-processing output files

DualSPHysics on roads produces two streams of output files:

1. A log file of the simulation called Run.out.

   It contains important information like the input parameters, the hardware configuration, the domain configuration, and the run-time progress.

   The driver script of § 3.2.5 saves this file in [simulation-root], the root of the output directory tree.

   We advise not to rely on the compute times reported in this file but in gross numbers – recall § 3.2.3.

   This file is part of the datasets.

2. Binary files, storing the states of the particles at the output frequency prescribed in the XML settings file, as mentioned in § 3.2.4.

   These binary files have format extensions bi4, obi4, ibi4. The resources of § 1.3 do not describe their file format specification; a developer can reverse-engineer these format specifications from the classes on input/output in the DualSPHysics open-source code – see for example https://forums.dual.sphysics.org/discussion/comment/2814, last accessed 23-2-2021.

   Binary files are important for restarting a simulation from the flow at a chosen output time ('hot start').

   The driver script of § 3.2.5 saved these files in the subdirectory simulation-root/data.

   These files are part of the datasets. Each dataset contains the pair PartInfo.ibi4 and Part_Head.ibi4, one PartOut_0000.obi4 file, 201 Part_????.bi4 files – the question marks indicate a frame number from 0000 to 0200.

   The typical size of a bi4 file for 82M particles is 3.6 GB.

3.2.8 Post-processing output files

The closed-source post-processing tool 'PartVTK v5.0.122 (09-07-2020)' has been used to extract from the binary files of § 3.2.7 information readable with ParaView.

- PartVTK is distributed in the subdirectory dsph-root/bin of § 3.2.1; refer to the subdirectory dsph-root/doc/help for the command-line arguments and options.
- With the settings given in § 3.2.5, PartVTK produces as many files in vtk format as there are bi4 files. These vtk files contain the states of the particles at the output time instants; they are the input for ParaView as outlined in § 3.2.9.

  These files are part of the datasets. They are named with the pattern WaterParticles_????.vtk where the question marks indicates a frame number from 0000 up to 0200. This means 201 vtk files per simulation and 804 files for the entire dataset of four simulations.

  The largest vtk file size in the dataset is 3.3 GB.

3.2.9 Visualisation

Visualisations of the flow field are also shared to help users appreciate the overall development of the dam break and identify the flow stages that are most interesting for them.

- These images have been rendered with ParaView, "an open-source multiple-platform application for interactive, scientific visualization" (https://en.wikipedia.org/wiki/ParaView). ParaView can also be used for the data processing of the vtk files.
- The temporal evolution of the density, particle identification number and velocity fields in the dataset simulations are shown as snapshots per output time in png format, 1604 files gathered in 12 archive files – see Figure 1.
- A playlist with the animations of the velocity and density fields at the four resolutions is available on YouTube at https://www.youtube.com/playlist?list=PLb_klyJ6w5QihDlztSqN0GRhT7awNnibe.

Recall that ParaView will draw each data point individually: a simulation with 82M particles entails a considerable visualisation task, both in terms of memory and compute power. Therefore, we have accelerated visualisation with a client/server arrangement of ParaView 5.7.1, using the Nvidia GPU used for computing as graphics server. To this end it has been necessary to enhance ParaView with the NVIDIA IndeX™ plug-in. Explaining this is beyond the scope of this document: see https://www.nvidia.com/en-us/data-center/index-paraview-plugin/, last accessed 23-3-2021, for an entry point.

3.3 Collection access

3.3.1 Compression

The datasets contain compressed files save a few exceptions.

Files have been compressed using the xz compression algorithm and file format. Compression with xz is lossless, is primarily based on the compression algorithm LZMA2, has open file-format specifications, and has been implemented in cross-platform software. See http://tukaani.org/xz/, last accessed 13 Nov 2020, for details on xz.

The namesake Linux utility used for compressing this dataset is xz (xz Utils) 5.2.4, using the library liblzma 5.2.4. This utility allows multithreading. The default compression level 6 is deemed to strike a compromise between the eventual decompression speed and the memory requirements in computers of varying level. Also, an integrity check has been done upon using the default CRC64 check type: a file checksum is included in the compressed file and the decompresser program verifies it. The GNU Bash command summarising the above action was `xz -T0 -6 -C crc64`.

The eventual file compression rate is around 2 for binary files and 3 for vtk files, depending on the native size – see Table 2. The compressed files have an xz extension appended to the original file name.

