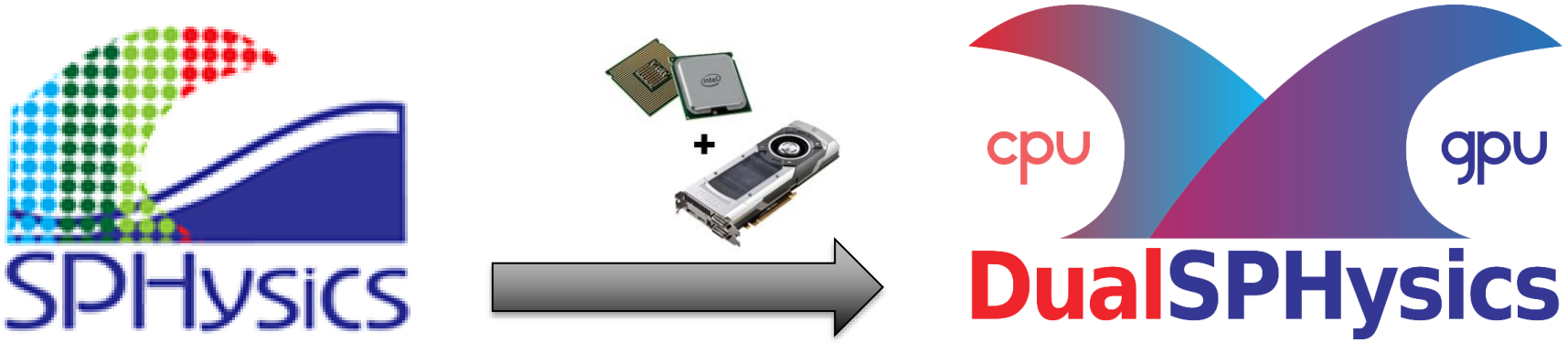
DualSPHysics: Multi-GPU implementation

José M. Domínguez, Iván Martínez-Estévez, Alejandro J.C. Crespo,
Moncho Gómez-Gesteira

DualSPHysics origin



- First release in 2007
- Written in Fortran90
- Many formulations
- Validated with high accuracy
- Too slow for large simulations

- First release in 2011
- CPU multicore and GPU implementation
- Written in C++, OpenMP and CUDA
- **Optimised for large simulations**

DualSPHysics solver

SPH HIGHLY PARALLELISED

GPU

NVIDIA CUDA

CPU

C++

GPU CPU

x100

OPEN SOURCE MODEL WITH OPEN LICENSE

LGPL Free Software

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```

DualSPHysics project

DEVELOPERS:

- Universidade de Vigo, Spain
- The University of Manchester, UK
- Università degli studi di Parma, Italy
- Universitat Politècnica de Catalunya, Spain
- New Jersey Institute of Technology, USA
- Imperial College London, UK

CONTRIBUTORS:

- Instituto Superior Tecnico, Lisbon, Portugal
- Science & Technology Facilities Council, UK
- Flanders Hydraulics Research, Belgium
- Universidad de Guanajuato, Mexico
- Universiteit Gent, Belgium
- Mälardalen University, Sweden
- University of Salerno, Italy
- TECNALIA. Inspiring Business, Spain
- ABB AB Corporation, Switzerland

…

POLITÉCNICA

tecnalia Inspiring Business

Imperial College London

Universidad de Guanajuato

UNIVERSITEIT GENT

UNIVERSITÀ DEGLI STUDI DI SALERNO

MÄLARDALEN UNIVERSITY SWEDEN

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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: 14,176 (73% Windows)

DUALSPHYSICS V4.0 (2016)
Downloads: 13,119 (72% Windows)

DUALSPHYSICS V4.2 (May 2018)
Downloads: 8,033

DUALSPHYSICS V4.4 (April 2019)
Downloads: 21,884

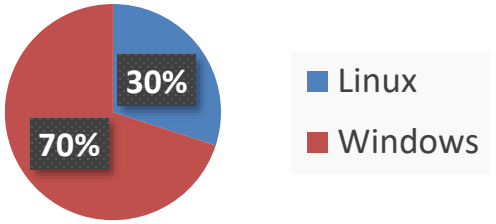
DUALSPHYSICS V5.0 (July 2020)
Downloads: 61,144

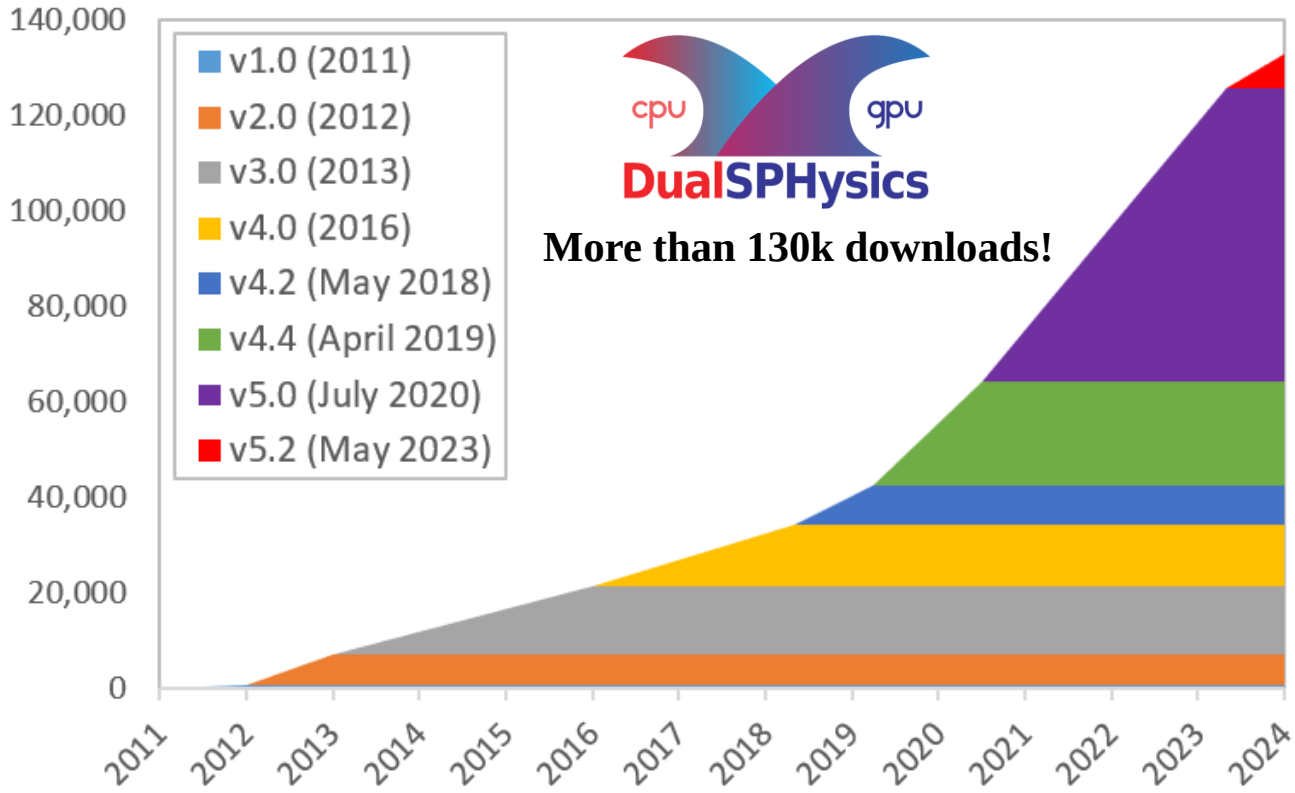
DUALSPHYSICS V5.2 (May 2023)
Downloads: 7,142

DUALSPHYSICS - ALL VERSIONS

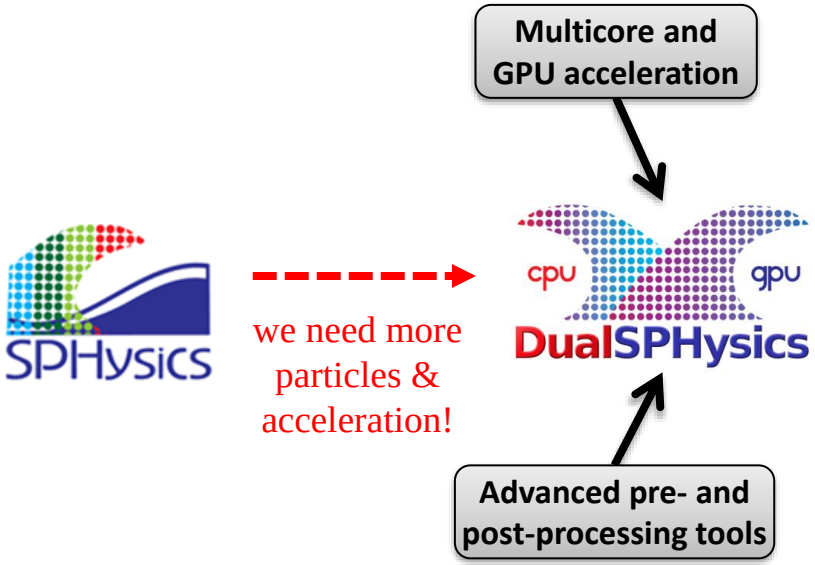
Downloads: 132,671 (70% Windows)

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



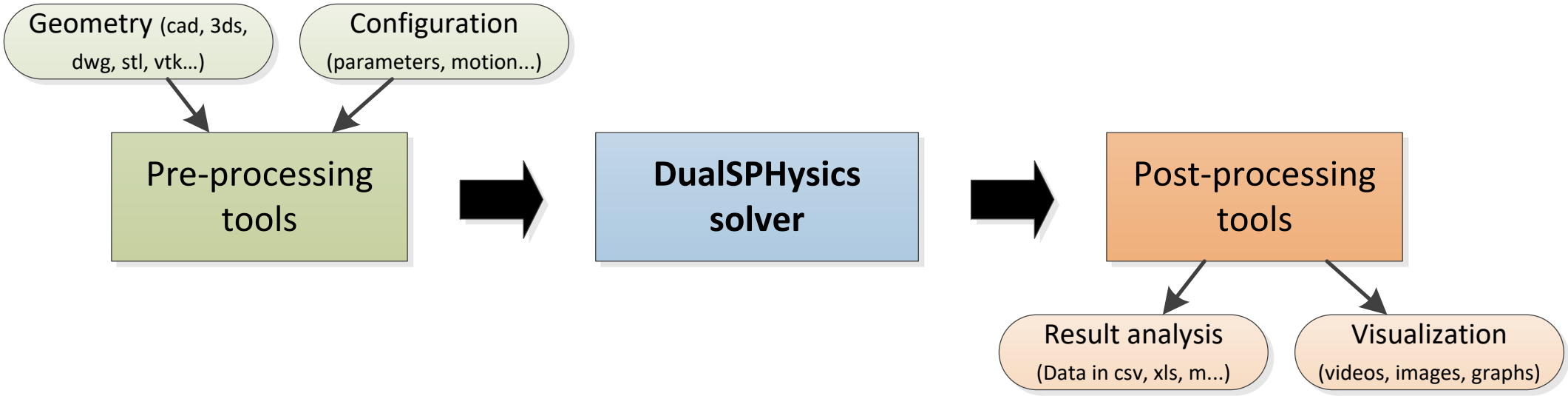


DualSPHysics evolution



DualSPHysics and tools

DSPH software 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.

