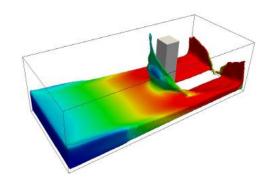
Structure of the DualSPHysics code















Dr José Manuel Domínguez Alonso jmdominguez@uvigo.es



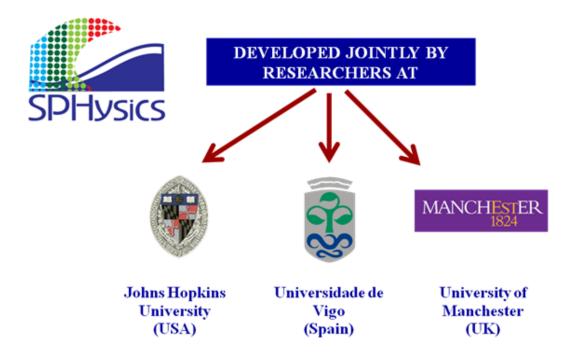
<u>Dr George Fourtakas</u> <u>Georgios.Fourtakas@postgrad.manchester.ac.uk</u>

Outline

- 1. DualSPHysics
 - 1.1. Origin of DualSPHysics
 - **1.2. Why GPUs?**
 - 1.3. DualSPHysics project
- 2. SPH formulation
- 3. Structure of code
 - 3.1. Stages of simulation
 - 3.2. Source files
 - 3.3. Object-Oriented Programming
 - 3.4. Execution diagram
- 4. Input & output files
- 5. Test cases online
- 6. Novelties in next release v4.0

1.1. Origin of DualSPHysics

The DualSPHysics code was created starting from SPHysics.



SPHysics is a numerical SPH solver developed for the study of free-surface problems.

It is a code written in Fortran90 with numerous options (different kernels, several boundary conditions, etc.), which has already demonstrated high accuracy in several validations with experimental results but it is too slow to apply to large domains.

1.1. Origin of DualSPHysics

The problem:

- SPH REQUIRES HIGH COMPUTATIONAL COST THAT INCREASES WHEN INCREASING THE NUMBER OF PARTICLES
- THE SIMULATION OF REAL PROBLEMS REQUIRES HIGH RESOLUTION WHICH IMPLIES SIMULATING MILLIONS OF PARTICLES

IT WAS NECESSARY TO INCREASE THE PERFORMACE OF THE CODE A FACTOR x100

Classic options:

- **OpenMP:** Distribute the workload among all CPU cores (\approx 4x)
- MPI: Combines the power of multiple machines connected via network (high cost).

New option:

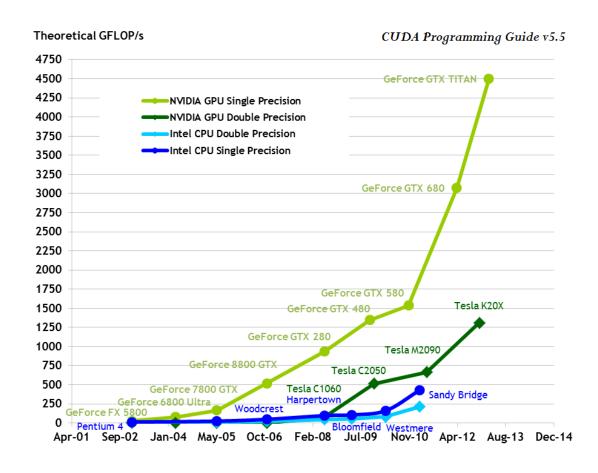
- **GPU:** Graphics cards with a high parallel computing power (cheap and accessible).

1.2. Why GPUs?

Graphics Processing Units (GPUs) are powerful parallel processors originally designed for graphics rendering.

Due to the development of the video games market and multimedia, their computing power has increased much faster than CPUs.

Now, GPUs can be used for general purpose applications, achieving speedups of x100 or more.



Advantages: GPUs provide the necessary computational power with very low cost and without expensive infrastructures.

Drawbacks: An efficient and full use of the capabilities of the GPUs is not straightforward.

1.2. Why GPUs?

GPUs are an accessible tool to accelerate SPH, many numerical methods in CFD and other computational methods



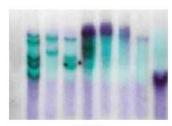
5X
Digital Content Creation
Adobe



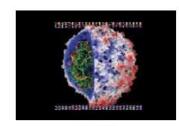
18X
Video Transcoding
Elemental Technologies



20X 3D Ultrasound TechniScan



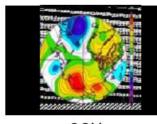
30X Gene Sequencing U of Maryland



36X
Molecular Dynamics
U of Illinois, Urbana-Champaign



50X
MATLAB Computing
AccelerEyes



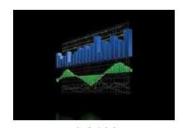
80X
Weather Modeling
Tokyo Institute of Technology



100X Astrophysics RIKEN



146X Medical Imaging U of Utah



149X
Financial Simulation
Oxford University

http://www.nvidia.com

1.2. Why GPUs?

TOP500 LIST – JUNE 2015

 R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
0	National Super Computer Center in Guangzhou China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	Titan - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	Mira - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945



First version in late 2009.

It includes **two implementations**:

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

- **GPU**: CUDA.

Both implementations optimized for best performance for each architecture.

Why two implementations?

This code can be used on machines with and without a GPU.

It allows us to make a fair and realistic comparison between CPU and GPU.

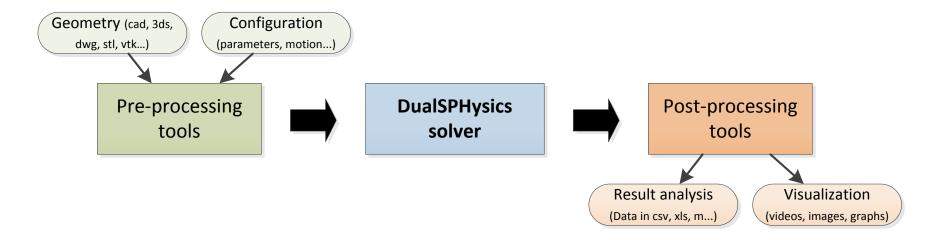
Some algorithms are complex and it is easy to make errors - difficult to detect. So they are implemented twice and we can compare results.

It is easier to understand the code in CUDA when you can see the same code in C++.

Drawback: It is necessary to implement and to maintain two different codes.



DSPH project includes:



Pre-processing tools:

- Converts geometry into particles.
- Provides configuration for simulation.

DualSPHysics solver:

- Runs simulation using SPH particles.
- Obtains data simulation for time intervals.

Post-processing tools:

- Calculates magnitudes using particle data.
- Generates images and videos starting form SPH particles.