Table 2 summarises the spatial resolution, number of fluid particles, and the size of the datasets for each resolution[1]. This count does not include visualisation files

3.3.2 Collection organisation and dataset inventory

Generally, compressed files are bundled into archive files to simplify their download, and archiving utilities often take care of compression and decompression under the covers. However, Table 2 shows that the overall size of a dataset is considerable: downloading it in one or even few blocks may be prohibitively heavy and long for many users. Hence we have opted for a mixed archiving strategy.

The simulation results are distributed as a collection of five datasets, accessible from https://doi.org/10.4121/c.5353691.

The five datasets are:

[1] At the time of uploading this collection we observed that the archive of 4TU.ResearchData reported the size of the datasets in binary form (GiB) and its unit in decimal form (GB). The values of Table 2 are in GB, so they seem to be smaller than shown in the online repository. For context on the file-size units see https://physics.nist.gov/cuu/Units/binary.html.

Figure 1: Example of flow field images distributed with the collection: density (top), particle identification number (middle), velocity (bottom)

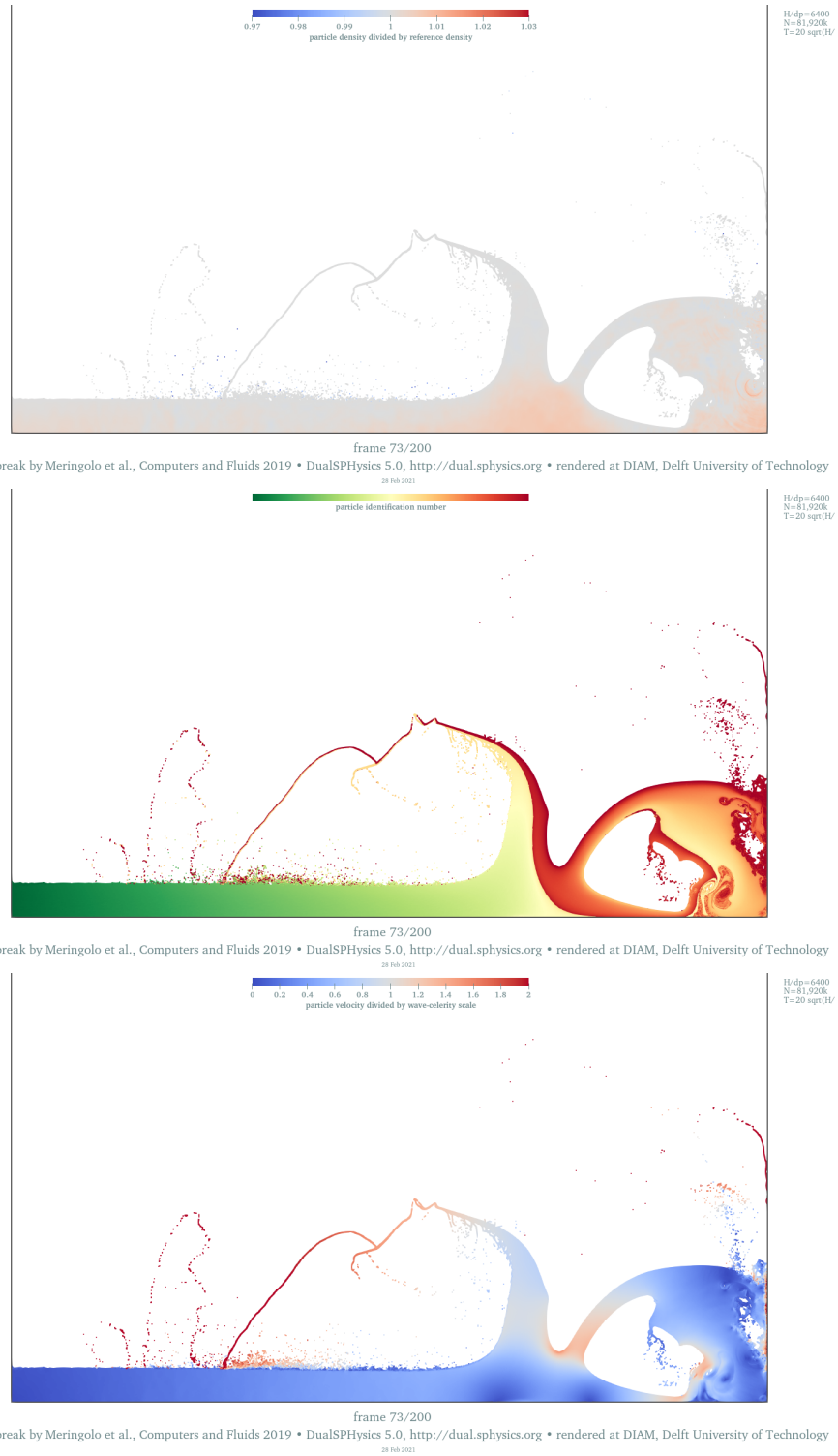

Table 2: Total sizes in GB before and after compression for the datasets for each simulation. Figures are rounded.

$H/\Delta p$	800	1600	3200	6400
Fluid particles (10^3)	1,280	5,120	20,480	81,920
Native	11	88	350	1,399
Compressed	9	36	140	549
Ratio	1.24	2.44	2.49	2.55

0. A 'main' dataset with referrer https://doi.org/10.4121/10.4121/14309240, containing
   (a) A human readable README file;
   (b) This one document, Commentary.pdf;
   (c) The images of the fields of velocity, density and particle identification number for each simulations: these frames are uncompressed and bundled in a 7z archive – see Figure 1 and § 3.3.5 on how to handle this format.
   (d) The compressed archive of DualSPHysics – recall § 3.2.1;
   (e) The 'patch file' Meringolo.patch containing the changes to the source code – recall § 3.2.1.
   (f) The input XML file Meringolo_Def.def – recall § 3.2.4.

   This dataset is meant as an entry point to guide the users as to where to find out in the ensuing datasets what is most useful for them. This also contains the material to reproduce the simulations.
1. The dataset for the simulation $H/\Delta p$=800, as in Tables 1 and 2, with referrer https://doi.org/10.4121/10.4121/14308883. It contains