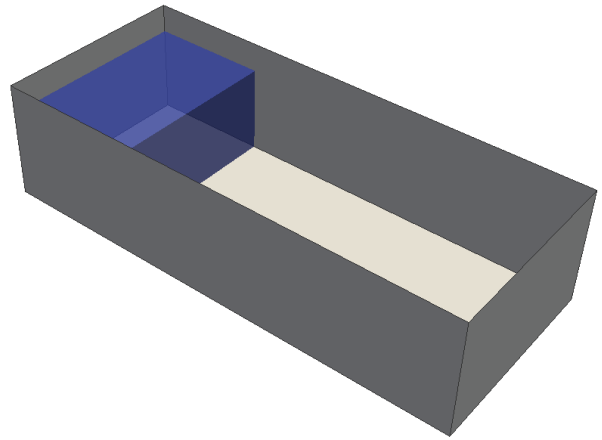
Post-processing tools:

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

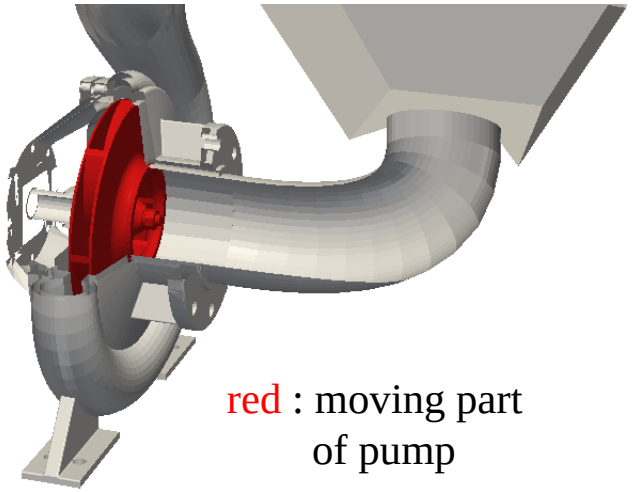
Advanced pre-processing for DualSPHysics

Simple XML file for boundary and fluid particles definition

```
<geometry>
 + <definition dp="0.005"></definition>
 − <commands>
     <setmkbound mk="0"/>
   − <drawbox>
       <boxfill>all^top</boxfill>
       <point x="0" y="0" z="0"/>
       <size x="1.6" y="0.7" z="0.4"/>
     </drawbox>
     <setmkfluid mk="0"/>
   − <drawbox>
       <boxfill>solid</boxfill>
       <point x="0" y="0" z="0"/>
       <size x="0.4" y="0.7" z="0.3"/>
     </drawbox>
   </commands>
</geometry>
```



…for motion and other behaviours definition

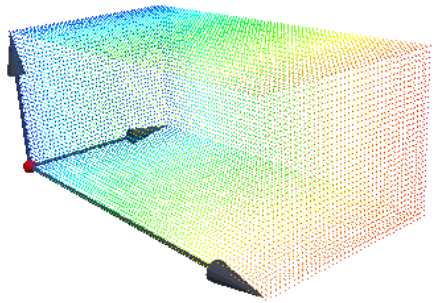


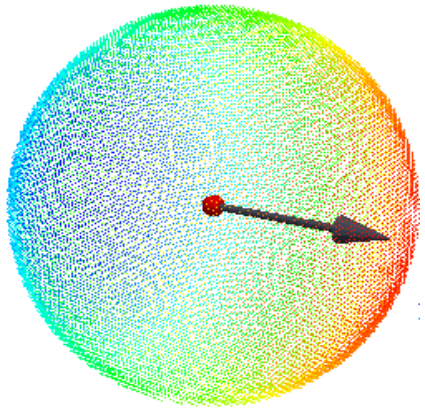
red : moving part of pump

```
<motion>
 − <objreal ref="2">
     <begin mov="1" start="0.5"/>
   − <mvrotace id="1" duration="20">
       <ace ang="300"/>
       <velini ang="90"/>
       <axisp1 x="-0.0176" y="-0.29" z="-0.7275"/>
       <axisp2 x="-0.0176" y="-0.49" z="-0.7275"/>
     </mvrotace>
   </objreal>
</motion>
```

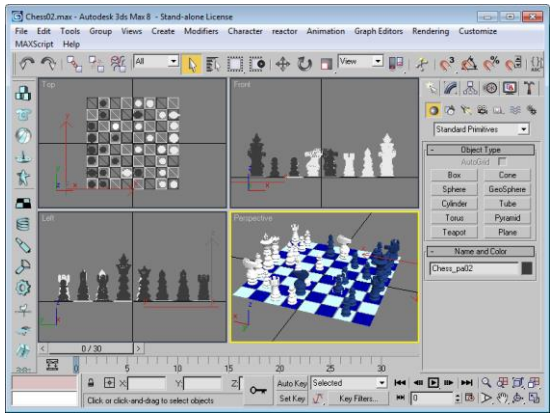
Advanced pre-processing for DualSPHysics

Basic parameterised shapes

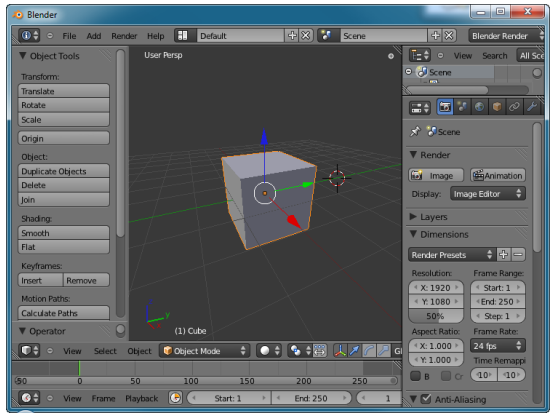




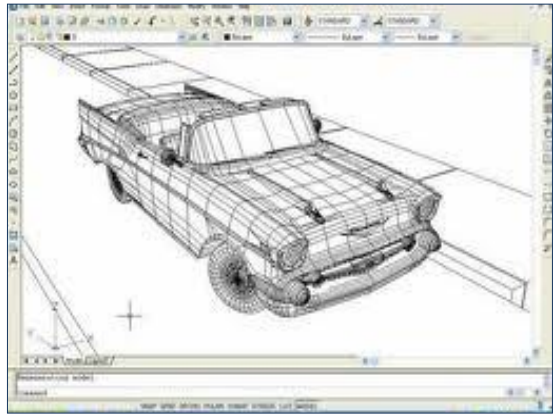
Complex 3D models from professional 3D modelling software



3D Studio Max

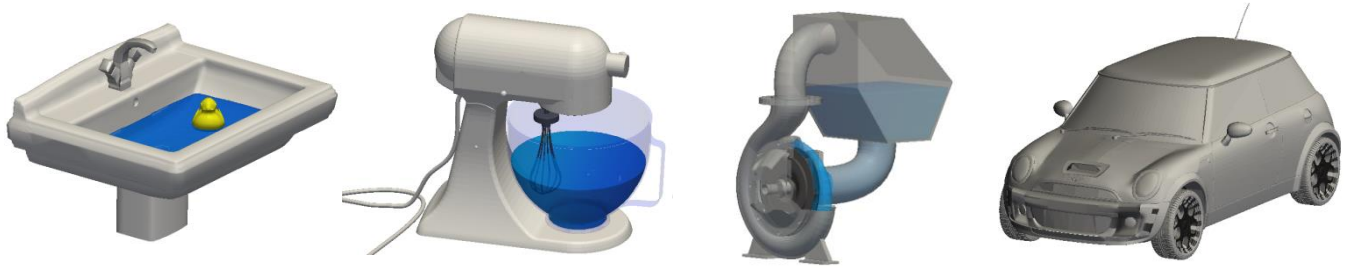


Blender

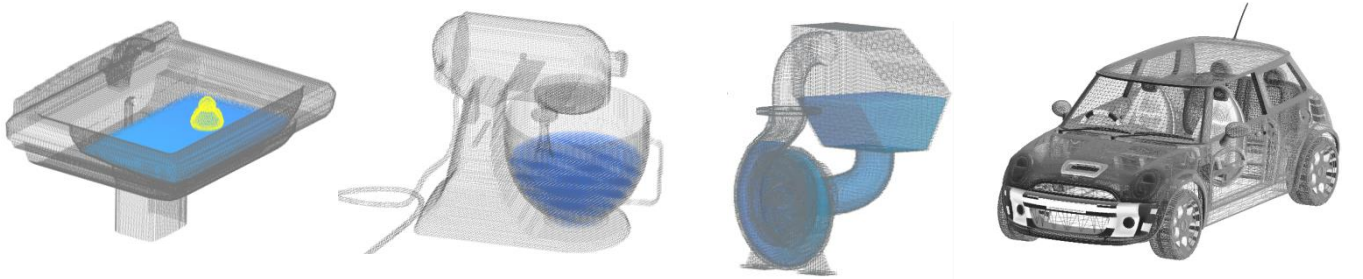


AutoCAD

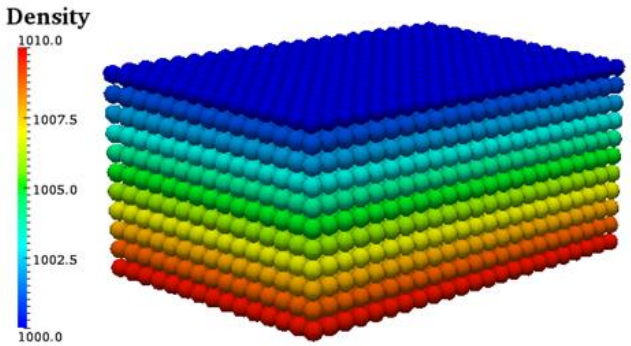
Shape model



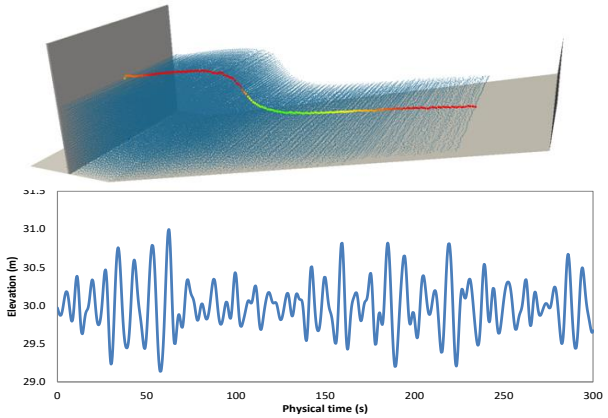
SPH particles



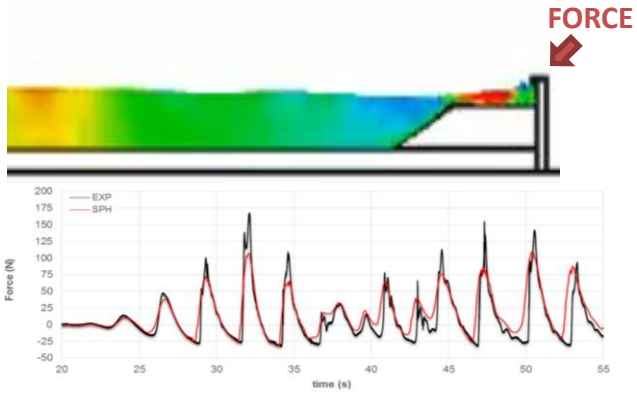
Main post-processing tools



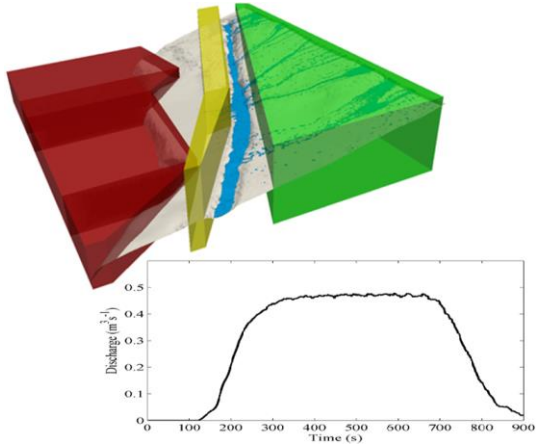
PartVTK: particle data visualisation



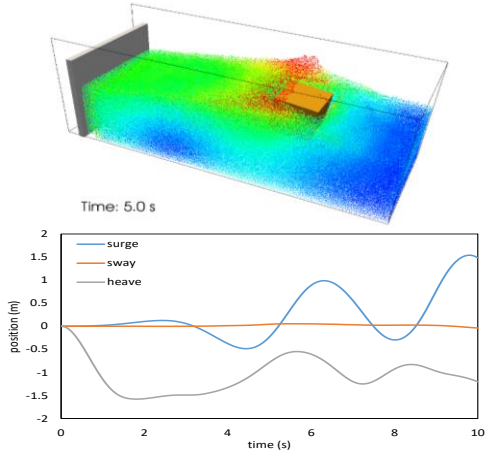
MeasureTool: velocity and water elevation calculation



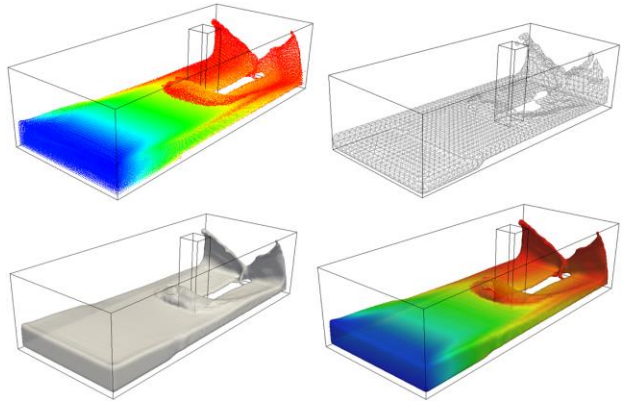
ComputeForces: force exerted by the fluid onto a boundary object