DualSPHysics





Universida_{de}Vigo



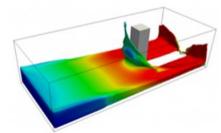
The University of Manchester

DualSPHysics is based on the Smoothed Particle Hydrodynamics model named SPHysics (www.sphysics.org).

The code is developed to study free-surface flow phenomena where Eulerian methods can be difficult to apply, such as waves or impact of dam-breaks on off-shore structures.

DualSPHysics is a set of C++ and CUDA codes to deal with real-life engineering problems.





Contact E-Mail: dualsphysics@gmail.com

www.dual.sphysics.org

DualSPHysics Users Workshop 2015, 8-9 September 2015, Manchester (United Kingdom)

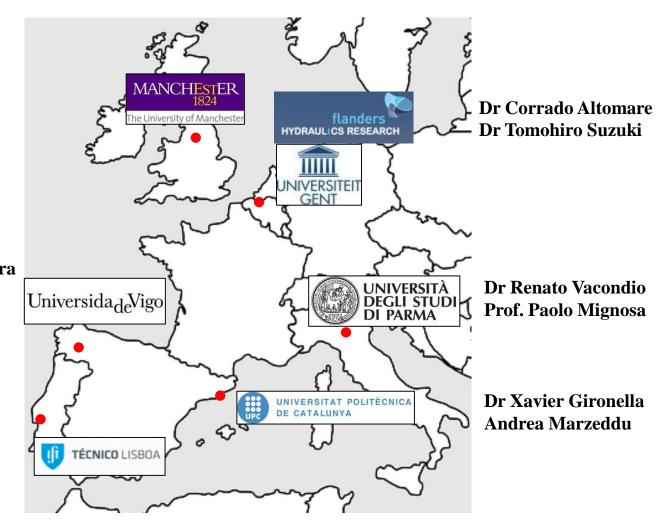


People working on DualSPHysics project:

Dr Benedict D. Rogers Dr Athanasios Mokos Dr Georgios Fourtakas Dr Stephen Longshaw Abouzied Nasar Prof. Peter Stansby

Prof. Moncho Gómez Gesteira Dr Alejandro J.C. Crespo Dr Jose M. Domínguez Dr Anxo Barreiro Orlando G. Feal Carlos Alvarado

Prof. Rui Ferreira Dr Ricardo Canelas



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2. SPH formulation

- 3. Structure of code
 - 3.1. Stages of simulation
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2. SPH formulation: DualSPHysics v3

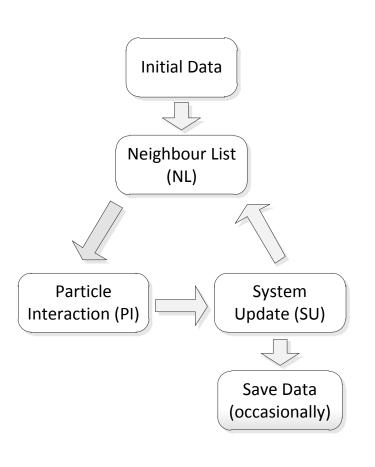
- Time integration scheme:
 - o Verlet [Verlet, 1967]
 - o Symplectic [Leimkhuler, 1996]
- Variable time step [Monaghan and Kos, 1999]
- Smoothing kernel functions:
 - o Cubic Spline kernel [Monagham and Lattanzio, 1985]
 - o Wendland kernel [Wendland, 1995]
- Weakly compressible approach using Tait's equation of state
- Density filter:
 - o Shepard filter [Panizzo, 2004]
 - o Delta-SPH formulation [Molteni and Colagrossi, 2009]
- Viscosity treatments:
 - o Artificial viscosity [Monaghan, 1992]
 - o Laminar viscosity + SPS turbulence model [Dalrymple and Rogers, 2006]
- Dynamic boundary conditions [Crespo et al., 2007]
- Floating objects [Monaghan et al., 2003]
- Periodic open boundaries

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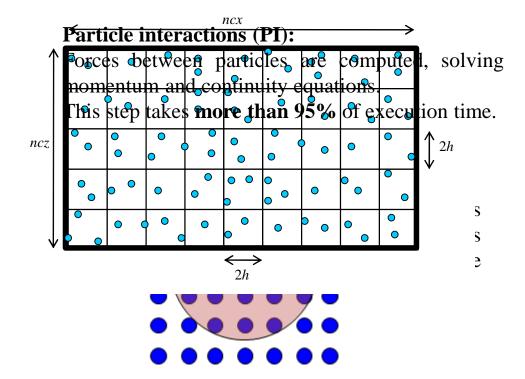
3.1. Stages of simulation

For the implementation of SPH, the code is organised in **3 main steps** that are repeated each time step till the end of the simulation.



Neighbour list (NL):

Particles are grouped in cells and reordered to optimise performance (memory access).



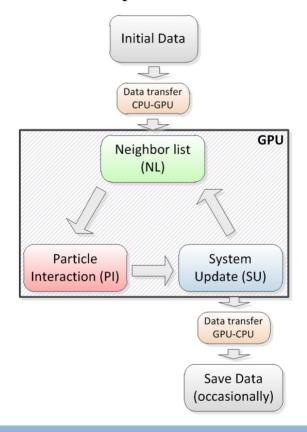
3.1. Stages of simulation

Full GPU implementation

- GPU is used in all steps (Neighbour List, Particle Interaction and System Update).
- All particle data is kept in GPU memory to avoid transfers CPU-GPU at each time step.

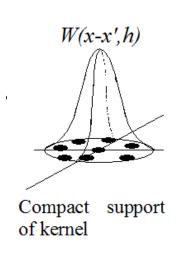
Particle Interaction (PI) System Update (SU) Save Data (occasionally)

GPU implementation

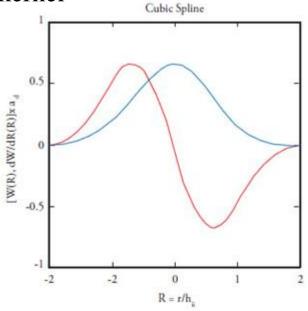


3.2. Source files

SPH smoothing kernel: This is the SPH smoothing kernel



$$W(R) = a_d \begin{cases} 1 - \frac{3}{2}R^2 + \frac{3}{4}R^3 & 0 \le R \le 1\\ \frac{1}{4}(2 - R)^3 & 1 \le R \le 2\\ 0 & R \ge 2 \end{cases}$$



NVIDIA CUDA kernel (C++ directives): This is not SPH related but refers to the CUDA function

```
__global__ void KerPreInteractionSimple(unsigned n,const double2 *posxy,const double *posz
,const float4 *velrhop,float4 *pospress,float cteb,float gamma)
{
    unsigned p=blockIdx.y*gridDim.x*blockDim.x + blockIdx.x*blockDim.x + threadIdx.x; //-Nº de la partícula
    if(p<n){|
        const float rrhop=velrhop[p].w;
        float press=cteb*(powf(rrhop*OVERRHOPCERO,gamma)-1.0f);
        double2 rpos=posxy[p];
        pospress[p]=make_float4(float(rpos.x),float(rpos.y),float(posz[p]),press);
    }
}</pre>
```

