Structure of the DualSPHysics code

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Outline

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   1.1. Origin of DualSPHysics
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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 PERFORMANCE OF THE CODE A FACTOR x100

Classic options:

- **OpenMP**: Distribute the workload among all CPU cores (≈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.

http://www.nvidia.com
1.2. Why GPUs?

http://www.top500.org/list/2015/06/

**TOP500 LIST – JUNE 2015**

*R*\(_{\text{max}}\) and *R*\(_{\text{peak}}\) values are in TFlops. For more details about other fields, check the TOP500 description.

<table>
<thead>
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<th><em>R</em>(_{\text{peak}}) (TFlop/s)</th>
<th>Power (kW)</th>
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1.3. DualSPHysics project

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.
1.3. DualSPHysics project

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.

Geometry (cad, 3ds, dwg, stl, vtk...)
Configuration (parameters, motion...)

Result analysis (Data in csv, xls, m...)
Visualization (videos, images, graphs)
1.3. DualSPHysics project

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
1.3. DualSPHysics project

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

Dr Corrado Altomare
Dr Tomohiro Suzuki

Dr Renato Vacondio
Prof. Paolo Mignosa

Dr Xavier Gironella
Andrea Marzeddu

DualSPHysics Users Workshop 2015, 8-9 September 2015, Manchester (United Kingdom)
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4. Input & output files

5. Test cases online

6. Novelties in next release v4.0
2. SPH formulation: DualSPHysics v3

• Time integration scheme:
  - Verlet [Verlet, 1967]
  - Symplectic [Leimkhuler, 1996]
• Variable time step [Monaghan and Kos, 1999]
• Smoothing kernel functions:
  - Cubic Spline kernel [Monaghham and Lattanzio, 1985]
  - Wendland kernel [Wendland, 1995]
• Weakly compressible approach using Tait’s equation of state
• Density filter:
  - Shepard filter [Panizzo, 2004]
  - Delta-SPH formulation [Molteni and Colagrossi, 2009]
• Viscosity treatments:
  - Artificial viscosity [Monaghnan, 1992]
  - 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.

**Initial Data**

**Neighbour List (NL):**
Particles are grouped in cells and reordered to optimise performance (memory access).

**Particle interactions (PI):**
Forces between particles are computed, solving momentum and continuity equations. This step takes more than 95% of execution time.

**System Update (SU):**

**Save Data (occasionally):**
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.
3.2. Source files

**SPH smoothing kernel:** This is the SPH smoothing kernel

\[
W(x-x', h) = \begin{cases} 
1 - \frac{3}{2} R^2 + \frac{3}{4} R^3 & 0 \leq R \leq 1 \\
\frac{1}{4} (2 - R)^3 & 1 \leq R \leq 2 \\
0 & R \geq 2 
\end{cases}
\]

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

```c++
__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;  // N° de la particula
    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);
    }
}
```
3.2. Source files

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<tr>
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Files:
- 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 and post-processing applications. They provide basic functionalities. Users do not need to modify them.

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| JSphVarAcc (.h .cpp) |
| Types.h |

| JSphCpu (.h .cpp) |
| JSphGpu (.h .cpp) |
| JSphGpu_ker (.h .cu) |

| JSphCpuSingle (.h .cpp) |
| JSphGpuSingle (.h .cpp) |

| JSphTimersCpu.h |
| JSphTimersGpu.h |

| JCellDivCpu (.h .cpp) |
| JCellDivGpu (.h .cpp) |
| JCellDivGpu_ker (.h .cu) |

| JCellDivCpuSingle (.h .cpp) |
| JCellDivGpuSingle (.h .cpp) |
| JCellDivGpuSingle_ker (.h .cu) |

| JPeriodicCpu (.h .cpp) |
| JPeriodicGpu (.h .cpp) |
| JPeriodicGpu_ker (.h .cu) |

| JGpuArrays (.h .cpp) |
### 3.2. Source files: Precompiled files

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Precompiled code in libraries.