FlowTool: flow rate in different areas

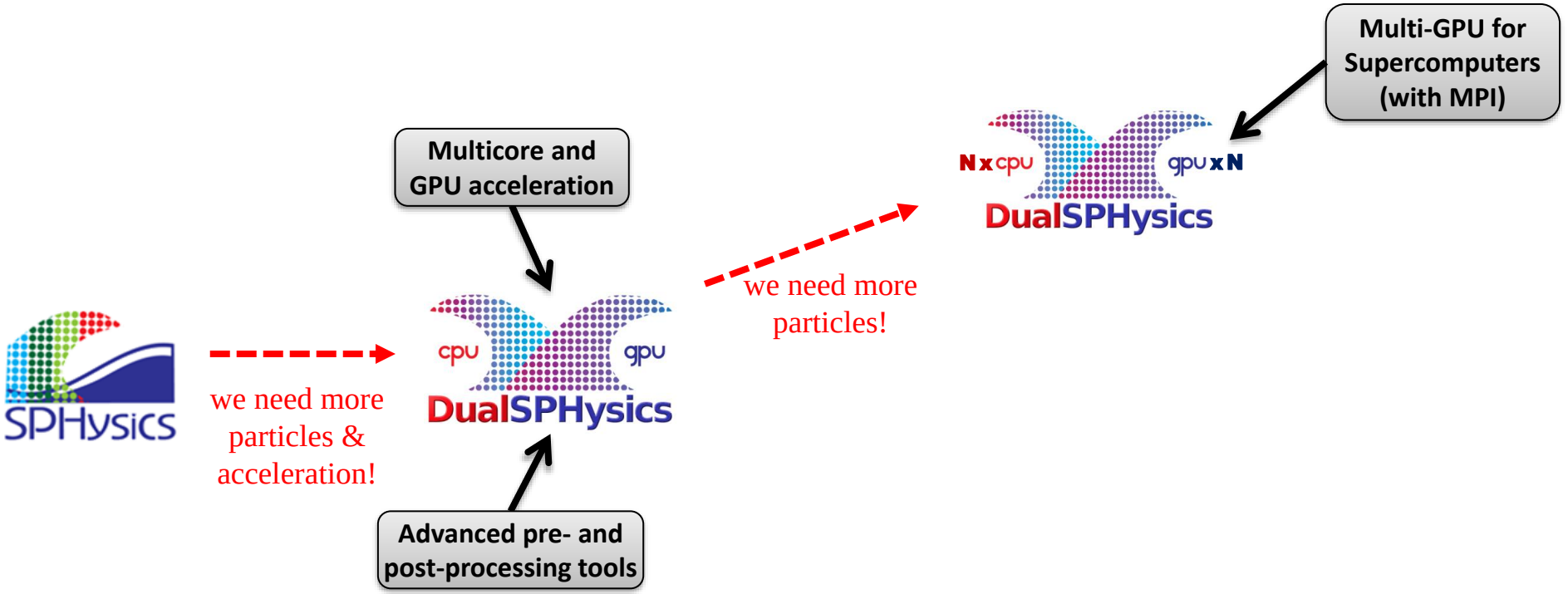


FloatingInfo: velocity, acceleration and motion of floating bodies



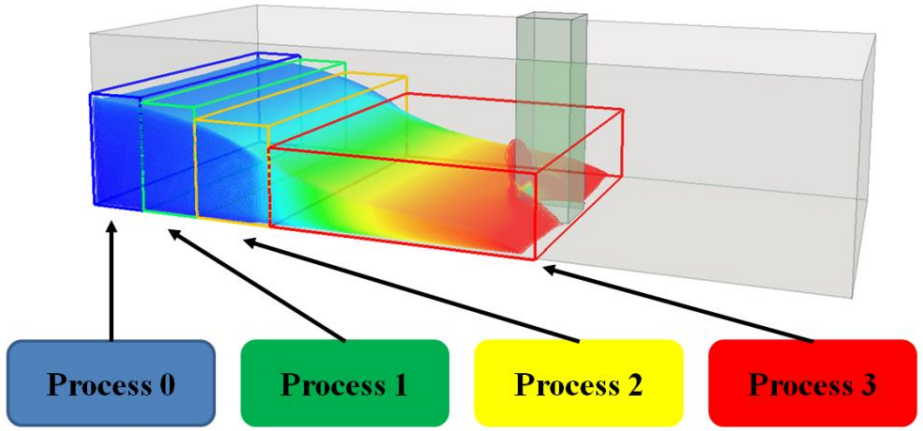
IsoSurface: efficient visualisation for large number of fluid particles

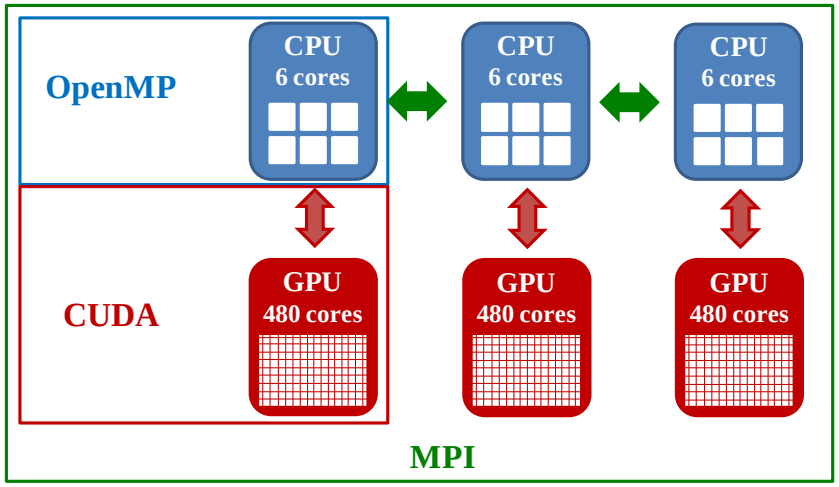
DualSPHysics evolution



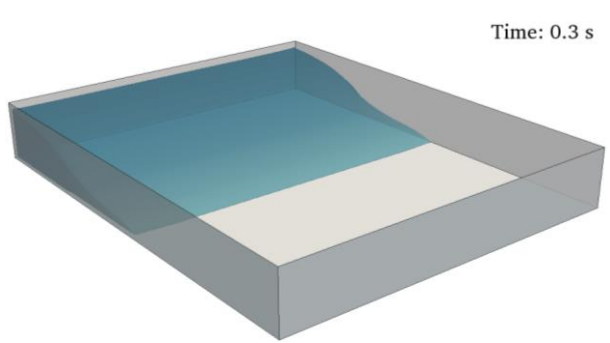
Multi-GPU for supercomputers using MPI

Physical domain division with dynamic load balancing





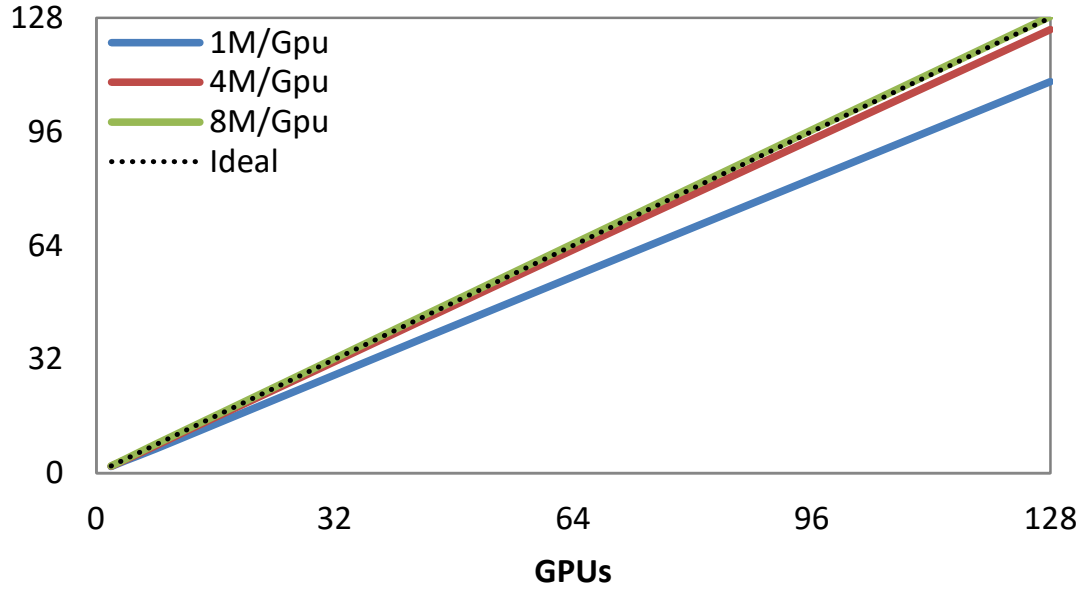
100% efficiency simulating 8M/GPU on 128 GPUs