3.2. Source files

Common	SPH on CPU	SPH on GPU	
Functions (.h .cpp)	main.cpp		
JException (.h .cpp)	JCfgRun (.h .cpp)		
JFloatingData (.h .cpp)	JSph (.h .cpp)		
JLog2 (.h .cpp)	JPartsLoad (.h .cpp)		
JObject (.h .cpp)	JPartsOut (.h .cpp)		
JObjectGpu (.h .cpp)	JSphDtFixed (.h .cpp)		
JPartData (.h .cpp)	JSphVarAcc (.h .cpp)		
JPtxasInfo (.h .cpp)	Types.1	n	
JSpaceCtes (.h .cpp)		<	
JSpaceEParms (.h .cpp)	JSphCpu (.h .cpp)	JSphGpu (.h .cpp)	
JSpaceParts (.h .cpp)		JSphGpu_ker (.h .cu)	
JSpaceProperties (.h.cpp)	ISah Causinala (h. ann)	ISah Causingle (h. ean)	
JRangeFilter (.h .cpp) JTimer.h	JSphCpuSingle (.h .cpp)	JSphGpuSingle (.h .cpp)	
JTimerCuda.h	JSphTimersCpu.h	JSphTimersGpu.h	
JVarsAscii (.h .cpp)			
TypesDef.h	JCellDivCpu (.h .cpp)	JCellDivGpu (.h .cpp) JCellDivGpu_ker (.h .cu)	
JFormatFiles2.h JFormatFiles2.lib / libjformatfiles2.a	JCellDivCpuSingle (.h .cpp)	JCellDivGpuSingle (.h .cpp) JCellDivGpuSingle_ker (.h .cu)	
JSphMotion.h JSphMotion.lib / libjsphmotion.a	JPeriodicCpu (.h .cpp)	JPeriodicGpu (.h .cpp) JPeriodicGpu_ker (.h .cu)	
JXml.h JXml.lib / libjxml.a		JGpuArrays (.h .cpp)	



40 C++ headers

33 C++ codes

4 CUDA headers

4 CUDA codes

3.2. Source files: Common files

Common files used in several pre-processing a				
Functions (.h .cpp) JException (.h .cpp) JFloatingData (.h .cpp) JLog2 (.h .cpp) JObject (.h .cpp) JObjectGpu (.h .cpp)		post-processing applications. They provide basic functionalities. Users do not need to modify them. JSphDtFixed (.h .cpp)		
JPartData (.h .cpp) JPtxasInfo (.h .cpp) JSpaceCtes (.h .cpp)		JSphVarAcc (.h .cpp) Types.h		
JSpaceEParms (.h .cpp) JSpaceParts (.h .cpp) JSpaceProperties (.h .cpp)		Cpu (.h .cpp)	JSphGpu (.h .cpp) JSphGpu_ker (.h .cu)	
JRangeFilter (.h .cpp) JTimer.h JTimerCuda.h	-	CpuSingle (.h .cpp) TimersCpu.h	JSphGpuSingle (.h .cpp) JSphTimersGpu.h	
JVarsAscii (.h .cpp) TypesDef.h JFormatFiles2.h		DivCpu (.h .cpp)	JCellDivGpu (.h .cpp) JCellDivGpu_ker (.h .cu) JCellDivGpuSingle (.h .cpp)	
JFormatFiles2.lib / libjformatfiles2.a JSphMotion.h		DivCpuSingle (.h .cpp) odicCpu (.h .cpp)	JCellDivGpuSingle (.h .cpp) JCellDivGpuSingle_ker (.h .cu) JPeriodicGpu (.h .cpp)	
JSphMotion.lib / libjsphmotion.a JXml.h JXml.lib / libjxml.a			JGpuArrays (.h .cpp)	

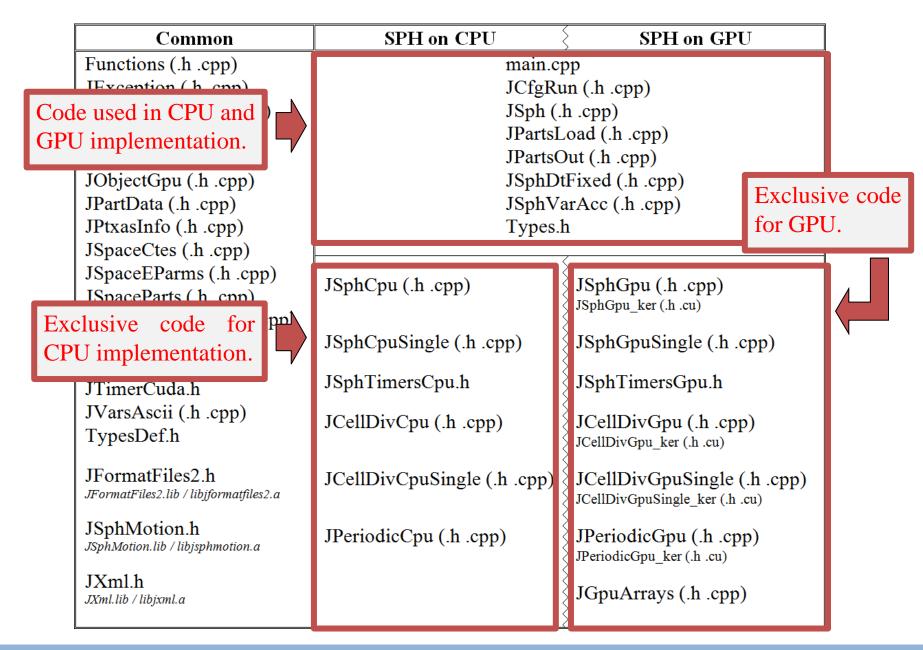
3.2. Source files: Precompiled files

Common	SPH on CPU	SPH on GPU		
Functions (.h .cpp)	main	ı.cpp		
JException (.h .cpp)	JCfgRun (.h .cpp)			
JFloatingData (.h .cpp)	JSph (.h .cpp)			
JLog2 (.h .cpp)	JPartsLoad (.h .cpp)			
JObject (.h .cpp)	JPartsOut (.h .cpp)			
JObjectGpu (.h .cpp)	JSphDtFixed (.h .cpp)			
JPartData (.h .cpp)	JSph	nVarAcc (.h .cpp)		
JPtxasInfo (.h .cpp)	Туре	es.h		
JSpaceCtes (.h .cpp)				
JSpaceEParms (.h .cpp)	JSphCpu (.h .cpp)	JSphGpu (.h .cpp)		
JSpaceParts (.h .cpp)	зорисра (.п.ерр)	JSphGpu_ker (.h .cu)		
JSpaceProperties (.h .cpp)		\		
JRangeFilter (.h .cpp)	JSphCpuSingle (.h .cpp)	SphGpuSingle (.h .cpp)		
JTimer.h	JSphTimersCpu.h	JSphTimersGpu.h		
JTimerCuda.h	Japin i intersepti.ii	Sopii i intersopu.ii		
JVarsAscii (.h .cpp)	JCellDivCov (h. con)	ICallDivCay (h. ann)		
TypesDef.h	Precompiled code in libraries.			
JFormatFiles2.h JFormatFiles2.lib / libjformatfiles2.a		sed in several pre-processing and		
ISph Matian h	post-processing applications. They provide basic functionalities.			
JSphMotion.h JSphMotion.lib / libjsphmotion.a				
JXml.h		JGpuArrays (.h .cpp)		
JXml.lib / libjxml.a		>		

