

Novelties on DualSPHysics v5.4

J.M. DOMÍNGUEZ

7th DualSPHysics Workshop

March 19, 2024 – Bari, Italy



Implementation of **Smoothed Particle Hydronynamics** method for **complex fluid dynamics** using HPC techniques











It includes **two implementations**:

- **CPU**: C++ and OpenMP.
- **GPU**: CUDA.

Both options optimized for the best performance of each architecture.

SPH HIGHLY PARALLELISED







DUALSPHYSICS TEAM

Project Leaders:

Dr José M. Domínguez. Universidade de Vigo, Spain
Dr Georgios Fourtakas. The University of Manchester, UK
Prof. Alejandro J.C. Crespo. Universidade de Vigo, Spain
Prof. Benedict D. Rogers. The University of Manchester, UK
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Dr Corrado Altomare. Universitat Politècnica de Catalunya – BarcelonaTech, Spain
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Project Coordinators:

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- Dr Orlando García Feal. Universidade de Vigo, Spain
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- •Dr Aaron English. The University of Manchester, UK
- •Iván Martínez Estévez. Universidade de Vigo, Spain
- •Dr Francesco Ricci. New Jersey Institute of Technology, US





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Latest incorporations to DualSPHysics team





Bonaventura

lván



Aaron



Francesco

New Wiki under development

Wiki Coordinator: Dr Bonaventura Tagliafierro



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- Very easy to customize
- Easy to maintain
- Easy to port
- Markdown for input source files
- It can build either websites or doc files (limited for now)
- Support for html as well

0 127.0	0.1-8000/formulation/hundamentals/
DualSPHy	sics
Main Theory manual	External Libraries
Theory manual SPH Implementation	SPH Formulation
Boundary conditions	Smoothed Particle Hydrodynamics (SPH) is a Lagrangian meshless method. The techniqu discretises a continuum using a set of material points or particles. When used for the simulatio of fluid dynamics, the discretised Navier-Stokes equations are locally integrated at the location or each of these particles, according to the physical properties of surrounding particles. The set on neighbouring particles is determined by a distance based function, either circular (two dimensional) or spherical (three-dimensional), with an associated characteristic length of smoothing length often denoted as <i>h</i> . At each timestep new physical quantities are calculate for each particle, and they then move according to the updated values.
	Inote The conservation laws of continuum fluid dynamics are transformed from their partial differential form to a form suitable for particle based simulation using integral equations base on an interpolation function, which gives an estimate of values at a specific point.
	SPH Fundamentals
	Typically this interpolation or weighting function is referred to as the kernel function W and ca take different forms, with the most common being cubic or quintic. In all cases however, it is designed to represent a function $F(\mathbf{r})$ defined in \mathbf{r}' by the integral approximation:
	$\mathbf{F}(\mathbf{r}) = \int_{\Omega} F(\mathbf{r}') W(\mathbf{r} - \mathbf{r}') \mathrm{d}\mathbf{r}', \tag{1}$
	where $oldsymbol{r}$ is the pointee and $oldsymbol{r}'$ a ne
	The smoothing kernel must fulfil several properties [@Monaghan_1992], Lorem ipsum ¹ dolor s

The new wiki will contain

- Structured content
- Provide walkthrough for template cases
- Anyone can maintain their page (or section)



Formulation and capabilities

- SPH approaches:
 - Single phase free-surface flow solver
 - Multi-phase: liquid and gas
 - Multi-phase: non-Newtonian flows
- Kernel functions:
 - Cubic Spline (Monaghan and Lattanzio, 1985)
 - Quintic Wendland (Wendland, 1995)
- Density diffusion Term:
 - Molteni (Molteni and Colagrossi, 2009)
 - Fourtakas (Fourtakas et al., 2019)
- Viscosity:
 - Artificial (Monaghan, 1992)
 - Laminar (Lo & Shao, 2002)
 - Laminar + SPS turbulence model (Dalrymple & Rogers, 2006)
- Weakly compressible approach using Tait's equation of state (Batchelor, 1974)



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- Time integration scheme:
 - Verlet (Verlet, 1967)
 - Symplectic (Leimkhuler, 1996)
- Variable time step (Monaghan and Kos, 1999)
- Shifting algorithm (Lind et al., 2012)
- Boundary conditions:
 - Dynamic boundary conditions (Crespo et al., 2007)
 - Modified Dynamic boundary conditions (English et al., 2022)
 - No-Slip Modified Dynamic boundary conditions
- Periodic open boundaries (Gómez-Gesteira et al., 2012)
- Inflow-outflow boundary conditions (Tafuni et al., 2018)
- MESH-IN: Meshed inlet offline coupling (Ruffini et al., 2023)
- External forces (Longshaw and Rogers, 2015)