Common files used in several pre-processing and post-processing applications.

They provide basic functionalities.
## 3.2. Source files: SPH files

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Exclusive source code files of DualSPHysics to implement the SPH model.
### 3.2. Source files: SPH files

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</tbody>
</table>

- **Code used in CPU and GPU implementation.**
- **Exclusive code for GPU.**
- **Exclusive code for CPU implementation.**
3.2. Source files: A starting point to modify DualSPHysics

<table>
<thead>
<tr>
<th>Common</th>
<th>SPH on CPU</th>
<th>SPH on GPU</th>
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<tr>
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</table>

Loads data and most of initialization functions are located here!!!!

Contains most of the CPU solver and the main PI solver.

Contains most of the GPU solver and the main PI solver.
### 3.2. Source files

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Complete description of each file in DualSPHysics Guide.
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

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

Diagram showing the execution flow of CPU operations, including:
- RUN
  - AllocMemory
  - RunCellDivide
    - CellDivSingle -> Divide
    - PreSort
      - CalcCellDomain
      - PreInteraction_Forces
    - InteractionCells
    - SPSCalcTau
    - ComputeRhop
  - Interaction_Forces
    - DtVariable
    - ComputeSymplecticPre
    - ComputeRhopEpsilon
    - RunCellDivide
    - PreInteraction_Forces
    - InteractionCells
    - SPSCalcTau
    - ComputeRhopEpsilon
  - ComputeSymplecticCorr
    - Interaction_Forces
    - DtVariable
    - RunFloating
3.4. Execution diagram: CPU interaction

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

Three execution modes:
- Single: One
- Static: multi
- Dynamic: n different

![Diagram of CPU interaction]

- **InteractSelf**
  - **ComputeForces**
- **InteractCelij**
  - **ComputeForces**
- **InteractSelf**
  - **ComputeForces**
- **InteractCelij**
  - **ComputeForces**
- **InteractSelf**
  - **ComputeForces**
- **InteractCelij**
  - **ComputeForces**

(ncz boxes)
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).

![Execution Diagram](image-url)
3.4. Execution diagram: GPU with CUDA kernels

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

Pre-Processing

GENCASE
- Case_Def.xml
- object.vtk
- object.stl
- object.ply

DUALSPHYSICS
- Run.out
- Part_xxxx.bi2
- PartOut.bi2
- Case_All.vtk
- Case_Bound.vtk
- Case_Fluid.vtk
- Case__Actual.vtk
- Case__Dp.vtk
- mov.dat
- Case.xml
- Case.bi2
- forces.csv

Post-Processing

PARTVTK
- PartFluid.vtk
- PartBound.vtk
- PartMoving.vtk
- PartFloating.vtk

BOUNDARYVTK
- Fixed.vtk
- Moving_xxxx.vtk
- Floating_xxxx.vtk

ISOSURFACE
- Surface_xxxx.vtk

MEASURETOOL
- Pressure.csv
- Velocity.csv
- Height_xxxx.vtk
- Acceleration.ascii
- PointsPos.csv
- Points.txt
4. Input & output files

- Data for moving boundaries
  - mov.dat
  - forces.csv

- Constants and configuration parameters for simulation
  - Case.xml
  - Case.bi2

- Binary file with particles data at initial instant
  - Part_xxxx.bi2
  - PartOut.bi2

- Binary file with particles data at each saved step
  - Run.out

- Binary file with excluded particles during simulation

- Text file with log of execution
  - forces.csv

*Created by GenCase BUT it can be also created by the user*
4. Input & output files: Format files

**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.

**BINAR Y 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).
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   3.4. Execution diagram

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

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.
5. Test cases online

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.
5. Test cases online

CASEFLOATING:

A floating box moves due to waves generated with a piston
5. Test cases online

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.
5. Test cases online

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.
5. Test cases online

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).
5. Test cases online

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.
5. Test cases online

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.
Outline

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   3.4. Execution diagram

4. Input & output files

5. Test cases online

6. Novelties in next release v4.0
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