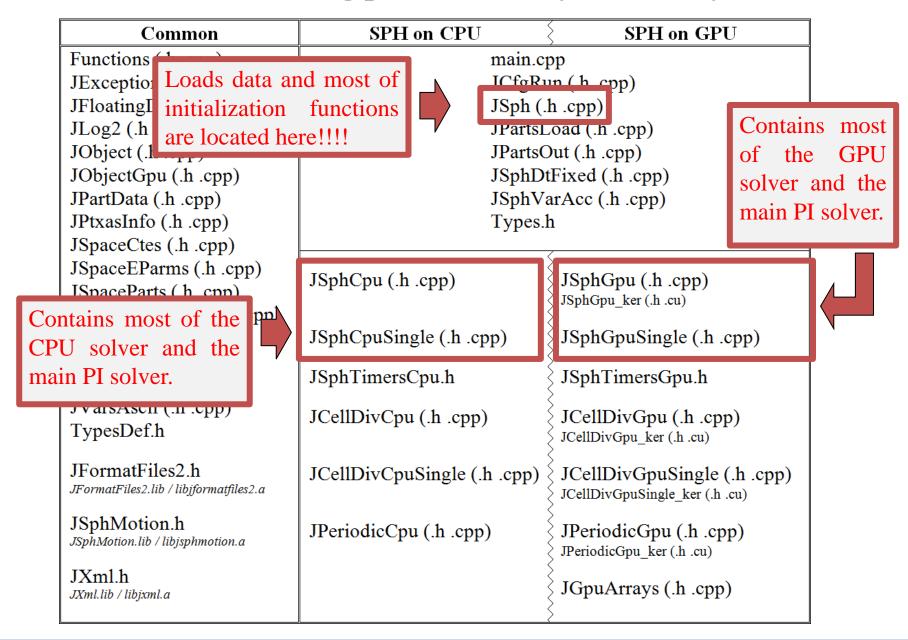
3.2. Source files: SPH files

Common	SPH on CPU	SPH on GPU
Exclusive source code files of DualSPHysics to implement the SPH model. JPartData (.h.cpp) JPtxasInfo (.h.cpp)	main.cpp JCfgRun (.h .cpp) JSph (.h .cpp) JPartsLoad (.h .cpp) JPartsOut (.h .cpp) JSphDtFixed (.h .cpp) JSphVarAcc (.h .cpp) Types.h	
JSpaceCtes (.h .cpp) JSpaceParms (.h .cpp) JSpaceParts (.h .cpp) JSpaceProperties (.h .cpp)	JSphCpu (.h .cpp)	JSphGpu (.h .cpp) JSphGpu_ker (.h .cu)
JRangeFilter (.h .cpp)	JSphCpuSingle (.h .cpp)	JSphGpuSingle (.h .cpp)
JTimer.h JTimerCuda.h	JSphTimersCpu.h	JSphTimersGpu.h
JVarsAscii (.h .cpp) TypesDef.h	JCellDivCpu (.h .cpp)	JCellDivGpu (.h .cpp) JCellDivGpu_ker (.h .cu)
JFormatFiles2.h JFormatFiles2.lib / libjformatfiles2.a	JCellDivCpuSingle (.h .cpp)	JCellDivGpuSingle (.h .cpp) JCellDivGpuSingle_ker (.h .cu)
JSphMotion.h JSphMotion.lib / libjsphmotion.a	JPeriodicCpu (.h .cpp)	JPeriodicGpu (.h .cpp) JPeriodicGpu_ker (.h .cu)
JXml.h JXml.lib / libjxml.a		JGpuArrays (.h .cpp)

3.2. Source files: SPH files



3.2. Source files: A starting point to modify DualSPHysics



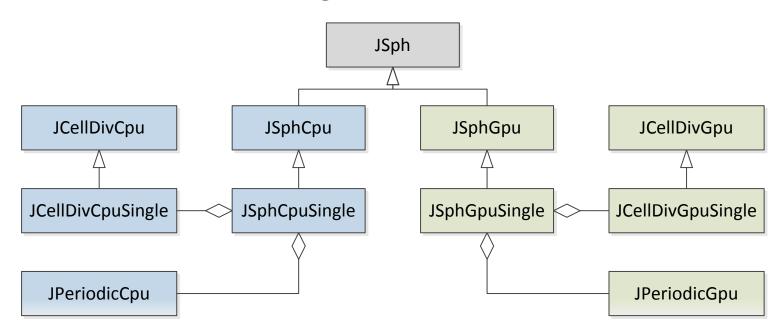
3.2. Source files

Common	SPH on CPU	SPH on GPU		
Functions (.h .cpp)	main.cpp			
JException (.h .cpp)	JCfgRun (.h .cpp)			
JFloatingData (.h .cpp)	JSph (.h .cpp)			
JLog2 (.h .cpp)	JPartsLoad (.h .cpp)			
JObject (.h .cpp)	JPartsC	JPartsOut (.h .cpp)		
JObjectGpu (.h .cpp)	JSphDt	tFixed (.h .cpp)		
JPartData (.h .cpp)		.h .cpp)		
JPtxasInfo (.h .cpp)				
JSpaceCtes (.h .cpp)	Complete description of each			
JSpaceEParms (.h .cpp)	file in DualSPHysics Guide. Gpu (.h .cpp)			
JSpaceParts (.h .cpp)	The in Dualst Hysics Guid	ou_ker (.h .cu)		
JSpaceProperties (.h .cp				
JRangeFilter (.h .cpp)	JSphCpuSingle (.h .cpp)	JSphGpuSingle (.h .cpp)		
JTimer.h	JSphTimersCpu.h	S JSphTimersGpu.h		
JTimerCuda.h	JSpii i intersepti.ii	Spiri intersopu.ii		
JVarsAscii (.h .cpp)	JCellDivCpu (.h .cpp)	JCellDivGpu (.h .cpp)		
TypesDef.h		JCellDivGpu_ker (.h .cu)		
JFormatFiles2.h	JCellDivCpuSingle (.h .cpp)	JCellDivGpuSingle (.h .cpp)		
JFormatFiles2.lib / libjformatfiles2.a		JCellDivGpuSingle_ker (.h .cu)		
JSphMotion.h	JPeriodicCpu (.h .cpp)	JPeriodicGpu (.h .cpp) ЉeriodicGpu_ker (.h .cu)		
JSphMotion.lib / libjsphmotion.a				
JXml.h		JGpuArrays (.h .cpp)		
JXml.lib / libjxml.a		(iii .opp)		