   (a) A human readable README file;
   (b) The preprocessing output of § 3.2.6, Meringolo.xml;
   (c) The log file of § 3.2.7, Run.out;
   (d) The binary files of § 3.2.7, recognizable by the name pattern Part*;
   (e) The vtk files of § 3.2.8, recognizable by the name pattern WaterParticles*;
2. Ditto for the simulation $H/\Delta p$=1600 with referrer https://doi.org/10.4121/10.4121/14309081;
3. Ditto for the simulation $H/\Delta p$=3200 with referrer https://doi.org/10.4121/10.4121/14309171;
4. Ditto for the simulation $H/\Delta p$=6400[2] with referrer https://doi.org/10.4121/10.4121/14309234.

3.3.3 Licensing

The collection and its parts are distributed by the 4TU.ResearchData repository under a CC-BY 4.0 license: https://creativecommons.org/licenses/by/4.0/. The referrers to access the dataset are given in § 3.3.2.

For the licensing information of DualSPHysics, see § 1.3.1 and § 3.2.1.

[2]This dataset may be under an initial embargo period; the online repository shows clearly whether this is still the case and the time left before release. Thanks for bearing with us.

3.3.4 Downloading

The largest compressed files are 1.8GB: with connection speeds of 5, 10, 50 Mbps and excluding any other network traffic overhead, the estimated time to download this is 46, 23 and 5 minutes respectively. The speeds above are lower bounds for DSL, cable and fibre connections.

3.3.5 Decompression

Beside with the xz utility itself in Unix-like systems, the data-set files can be decompressed in several ways.

- Among open and free software, 7-zip works on a wide range of Windows operating systems and is described in more detail at https://www.7zip.org/ (last accessed 13 Nov 2020).
  It has also has been ported into Linux as the p7zip package (https://sourceforge.net/projects/p7zip/, last accessed 13 Nov 2020; this may already be available from the package repositories of Linux distributions, like Ubuntu. Conveniently, 7-zip exploits multithreading.
- Commercial utilities are generally able to handle xz formats. An example is WinZip, available for Windows and Mac operating systems: see https://www.winzip.com/win/en/7-zip-file.html, last accessed 13 Nov 2020.

The same utilities are able to extract the content of 7z archives.

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Prof Kees Vuik of the Delft Institute of Applied Mathematics at the Delft University of Technology has supervised the research as Principal Investigator and approved of the release of this document and collection of datasets.

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