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

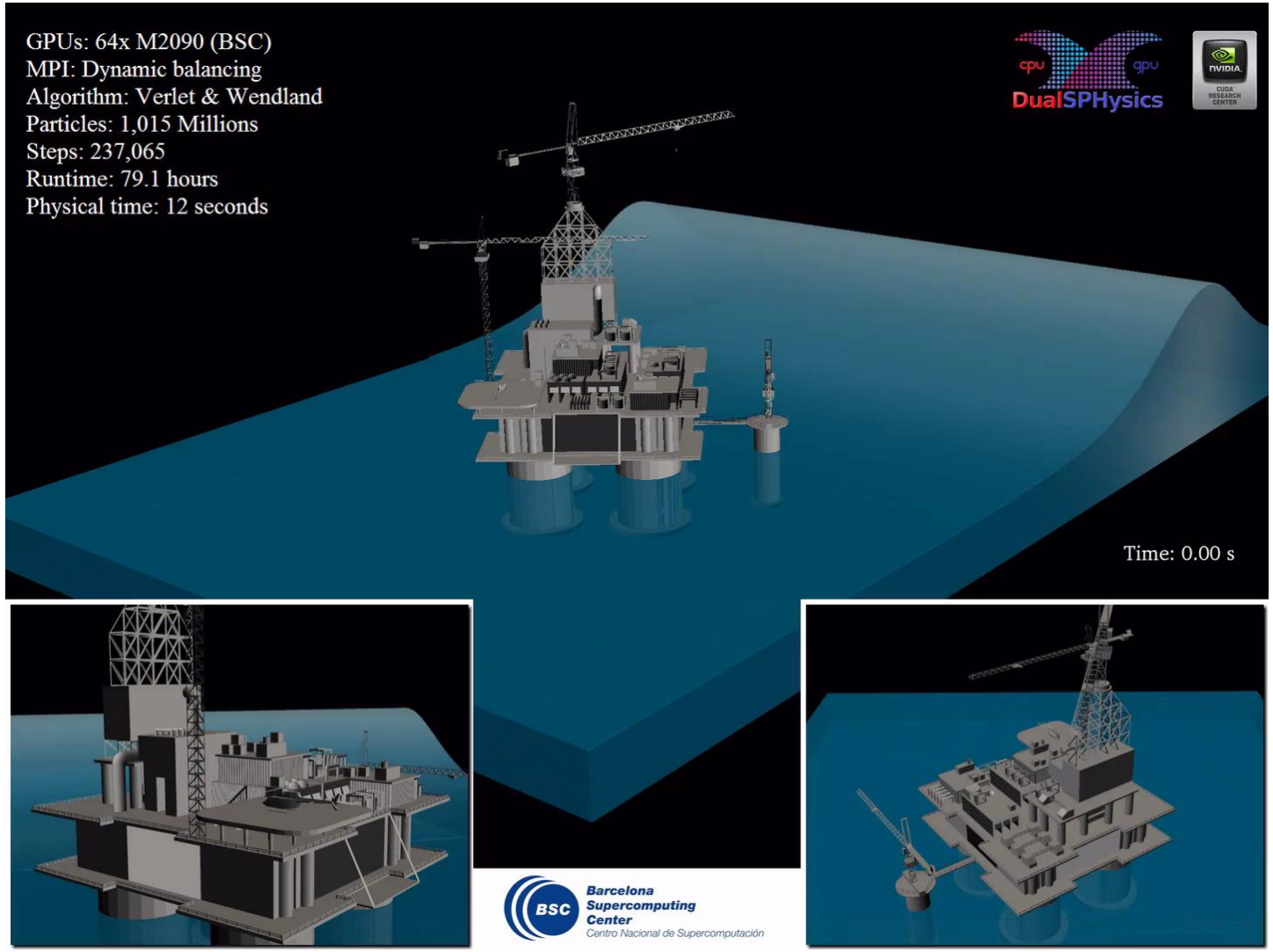
128×

Speedup - Weak scaling



Multi-GPU for supercomputers using MPI

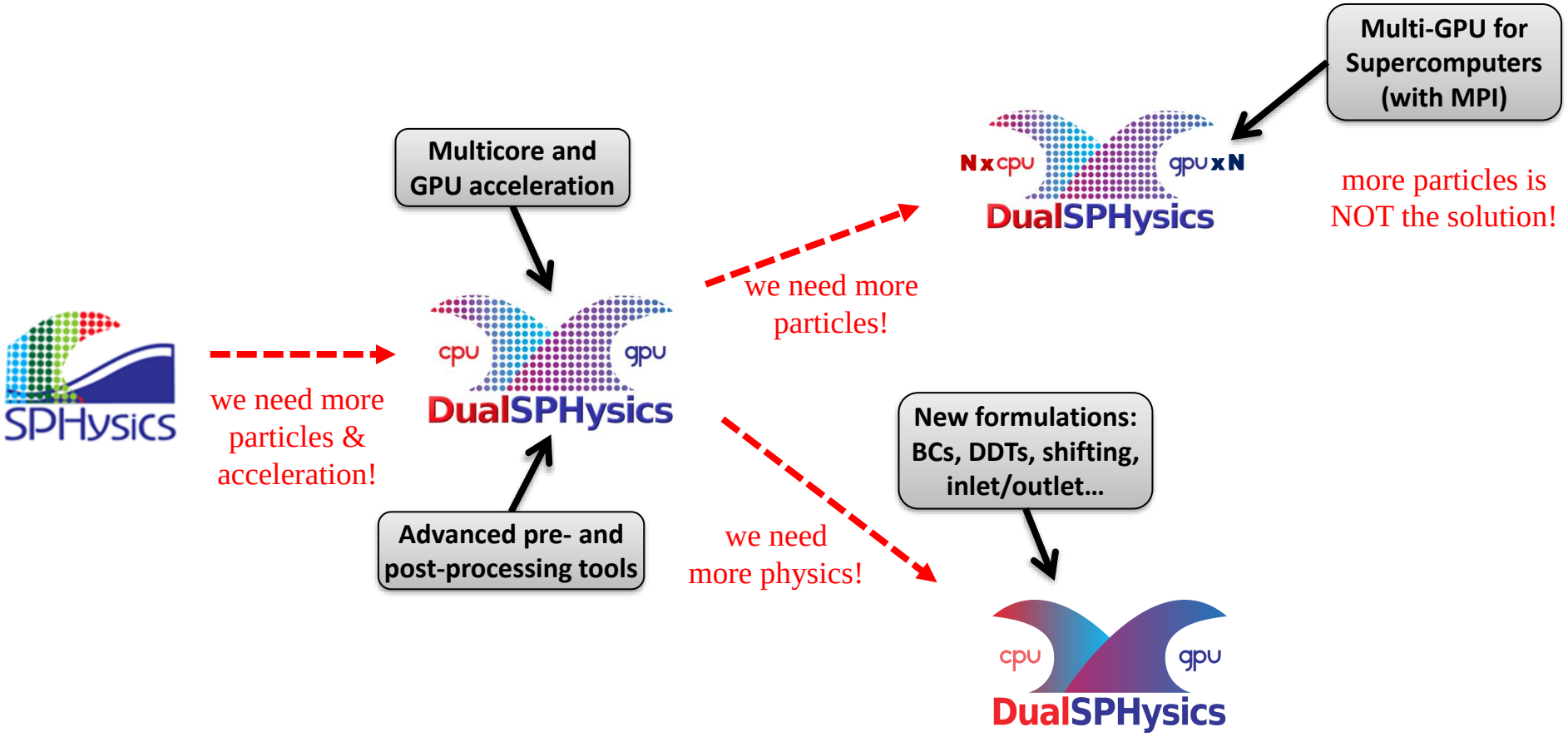
Largest full SPH free-surface fluid simulation in 2013. More than 1 billion particles!!



- Large wave interaction with oil rig using **10^9 particles**.
- More than 237,000 simulation steps to simulate **12 physical seconds**.
- **79.1 hours** using **64 GPUs** Tesla M2090.
- **Huge complexity** for pre-processing, simulation and post-processing.

- Very interesting challenge but not very useful.
- Access to a supercomputer is required.
- Too much effort for practical use.
- Many particles do **not allow modelling of complex problems** involving different physical phenomena.

DualSPHysics evolution



DualSPHysics formulation I

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

- 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)
  - *Antuono (Antuono et al., 2012)*
  - *Green (Green et al., 2019)*

- Viscosity:
  - Artificial (Monaghan, 1992)
  - Laminar (Lo and Shao, 2002)
  - Laminar + SPS turbulence model (Dalrymple and Rogers, 2006)

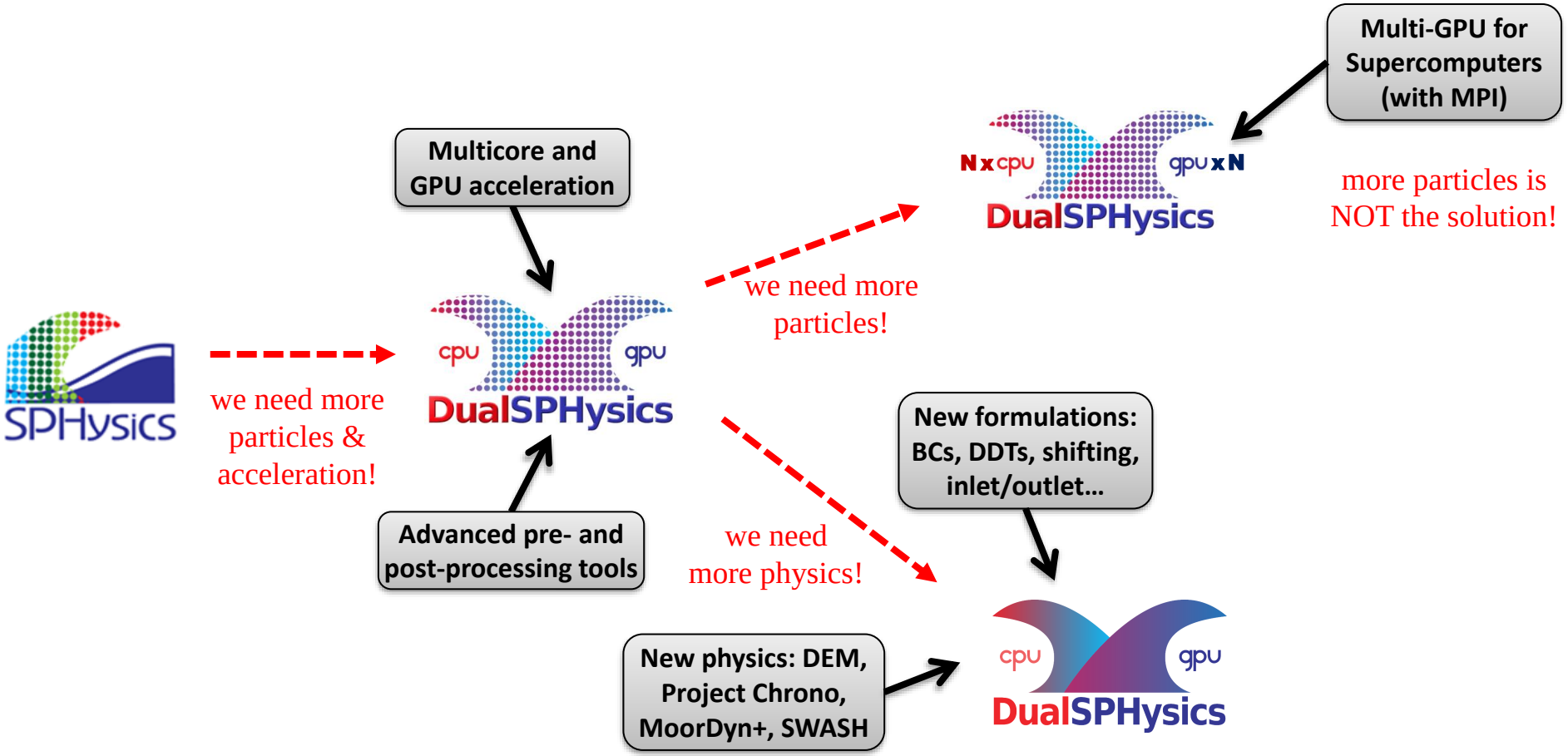
- Weakly compressible approach using Tait's equation of state (Batchelor, 1974)

DualSPHysics formulation II

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

- 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., 2021)
- Floating objects (Monaghan et al., 2003)
- Periodic open boundaries (Gómez-Gesteira et al., 2012)
- Inflow-outflow boundary conditions (Tafuni et al., 2018)

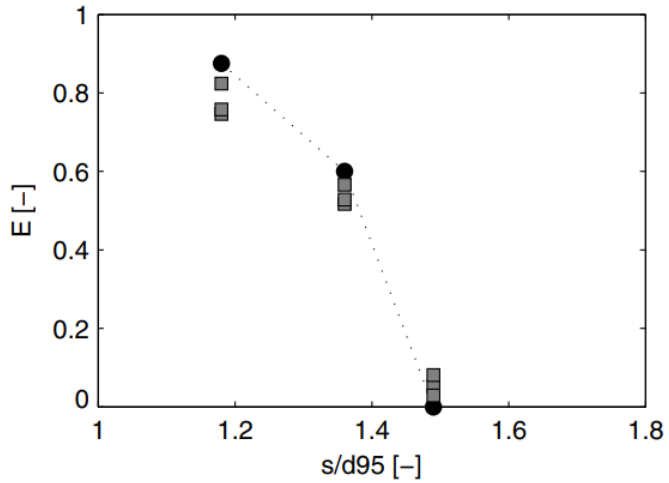
DualSPHysics evolution

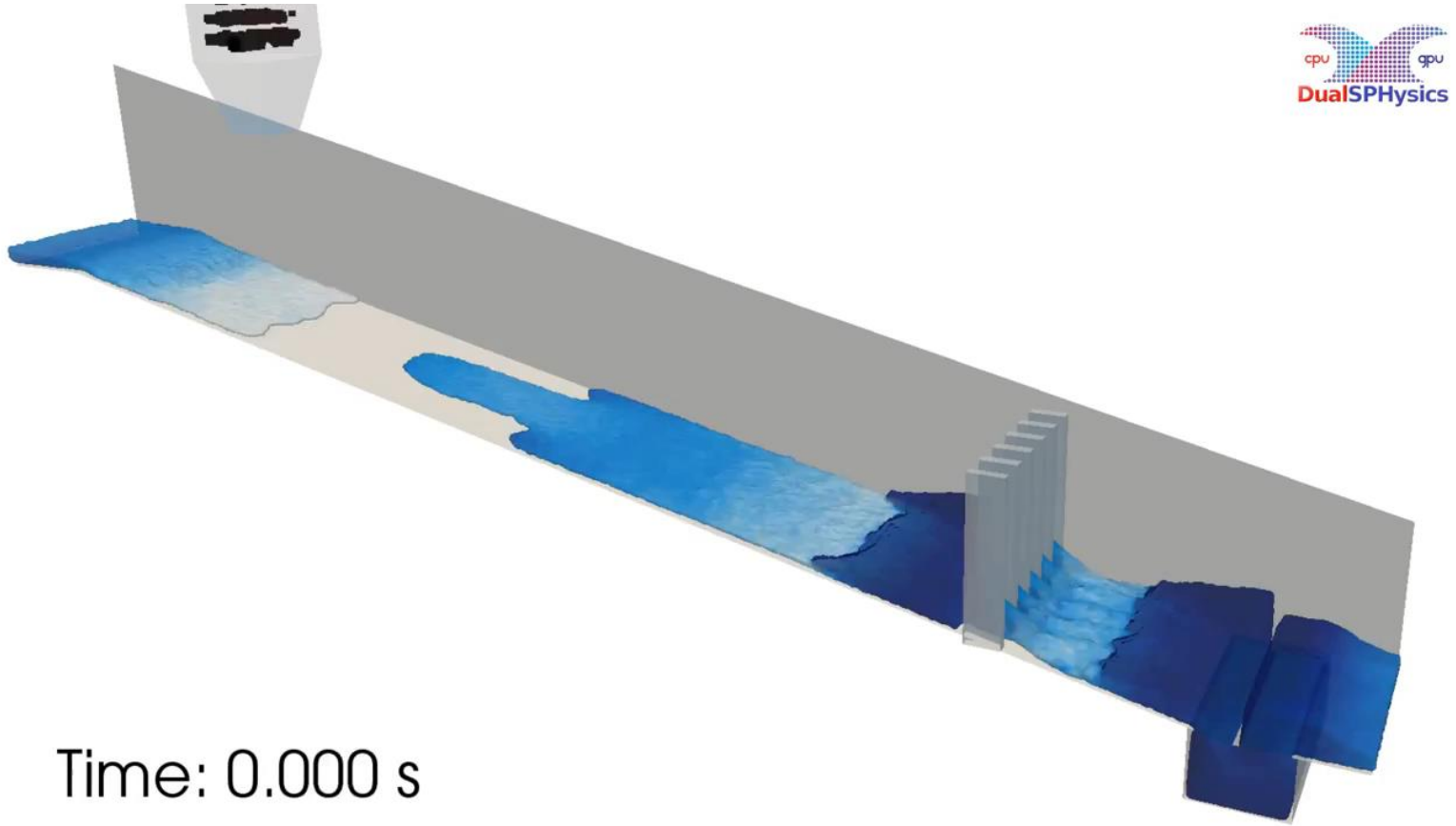


Coupling with other models

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

- **Coupling with Discrete Element Method (Canelas et al., 2016; Canelas et al., 2017)**