3.3. Object-Oriented Programming

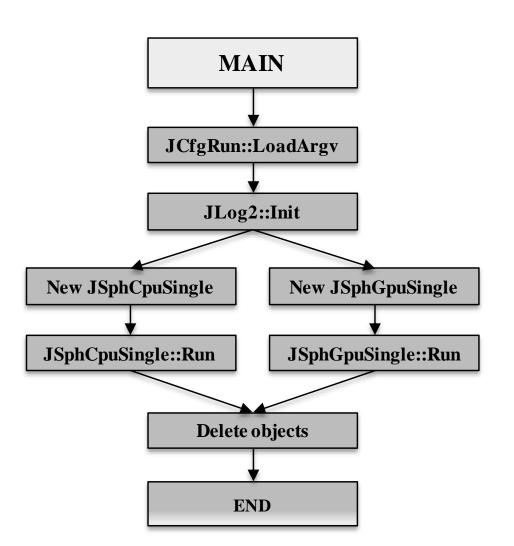
DualSPHysics uses Object-Oriented Programming (OOP) to organise the code. However, the particles data is stored in arrays to improve the performance. Class name matches the file name.

Diagram main classes



3.4. Execution diagram: Main

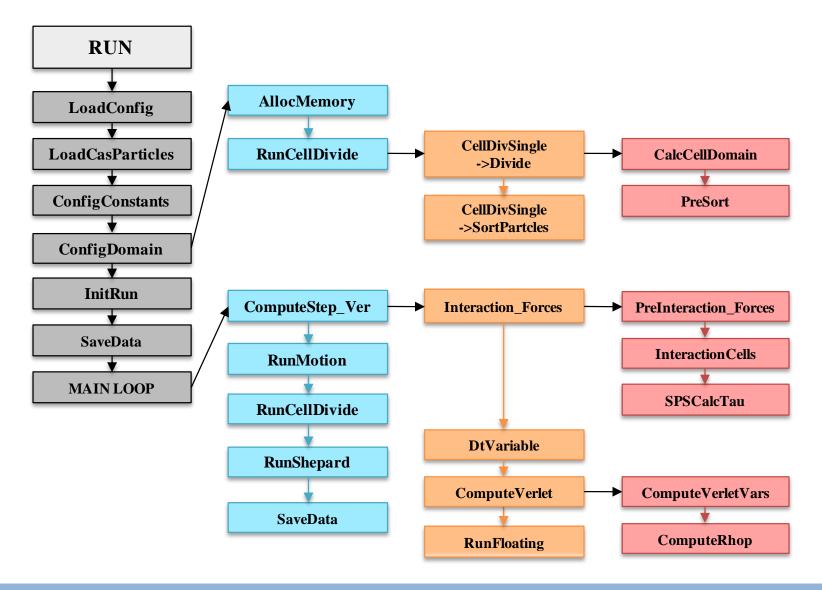
The execution of DualSPHysics begins in function main() in file main.cpp



- Loads parameters from command line
- Initializes log file
- Creates object for execution on Cpu or Gpu
- Executes method Run() of SPH object to start simulation
- Deletes objects and frees memory

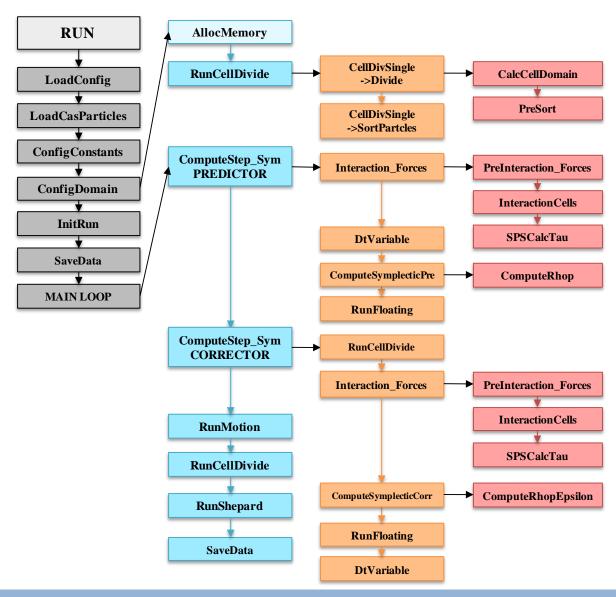
3.4. Execution diagram: CPU

CPU execution using **Verlet** algorithm (JSphCpuSingle::Run() in JSphCpuSingle.cpp).



3.4. Execution diagram: CPU

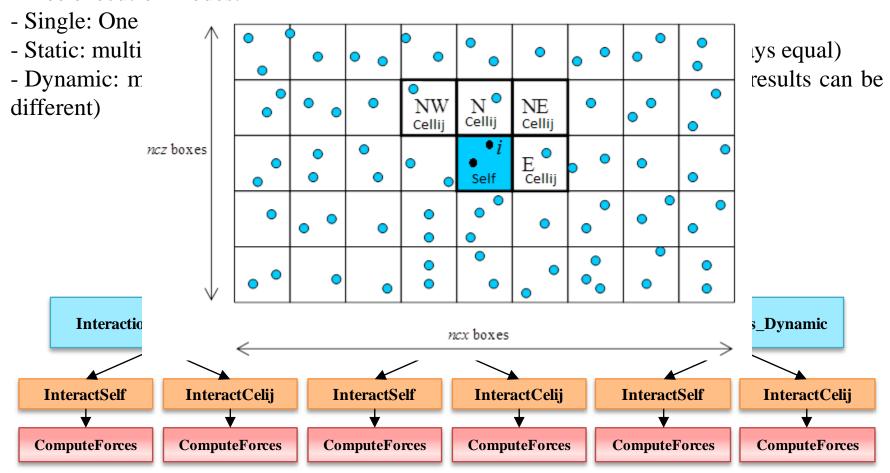
CPU execution using **Symplectic** algorithm (JSphCpuSingle::Run() in JSphCpuSingle.cpp).



3.4. Execution diagram: CPU interaction

InteractionCells performs the interaction between particles to calculate forces or Shepard correction.