Formulation and capabilities

- Floating objects (Monaghan et al., 2003)
- Floating objects with mDBC support
- Full-integrated lagrangian formulation for flexible fluid-structure interaction (O'Connor et al., 2021)
- Coupling with Discrete Element Method (Canelas et al., 2016)
- Coupling with Project Chrono (Canelas et al., 2018; Martínez-Estévez et al., 2022)
- Coupling with MoorDyn (Domínguez et al., 2019)
- Piston- and flap-type long-crested second-order wave generation (Altomare et al., 2017)
- Solitary waves (Domínguez et al., 2019)
- Focused waves (Whittaker et al., 2017)
- Passive and Active Wave Absorption System (Altomare et al., 2017)
- Relaxation Zone method and coupling with wave propagation models (Altomare et al., 2018)
- Non-linear wave generation and absorption using open boundaries (Verbrugghe et al., 2019)
- Variable resolution based on domain decomposition (Ricci et al., 2024) BETA version



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COMPLETE TOOLKIT

- SPH solver
- Pre-processing tools
- Post-processing tools but also...
- Graphical User Interface
- Advanced visualisation

VisualSPHysics (Advanced visualisation tool)







DualSPHysics downloads

DUALSPHYSICS V1.2 (2011)

Downloads: 701 (65% Windows)

DUALSPHYSICS V2.0 (2012) Downloads: 6,472 (71% Windows)

DUALSPHYSICS V3.0 (2013-2015)

Downloads: 14,210 (73% Windows)

DUALSPHYSICS V4.0 (2016) Downloads: 13,150 (72% Windows)

DUALSPHYSICS V4.2 (May 2018) Downloads: 8,076

DUALSPHYSICS V4.4 (April 2019) Downloads: 21,921

DUALSPHYSICS V5.0 (July 2020) Downloads: 61,240

DUALSPHYSICS V5.2 (May 2023) Downloads: 8,163

DUALSPHYSICS - ALL VERSIONS

Downloads: 133,933 (70% Windows)

https://dual.sphysics.org/downloads/





SPH solver novelties:

- New variable resolution method with binaries and test cases
- New mDBC no-slip option
- Major improvement in inlet-outlet by using mesh data (MESH-IN)
- Full-integrated lagrangian formulation for flexible fluid-structure interaction.
- Laminar viscosity option without SPS turbulence model (better and faster results).
- Filter options for output particle data (space saving)
- Improved implementation for particle arrays on CPU and GPU
- New simpler and faster implementation for few floating bodies

Pre-processing novelties (*GenCase*):

- Supports new XML-VTK formats automatically (VTK,VTP, VTU)
- Supports new VTM file format with filters according to index or surface name
- External geometries with a huge number of triangles are supported
- Major performance and memory usage improvements on advanced drawing mode
- Significant performance improvements on automatic normal calculation
- Supports output files larger than 4 GB to generate hundreds of millions of particles



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Post-processing novelties:

- Much faster motion processing without data loading (*FloatingInfo & BoundaryVtk*)
- More floating body information on fluid forces and external forces (*FloatingInfo*)
- Higher frequency output on moving and floating bodies (*BoundaryVtk & FloatingInfo*)
- Moment force calculation on intrinsic and extrinsic axis (*ComputeForces*)
- Improved area selection for flow calculation by XML file with many options (*FlowTool*).



Variable resolution in DualSPHysics (Ricci et al., 2024)

- New method based on domain decomposition.
- Allows you to define higher resolution areas within the simulation.
- Very useful to reduce the number of particles and execution time.
- Enables detailed simulations previously impossible without a supercomputer.
- Includes several interesting capabilities... See Ricci's talk

v5.4 includes binaries and test cases





F. Ricci, R. Vacondio, A. Tafuni. 2024. Multiscale Smoothed Particle Hydrodynamics based on a domain-decomposition strategy. Comput. Methods Appl. Mech. Engrg. 418: 116500. doi:10.1016/j.cma.2023.116500



New mDBC no-slip option

- mDBC provides better results with lower resolution.
- mDBC setup is more complicated than DBC and present some issues.
- New formulation avoids particle jumping when kernel support is not complete.
- The new no-slip option is essential for the accurate modelling of some applications.
- More details in English's talk.