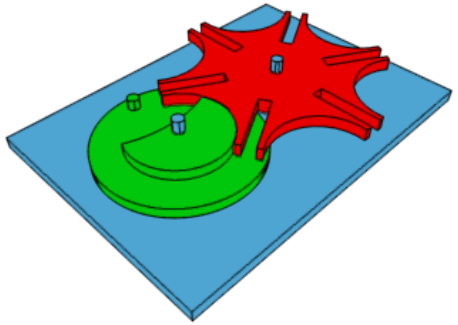


Coupling with other models

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

- Coupling with Discrete Element Method (Canelas et al., 2016)
- **Coupling with Project Chrono (Canelas et al., 2018; Martínez-Estévez et al., 2022)**

Project Chrono is a **physics-based** modeling and simulation **library** based on a **platform-independent**, **open-source** design (http://projectchrono.org).



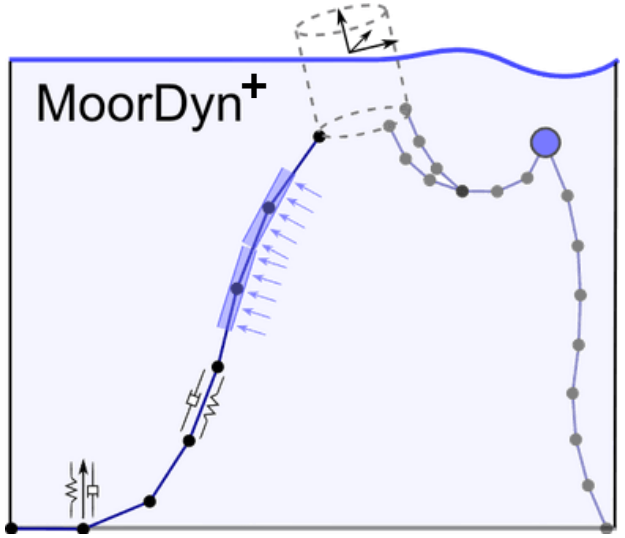
- Wide set of joints (spherical, revolute joint, prismatic, universal joint, with limits, etc.).
- Unilateral constraints.
- Exact Coulomb friction model, for precise stick-slip of bodies.
- Springs and dampers, even with non-linear features.
- Recent support for linear and nonlinear Finite Element Analysis - Euler-Bernoulli beams, bars, shells, cables.

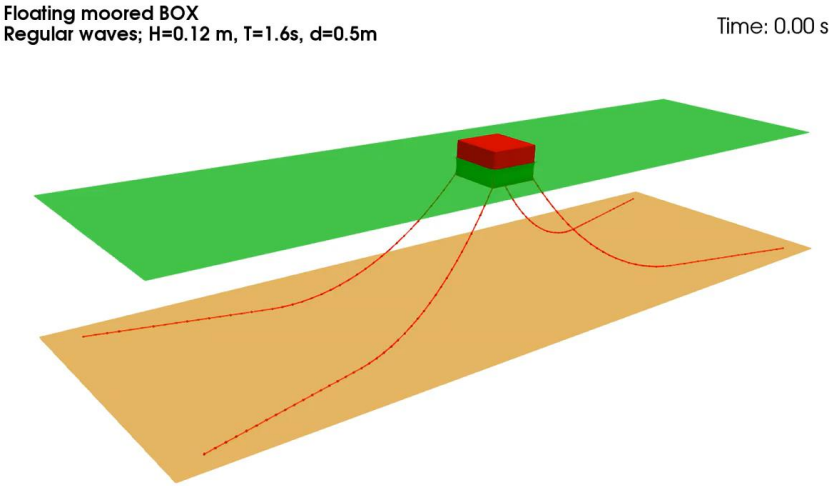
Coupling with other models

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

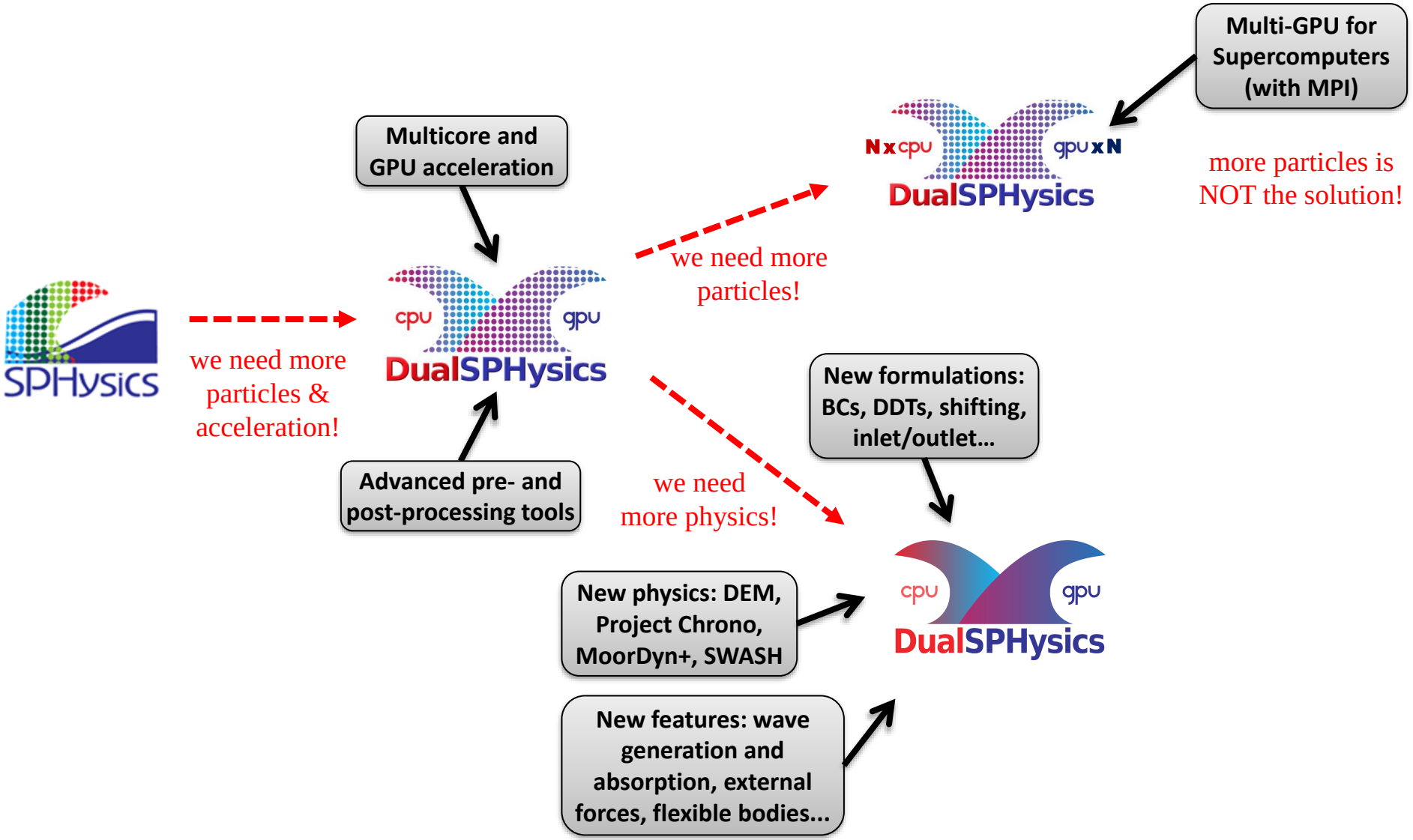
- Coupling with Discrete Element Method (Canelas et al., 2016)
- Coupling with Project Chrono (Canelas et al., 2018; Martínez-Estévez et al., 2022)
- **Coupling with MoorDyn+ (Domínguez et al., 2019)**

MoorDyn+ is an open-source dynamic mooring line model that uses a lumped-mass formulation for modelling axial elasticity, hydrodynamics, and bottom contact.





DualSPHysics evolution



DualSPHysics features

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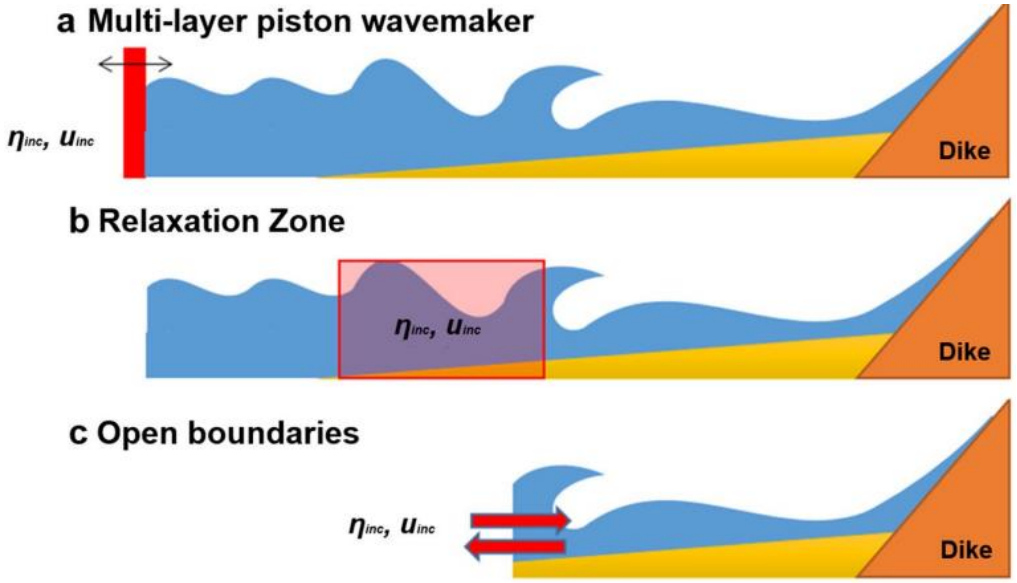
Ocean engineering features:

- 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)