Three execution modes:

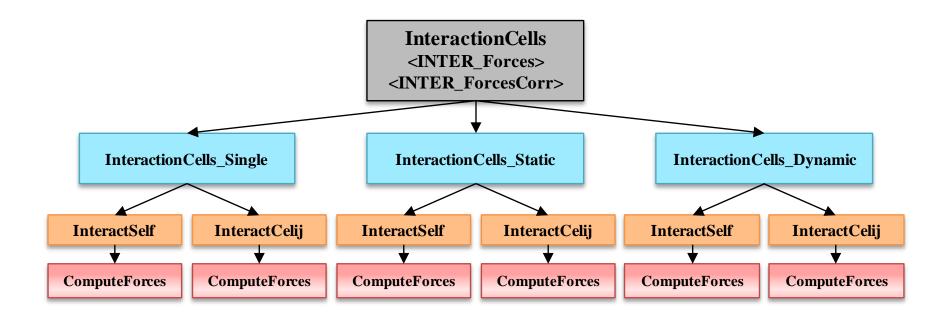


3.4. Execution diagram: CPU interaction

The interaction between particles is performed by cells:

- Interaction between particles in the same cell (InteractSelf)
- Interaction between particles from one cell with particles from another cell (InteractCelij)

The method **ComputeForces** performs the interaction between two particles **to calculate forces**.



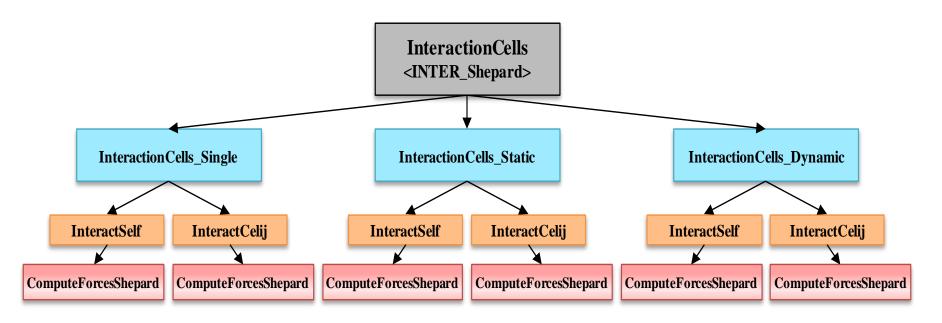
3.4. Execution diagram: CPU interaction

The interaction between particles is performed by cells:

- Interaction between particles in the same cell (InteractSelf)
- Interaction between particles from one cell with particles from another cell (InteractCelij)

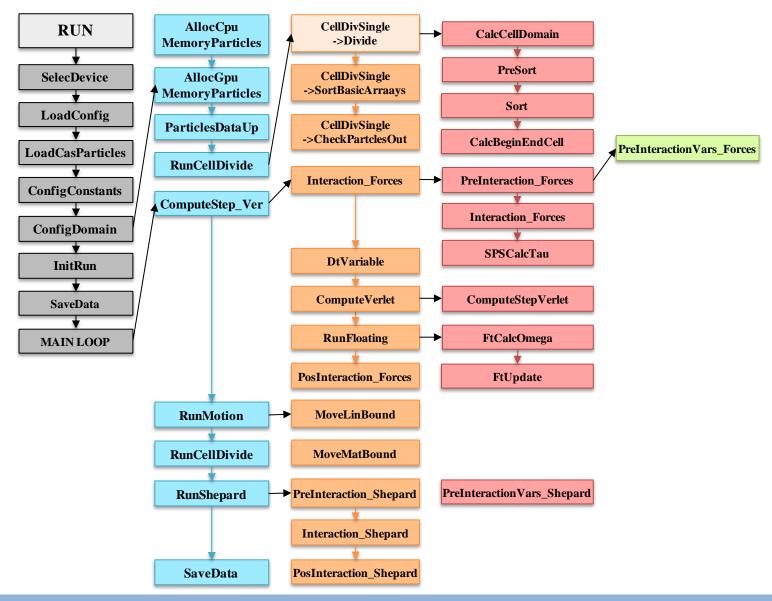
The method ComputeForces performs the interaction between two particles to calculate forces.

The method **ComputeForcesShepard** performs the interaction between two particles **to** calculate **Shepard correction**.



3.4. Execution diagram: GPU

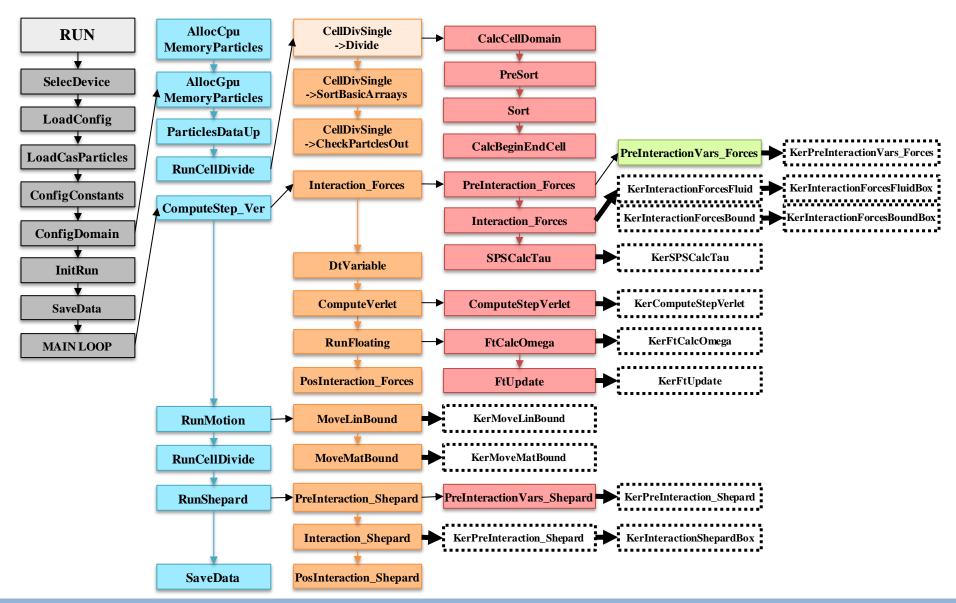
GPU execution using **Verlet** algorithm (similar to CPU execution).



DualSPHysics Users Workshop 2015, 8-9 September 2015, Manchester (United Kingdom)

3.4. Execution diagram: GPU with CUDA kernels

The C++ methods call CUDA kernels to execute each task on GPU.