A. English, J.M. Domínguez, R. Vacondio, A.J.C. Crespo, P.K. Stansby, S.J. Lind, L. Chiapponi, M. Gómez-Gesteira. 2022. **Modified dynamic boundary conditions (mDBC) for general-purpose smoothed particle hydrodynamics (SPH):** application to tank sloshing, dam break and fish pass problems. Computational Particle Mechanics, 9(5): 911-925. <u>doi:10.1007/s40571-021-00403-3</u>

Inlet condition by using mesh data (MESH-IN)

Parabolic velocity Z Z Ζ • Full control of velocity (magnitude and direction) Inlet velocity throughout the inlet area. profiles in \rightarrow • Full control of elevation throughout the inlet area. v5.2 2.7 3 vel [m/s] 2 vel [m/s] 3 vel [m/s] CaseJet3dMeshVel1 CaseJet3dMeshVelDir Variable velocity according to position (x,y,z) Inlet in **v5.4** enables: Variable 3-components velocity according to postition elocity [m/s] Velocity-Y [m/s] • Full custom velocity profile **DualSPHysics DualSPHysics** • Full custom velocity direction. • Fixed or variable in time. Examples available at examples\inletmesh\01 Basic Particles (max): 20,390 Particles (max): 9,087 Physical time: 8 s

Uniform velocity

Linear velocity

Runtime(RTX 3080): 63 s



Physical time: 5 s

Runtime(RTX 3080): 30 s



Inlet condition by using mesh data (MESH-IN)

- Full control of velocity (magnitude and direction) throughout the inlet area.
- Full control of elevation throughout the inlet area.

Example available at examples\inletmesh\01_Basic





Inlet condition by using mesh data (MESH-IN)

- Full control of velocity (magnitude and direction) throughout the inlet area.
- Full control of elevation throughout the inlet area.
- The velocity and elevation values are defined in a grid by using a simple CSV file.
- The interpolated value from the data grid is applied at each inlet position.

	Velocity [m/s]

	А	В	С	D	E	F	G	н	I	J	К	L	М	N
1	Format	DataName	DataUnits	DataType	Data12	Npt1	Npt2	Npt3	PtRef.x [m]	PtRef.y	PtRef.z	Vec1.x [m]	Vec1.y	Vec1.z
2	JMeshTDatas	Vel	[m/s]	float3	true	4	1	53	0	0	0	0	1	0
3	time [s]	v(0:0).x	v(0:0).y	v(0:0).z	v(1:0).x	v(1:0).y	v(1:0).z	v(2:0).x	v(2:0).y	v(2:0).z	v(3:0).x	v(3:0).y	v(3:0).z	
4	0	4	0	0	4	0	0	4	0	0	4	0	0	
5	1	4	0	0	4	0	0	4	0	0	4	0	0	
6	1.5	2.828	2.828	0	2.828	2.828	0	2.828	2.828	0	2.828	2.828	0	
7	2	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	
8	3	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	
9	3.5	2.309	-2.309	2.309	2.309	-2.309	2.309	2.309	-2.309	2.309	2.309	-2.309	2.309	
10	4	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	
11	4.5	2.309	-2.309	2.309	2.309	-2.309	2.309	2.309	-2.309	2.309	2.309	-2.309	2.309	
12	5	4	0	0	4	0	0	4	0	0	4	0	0	
13	5.5	4	0	0	4	0	0	4	0	0	4	0	0	
14	6	2.309	-2.309	2.309	2.309	-2.309	2.309	2.309	2.309	2.309	2.309	2.309	2.309	
15														

CSV file with 3-component velocity in 12 grid points (available at examples\inletmesh\01_Basic)

Complex inlet changing velocity and height according to mesh data in two CSV files generated by Python scripts in a simple way (available at examples\inletmesh\02 Complex).



Inlet condition by using mesh data (MESH-IN)

- Inlet input data can be generated manually or obtained from a simulation.
- The gauge system in DualSPHysiscs allows to record the velocity field and the fluid elevation in an area.
- Mesh data is stored in CSV or binary format (.mbi4).