DualSPHysics features

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

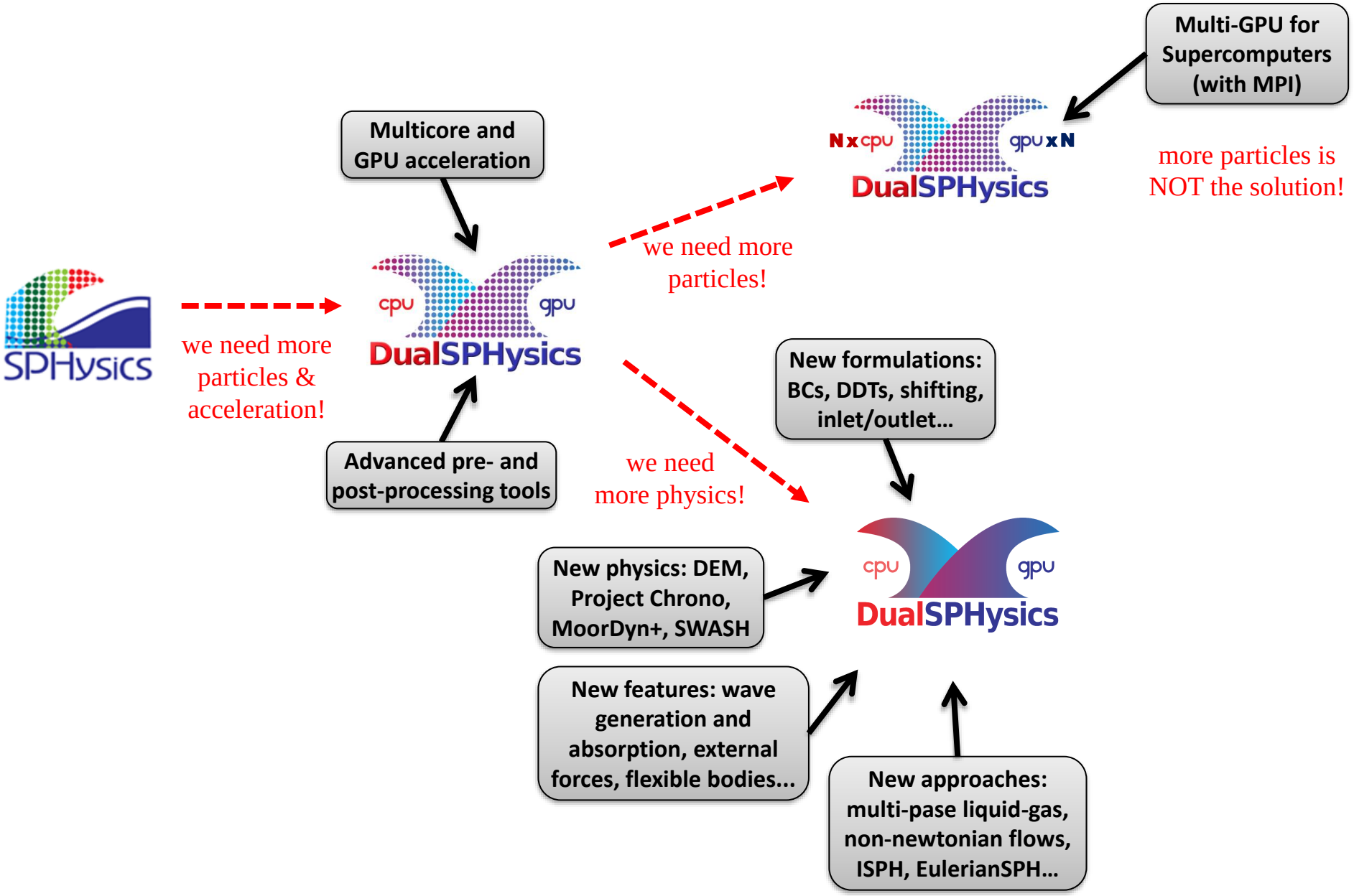
Ocean engineering features:

- 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)

Flexible body approaches:

- Lagrangian formulation for flexible fluid-structure interaction (O'Connor et al., 2021)
- Flexible beams based on co-rotating rigid elements using Project Chrono (Capasso et al., 2022)
- SPH coupling with FEA structural solver using Project Chrono (Martínez-Estévez et al., 2023)

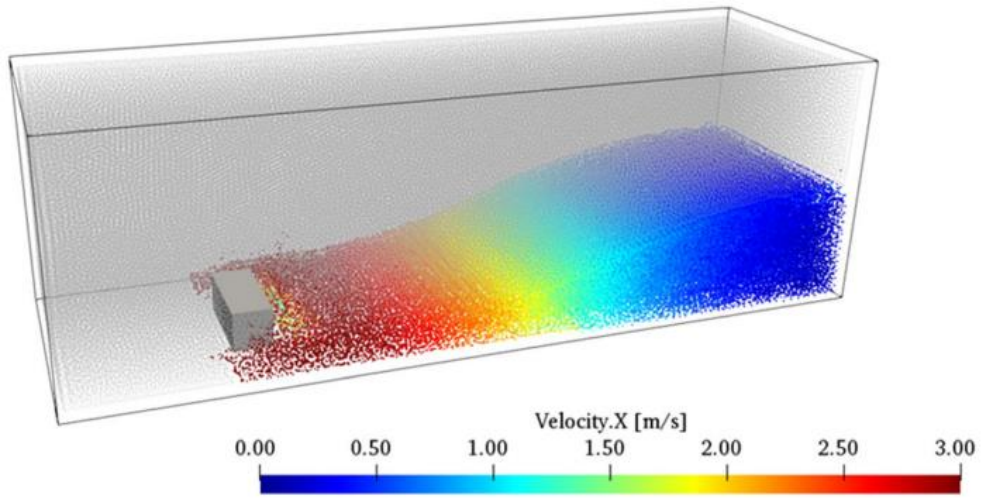
DualSPHysics evolution



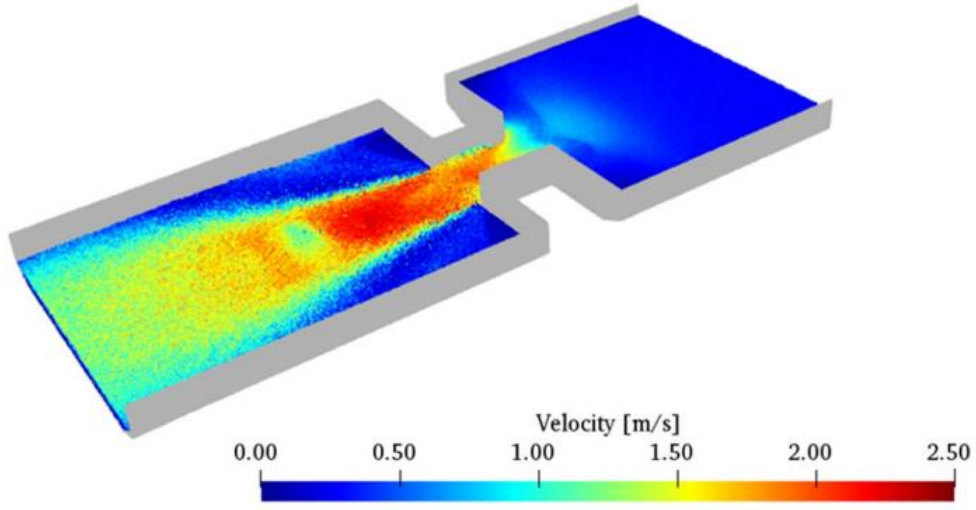
Other DualSPHysics approaches

J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2021. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. doi:10.1007/s40571-021-00404-2

- Multi-phase: liquid and gas (Mokos et al., 2015)
- Multi-phase: non-Newtonian flows (Fourtakas and Rogers, 2016)
- Incompressible SPH (Chow et al., 2018)
- Eulerian incompressible SPH (O'Connor et al., 2022)