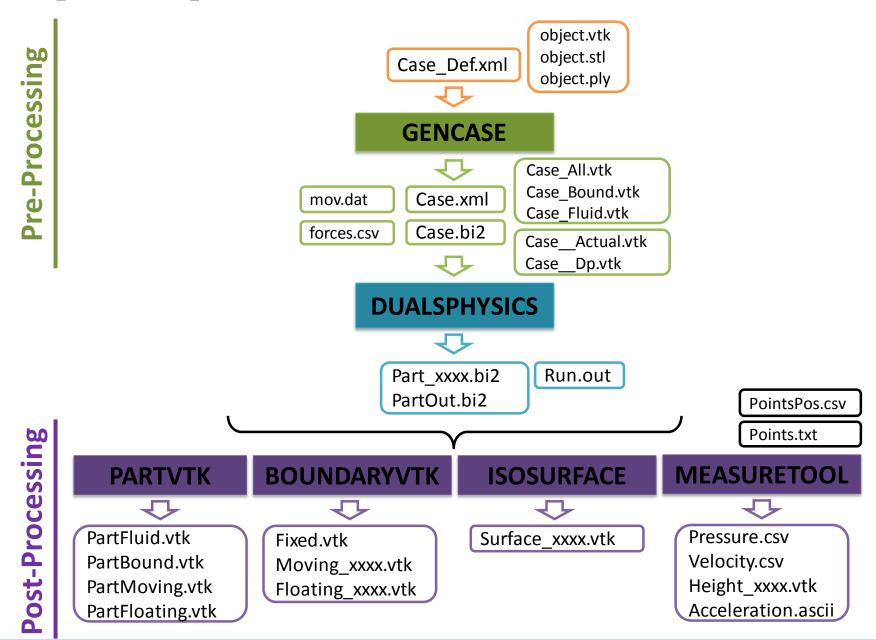
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 - 3.1. Steps of simulation
 - 3.2. Source files
 - 3.3. Object-Oriented Programming
 - 3.4. Execution diagram

4. Input & output files

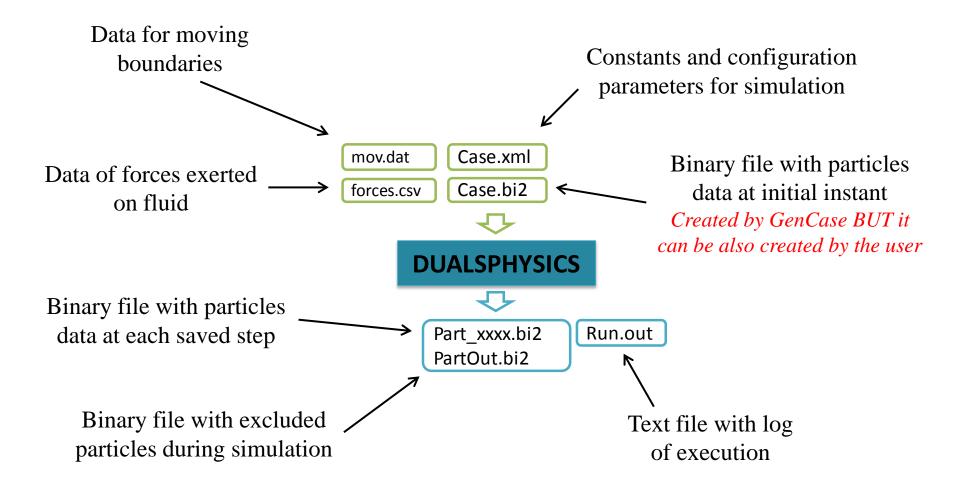
- 5. Test cases online
- 6. Novelties in next release v4.0

4. Input & output files



DualSPHysics Users Workshop 2015, 8-9 September 2015, Manchester (United Kingdom)

4. Input & output files



4. Input & output files: Format files

Case.xml

XML File

- The eXtensible Markup Language is textual data format compatible with any hardware and software.
- Information is structured and organised by using labels.
- They can be edited easily using any text editor.

Case.bi2

Part_xxxx.bi2
PartOut.bi2

BINARY File

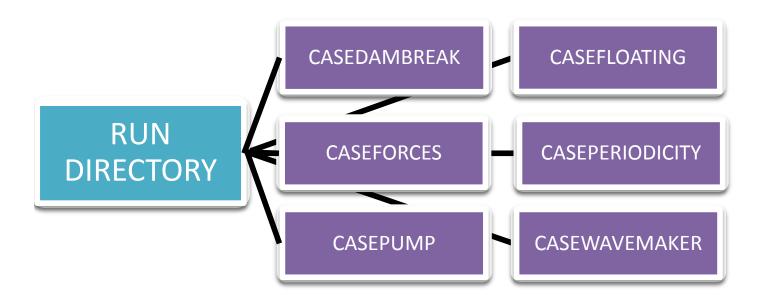
- Binary format consumes at least six times less memory than text (ASCII) format.
- Reading or writing is several times faster using a binary format.
- A special code is required to read the data (JPartData.cpp/.h).

Outline

- 1. DualSPHysics
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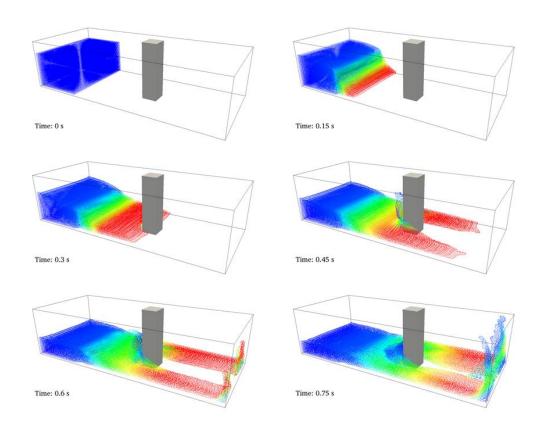
Some demonstration cases are included in the DualSPHysics package to show:

- Fixed boundaries
- Moving boundaries & piston wavemaker
- Complex geometries imported from external files
- Periodic boundaries
- Floating objects



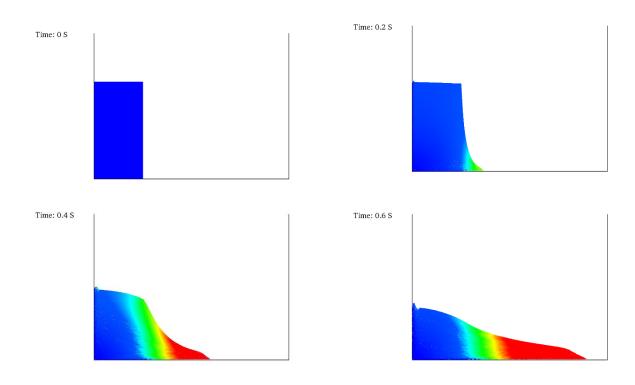
CASEDAMBREAK:

The first test case consists of a 3-D dam break impacting on a structure inside a tank. There are no moving boundaries in this simulation.