Full simulation field velocity and elevation (at red lines) generating a mesh data file (.mbi4) G. Ruffini, J.M. Domínguez, R. Briganti, C. Altomare, J. Stolle, A.J.C. Crespo, B. Ghiassi, S. Capasso, P. Girolamo. 2023. **MESH-IN: A MESHed INlet offline coupling method for 3-D extreme hydrodynamic events in DualSPHysics.** Ocean Engineering, 268: 113400. <u>doi:10.1016/j.oceaneng.2022.113400</u>

Example available at examples\inletmesh\03_Dambreak

CaseDamOpen2d_MakeData (saves flow data for MESH-IN simulations)

> CaseDamOpen2d_MeshIN_x120 (MESH-IN simulation at x=1.2m)

Reduced inlet simulation uses mesh data file to reproduce flow properties.



CaseDamOpen2d_MeshIN_x350 (MESH-IN simulation at x=3.5m)



Inlet condition by using mesh data (MESH-IN)

- 2-D or 3-D flow data can be obtained from a simplified simulation or from another source.
- Flow data can be used in:
 - New simulations with different setups.
 - The duration of the simulation can be reduced to the interval of interest.
 - The simulation domain can be reduced to the area of interest.
 - The resolution can be changed and
 2-D data can be used for 3-D simulations.



Solitary wave and floating body example available at examples\inletmesh\04_SolitaryWaveFt



OCEAN

G. Ruffini, J.M. Domínguez, R. Briganti, C. Altomare, J. Stolle, A.J.C. Crespo,
B. Ghiassi, S. Capasso, P. Girolamo. 2023. MESH-IN: A MESHed INlet offline
coupling method for 3-D extreme hydrodynamic events in DualSPHysics.
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 - The resolution can be changed and
 2-D data can be used for 3-D simulations.

3-D validation of MESH-IN

(Ruffini et al., 2023)



3-D validation of MESH-IN available at examples\inletmesh\05_DambreakGate



G. Ruffini, J.M. Domínguez, R. Briganti, C. Altomare, J. Stolle, A.J.C. Crespo, B. Ghiassi, S. Capasso, P. Girolamo. 2023. **MESH-IN: A MESHed INlet offline coupling method for 3-D extreme hydrodynamic events in DualSPHysics.** Ocean Engineering, 268: 113400. <u>doi:10.1016/j.oceaneng.2022.113400</u>



Improvements to Flexible FSI (FlexStruc)

- Full-integrated FlexStruc code in DualSPHysics v5.4.
- Improved error checking when specifying Poisson ratio for different constitutive models.
- Improved specification of zero, single or multiple mkclamp objects.

<flexstrucbody mkbound="2" mkclamp="0,1">



- Initial implementation with mDBC.
 - o Currently disabled by default as still in development
 - Can enable by uncommenting
 DISABLE_FLEXSTRUC_MDBC in *DualSphDef.h*
 - Use at own risk! (issues with particle penetration)









J. O'Connor, B.D. Rogers. 2021. A fluid-structure interaction model for free-surface flows and flexible structures using smoothed particle hydrodynamics on a GPU. Journal of Fluids and Structures, 104. doi:10.1016/j.jfluidstructs.2021.103312

Filter options for output particle data (space saving)

- Long and/or high resolution simulations generate an huge volume of output data (890 MB per 10M particles).
- It creates memory space problems and high post-processing run times.
- New option allows you to select the particles you need for post-processing and ignore the rest.
 - Several options for particle filtering (position, type, mk...)
 - Several options to combine different filters.
 - Filtering particles around moving or floating objects is also possible.

Full output data requires 5.8 GB and filtered output data 0.9 GB (**6.6 times less required space**)





Other SPH solver improvements:

- Laminar viscosity option without SPS turbulence model is enabled.
 - Laminar + SPS is too dissipative, so it is recommended only for high resolution and turbulent flows (as shown in Tagliafierro's talk).
 - \circ Laminar without SPH is faster (~30%).
- Significant improvements in the code (only for developers).
 - New implementation for particle arrays on CPU and GPU. Some tasks are now automatic and it is easier to add new properties.
 - New simpler and faster implementation for floating bodies among CPU and GPU.
 - Significant simplification in different parts (gauges, inlet/outlet, some formulations...).