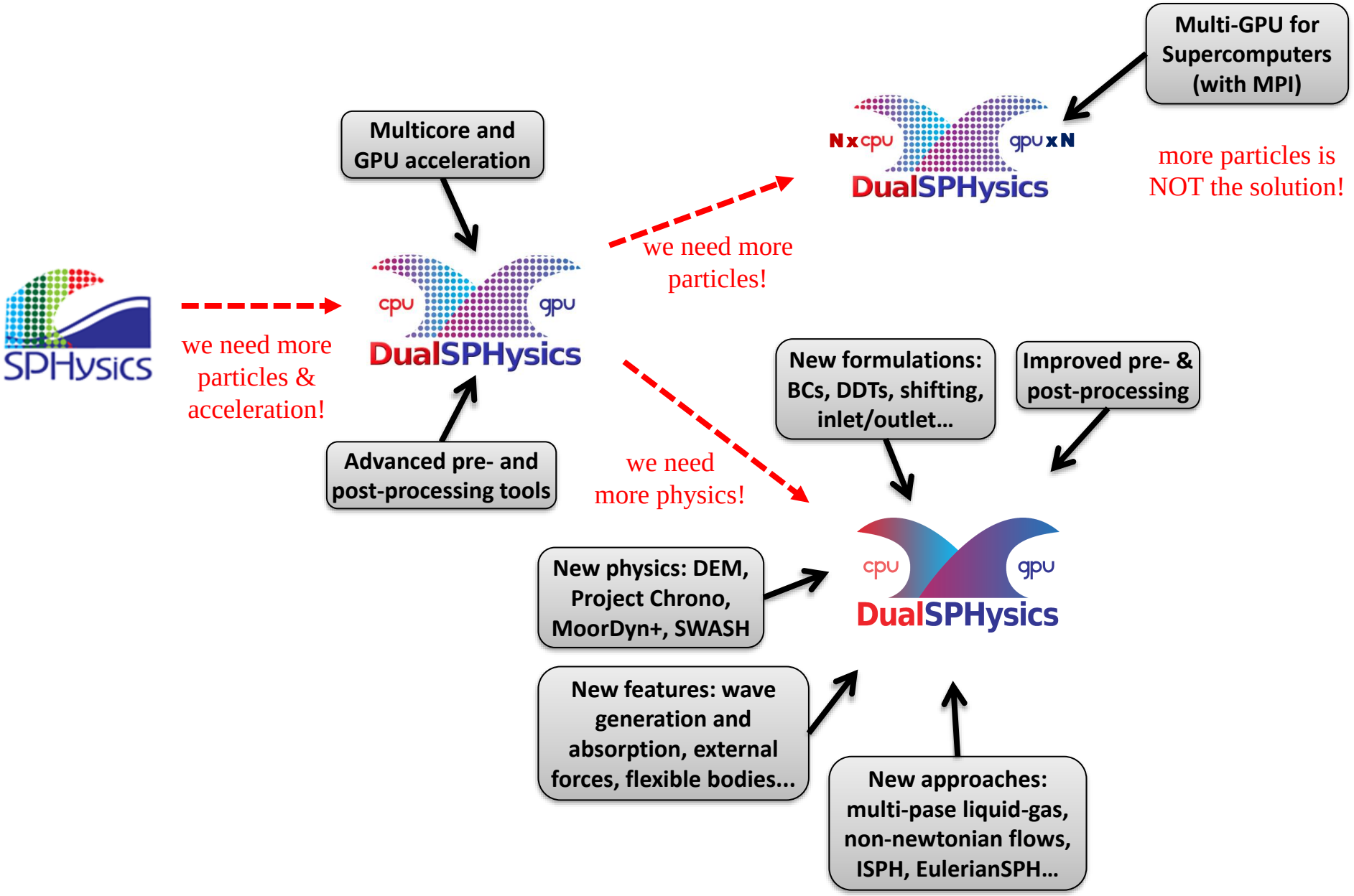


Liquid and gas: 3-D dam break impacting an obstacle

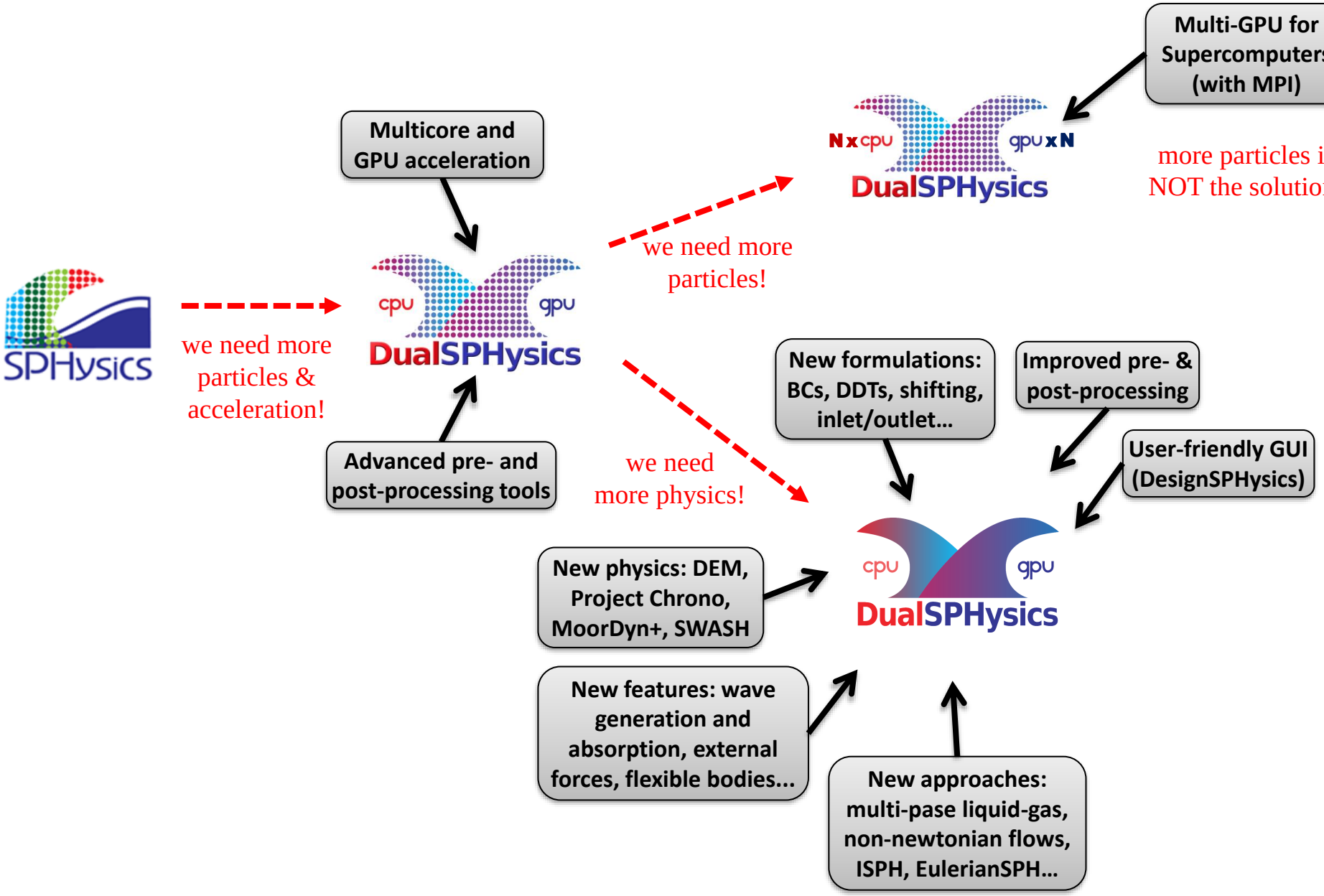


non-Newtonian flows: 3-D dam break over an erodible bed

DualSPHysics evolution

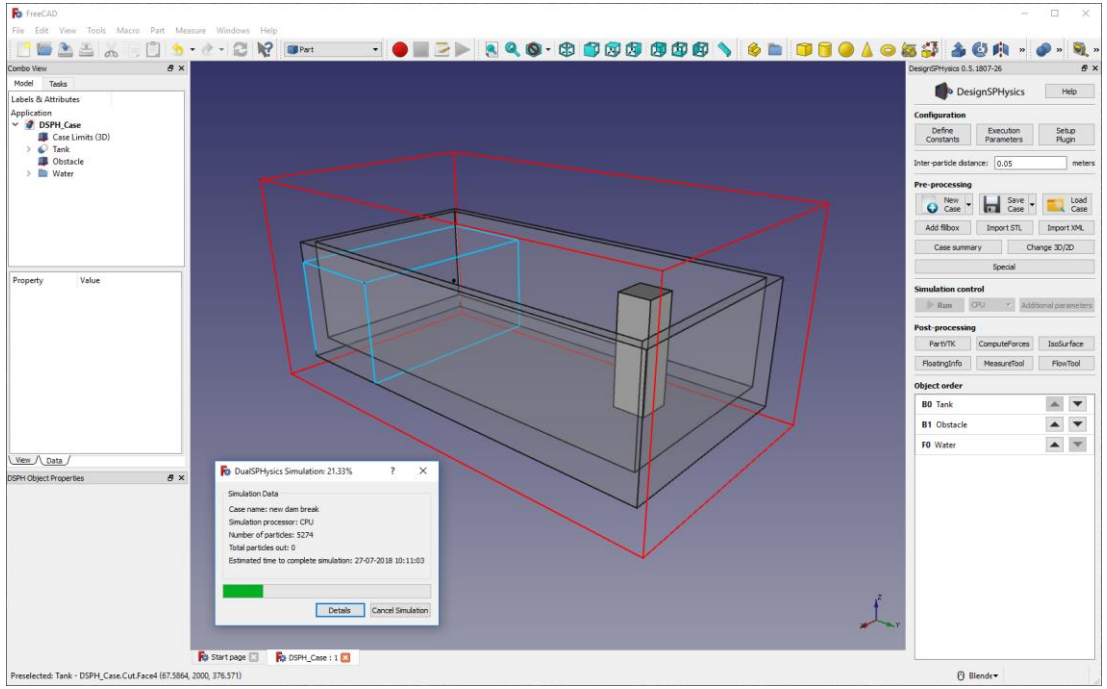


DualSPHysics evolution



DesignSPHysics: Graphical User Interface for DualSPHysics

CREATES THE XML FOR YOU



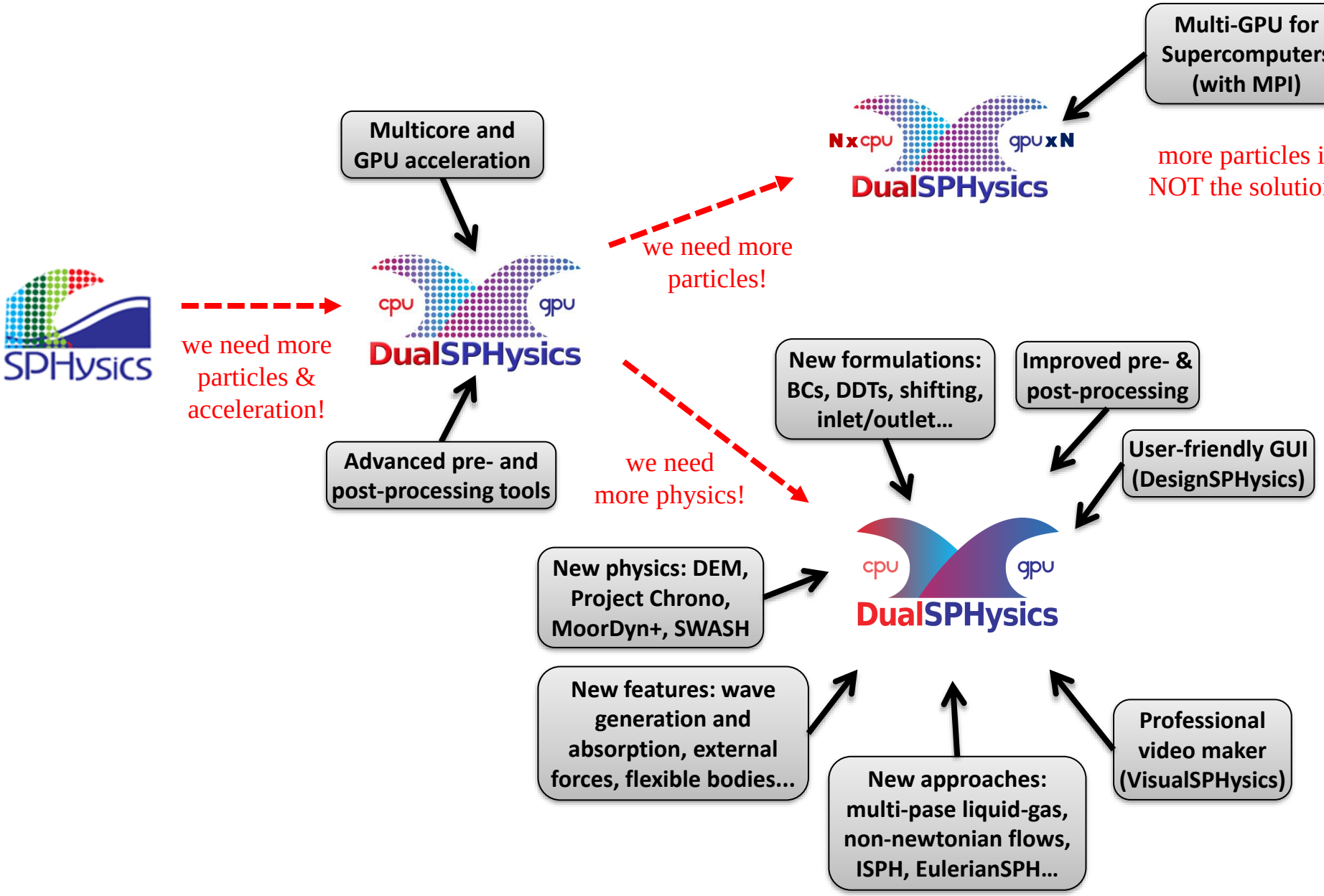
FreeCAD
Open Source parametric 3D CAD modeler

python™

DesignSPHysics is a **complete software** that allows the user to

1) create a new case,
2) execute the simulation and then
3) analyse the results
    3.1) by visualising the particles
    3.2) by computing physical magnitudes of interest

DualSPHysics evolution

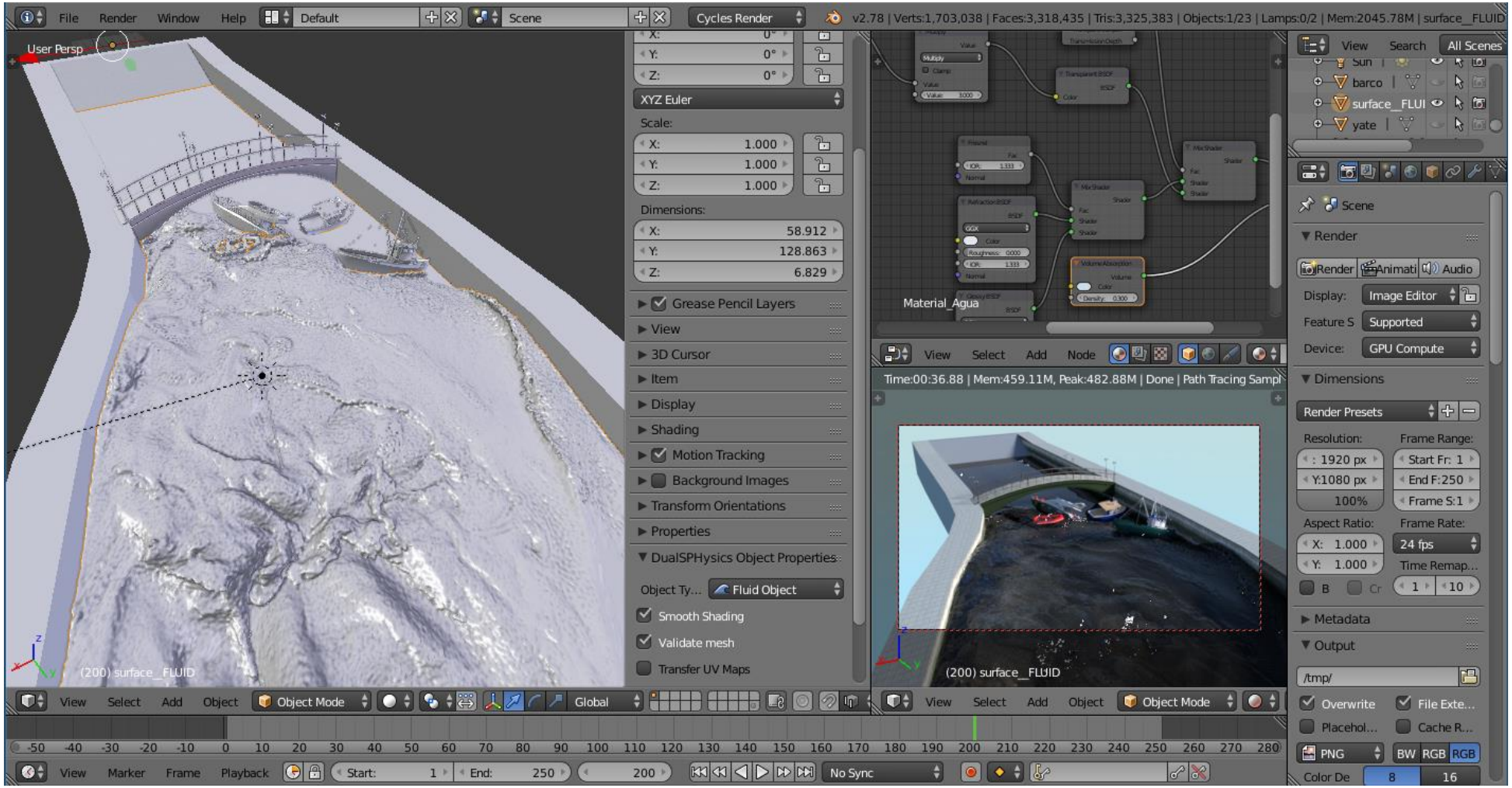


VisualSPHysics: Advanced visualisation tools

Advanced visualisation using Blender with **VisualSPHysics**: http://visual.sphysics.org/

O. García-Feal, A.J.C. Crespo, M. Gómez-Gesteira. 2021. **VisualSPHysics: advanced fluid visualization for SPH models.** Computational Particle Mechanics. doi: 10.1007/s40571-020-00386-7

blender + python



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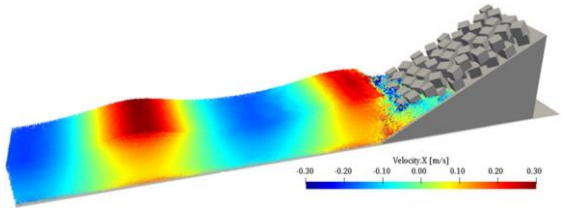
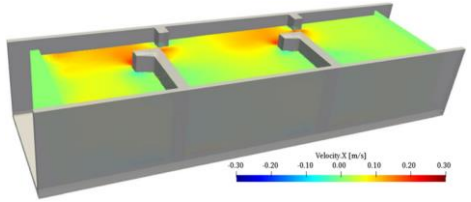
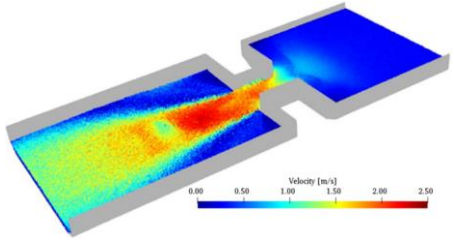
DualSPHysics is now ready for very complex multiphysics simulations!!