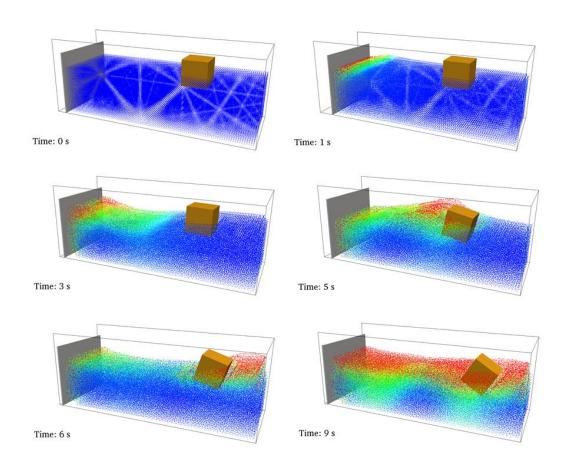
CASEDAMBREAK:

A validation in 2-D is also included for a different dam break where the experimental data of Koshizuka and Oka, 1996 can be numerically reproduced



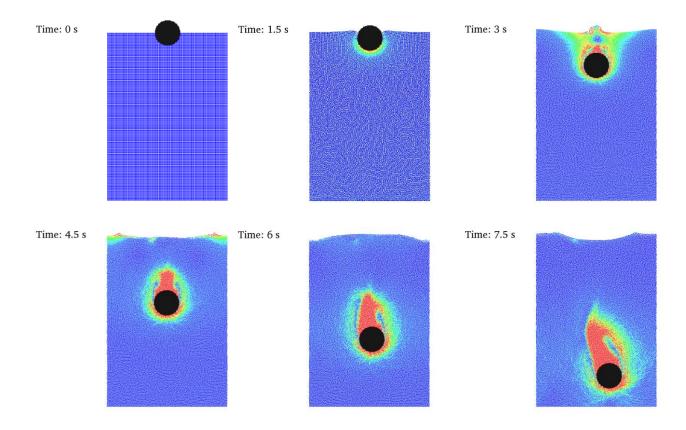
CASEFLOATING:

A floating box moves due to waves generated with a piston



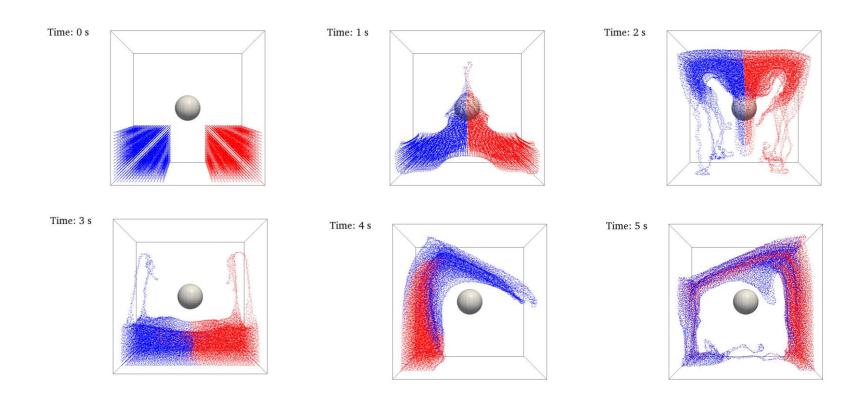
CASEFLOATING:

The 2-D case of fluid-structure interaction is also provided. The text files included in the folder contains the experimental displacement and velocity of experiments in Fekken, 2004 and Moyo and Greenhow, 2000.



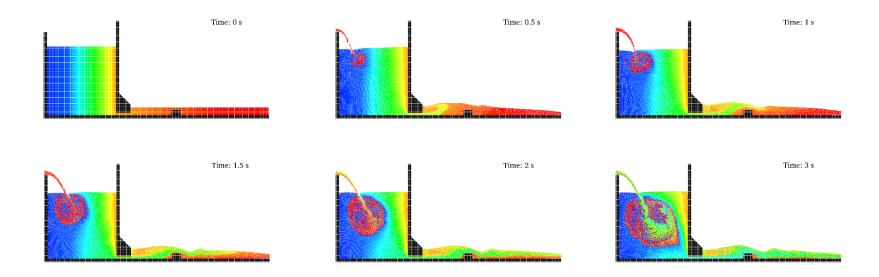
CASEFORCES:

This is a new test case where external forces are applied to the system. The external forces can be loaded from the files varAccInputFile_0.csv and varAccInputFile_1.csv.



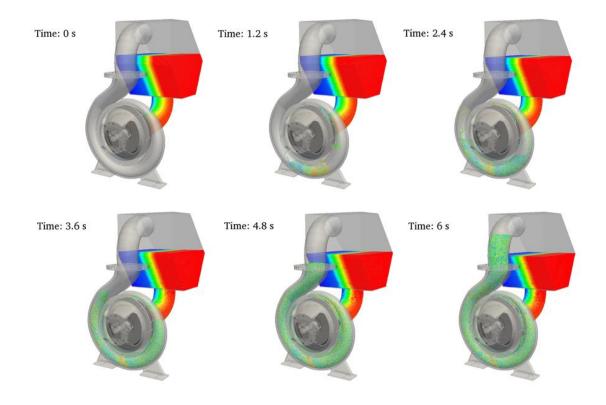
CASEPERIODICITY:

This test case is an example of periodicity applied to 2D case where particles that leave the domain through the right side are introduced through the left side with the same properties but where the vertical position can change (with an increase of +0.3 in Z-position).



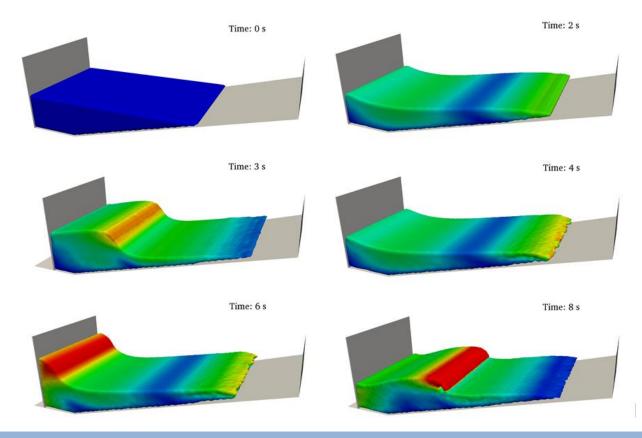
CASEPUMP:

This 3D test case loads an external model of a pump with a fixed (pump_fixed.vtk) and a moving part (pump_moving.vtk). The moving part describes a rotational movement and the reservoir is pre-filled with fluid particles.



CASEWAVEMAKER:

CaseWavemaker simulates several waves breaking on a numerical beach. A wavemaker is performed to generate and propagate the waves. In this test case, a sinusoidal movement is imposed to the boundary particles of the wavemaker



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6. Novelties in next release v4.0

- 1) New CPU structure that mimics the GPU threads.
- 2) New GPU structure with the code better organized Easy to follow and modify by the user.
- 3) Double precision implementation; several options.
- 4) Floating bodies formulation is corrected.
- 5) Delta-SPH of Molteni&Colagrossi plus others (to be confirmed)
- 6) Shifting algorithm
- 7) New wave generation (regular, irregular by given H/Hs, T/Tp and depth)
- 8) Source code of DEM (Discrete Element Method)
- 9) Multi-phase liquid-sediment solver release v3.2 (September 2015)

Check the website for news / releases / info