Main novelties in v5.4 for pre-processing

New formats are supported

- Supports new XML-VTP format (PolyData datasheet, ASCII/binary/appended, base64/raw).
- Supports new XML-VTU format (UnstructuredGrid datasheet, ASCII/binary/appended, base64/raw) generated by clipping operations in ParaView.
- Different variants of VTK, VTU and VTP files are supported by the <DRAWFILEVTK> operation transparently to the user.

```
<drawfilevtk file="File.vtk"/>
<drawfilevtk file="File.vtp"/>
<drawfilevtk file="File.vtu"/>
```

- Supports new VTM format that groups multiple named surfaces into VTP and VTU files.
- VTM files are supported by the new XML operation <DRAWFILEVTM> for regular and advanced drawing mode, and includes multiple filtering options (by surface name or id) and assignment of different MK values.

```
<drawfilevtm file="Surfaces.vtm">
   <onlysurfaces index="0-3"/>
   <onlysurfaces index="4,8,6,9" mkbound="40-42,49"/>
   <onlysurfaces name="Solid1,Solid2"/>
   <onlysurfaces name="Solid3" mkbound="3"/>
   <onlysurfaces name="Solid4" mkbound="44"/>
</drawfilevtm>
```



Main novelties in v5.4 for pre-processing

GenCase improvements for huge complex geometries and large testcases

- New algorithms to support external geometries with a huge number of triangles (+30M).
- Split processing of large files to **avoid out-of-memory problems**.
- Major **performance improvements on advanced drawing mode** for large geometries (**speedup 100x**).
- Significant **performance improvements on automatic normal calculation** for large geometries (**speedup 5x**).
- Supports output files larger than 4 GB to generate hundreds of millions of particles.



Main novelties in v5.4 for post-processing

Performance improvements and new options

• Extrinsic and intrinsic moment force calculation (ComputeForces).





Main novelties in v5.4 for post-processing

Performance improvements and new options

- Extrinsic and intrinsic moment force calculation (ComputeForces).
- Improved area selection for flow calculation by XML file with many options (*FlowTool*).

```
<flowtool boxes>
   <box8pt name="Domain1">
                                                         <boxangle name="Domain4">
       <point x="0.0" y="0.2" z="0.0" />
                                                             <point x="1.2783" y="-0.7755" z="1.1631" />
       <point x="0.0" y="0.0" z="0.0" />
                                                             <angle x="3" y="-4" z="5" />
       <point x="0.1" y="0.0" z="0.0" />
                                                             <size x="0.0792" y="0.1135" z="0.0621" />
       <point x="0.1" y="0.2" z="0.0" />
                                                         </boxangle>
       <point x="0.0" y="0.2" z="0.4" />
                                                         <boxanglediv name1="Domain5a" name2="Domain5b">
       <point x="0.0" y="0.0" z="0.4" />
                                                             <divide axis="y" />
       <point x="0.1" y="0.0" z="0.4" />
                                                             <point x="1.2783" y="-0.7755" z="1.1631" />
       <point x="0.1" y="0.2" z="0.4" />
                                                             <angle x="3" y="-4" z="5" />
   </box8pt>
                                                             <size x="0.0792" y="0.1135" z="0.0621" />
   <box2pt name="Domain2">
                                                         </boxanglediv>
       <point x="1.2783" y="-0.7755" z="1.1631" />
                                                     </flowtool boxes>
       <point x="1.3" y="-0.7" z="1.2" />
   </box2pt>
   <boxsize name="Domain3">
       <point x="1.2783" y="-0.7755" z="1.1631" />
       <size x="0.0792" y="0.1135" z="0.0621" />
   </boxsize>
```



Main novelties in v5.4 for post-processing

Performance improvements and new options

- Moment force calculation on **intrinsic and extrinsic** axis (*ComputeForces*)
- **Improved area selection** for flow calculation by XML file with **many options** (*FlowTool*).
- **Much faster motion processing** since it is computed during the simulation and the reading of output data is avoided. (*FloatingInfo & BoundaryVtk*). Almost instantaneous execution!
- More floating body information on fluid forces and external forces (*FloatingInfo*).
 - External linear and angular forces (moorings and imposed forces).
 - Linear and angular forces from fluid.
 - Linear and angular acceleration before constrints.
- Higher frequency output on moving and floating bodies (*BoundaryVtk & FloatingInfo*).

<parameter key="TimeOutExtra" value="0.001" comment="Time out for extra output data on motion and floating information"</pre>



DualSPHysics performance



Testcase for performance test

Dam break flow impacting an obstacle (experiment by kleefsman et al., 2005). 2 physical seconds of simulation.





SPH HIGHLY PARALLELISED