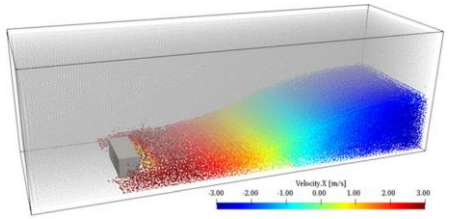
Armour breakwater



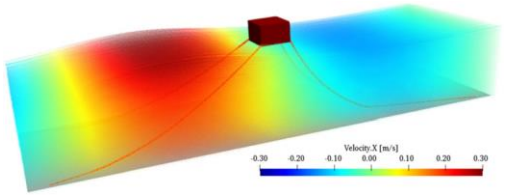
Vertical slot fishway



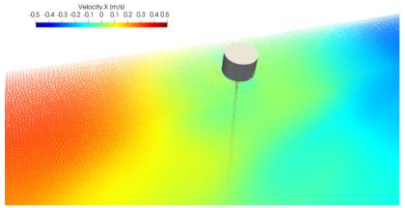
Non-Newtonian dam break



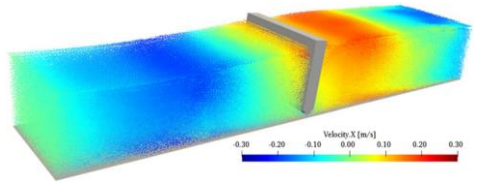
Dam break with liquid & gas



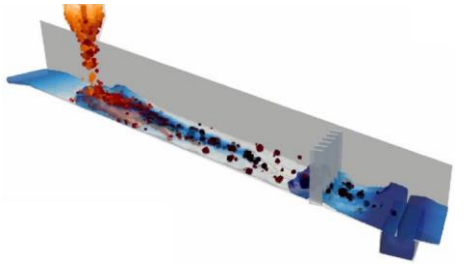
Moored floating body



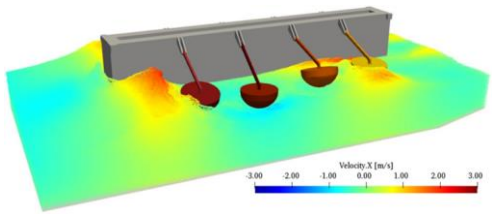
Moored point absorber



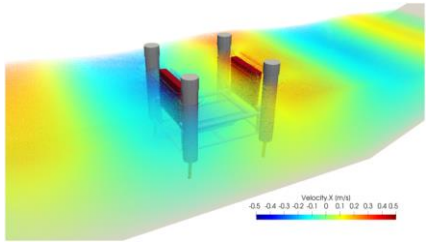
Oscillating wave surge converter



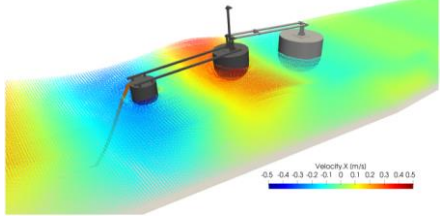
Debris flow with DEM



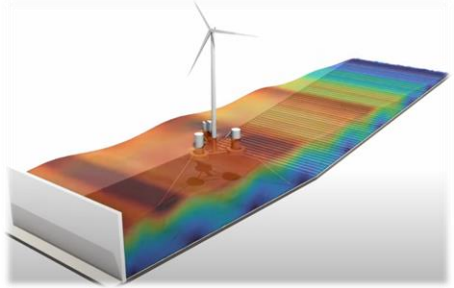
Wave star machine



Floating oscillating wave surge converter



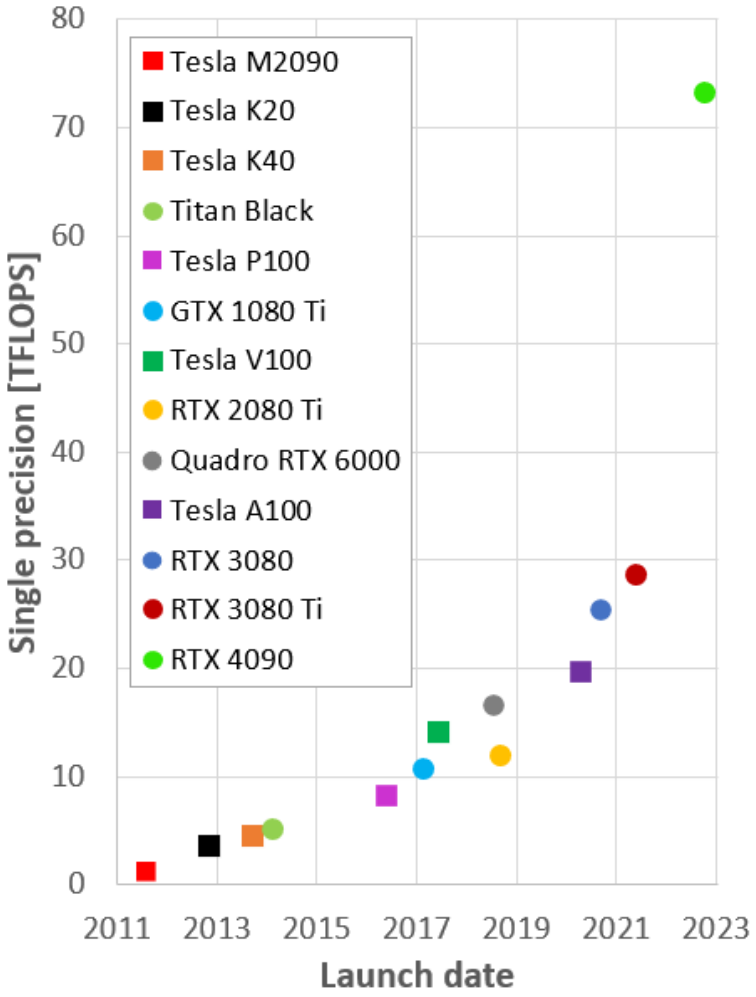
Multi-body attenuator M4

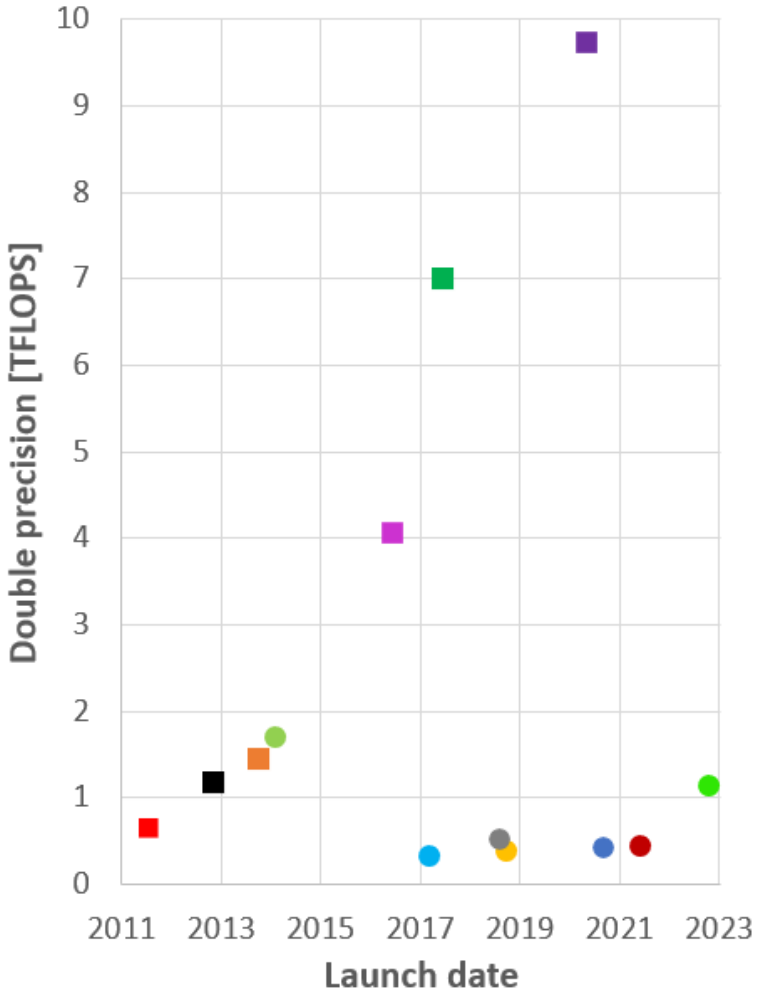


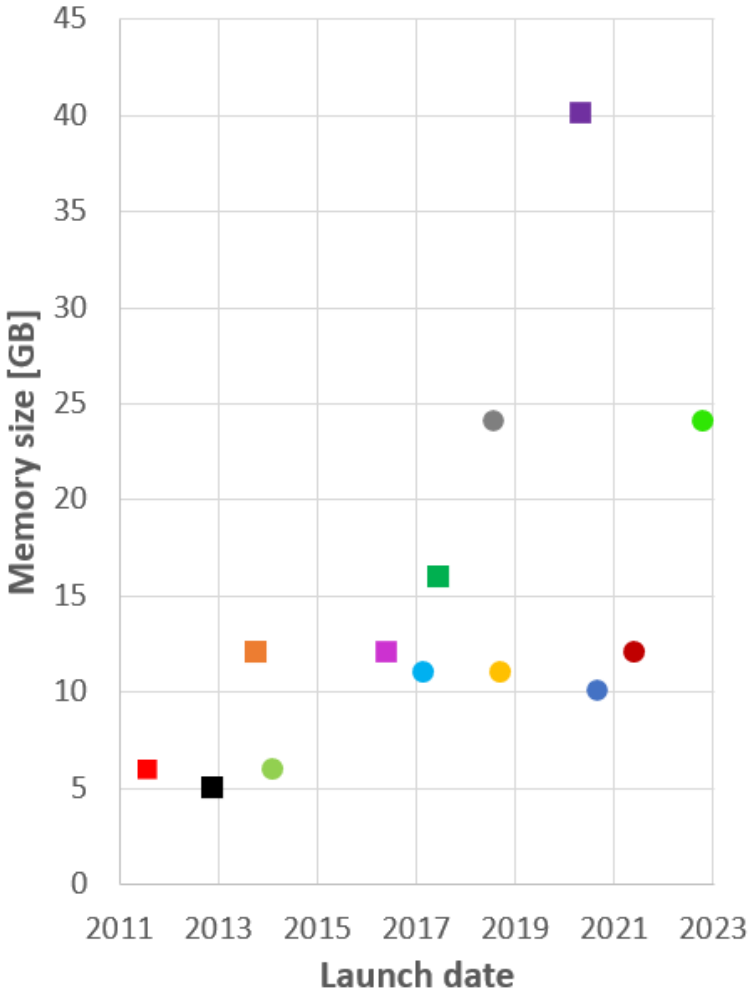
Floating wind turbine

What about DualSPHysics performance?

- **All new features are implemented to maximise performance**
- **Continuous re-implementation to improve performance without major complexity increase**
- **DualSPHysics takes advantage of the continuous performance improvement of the new GPU models**







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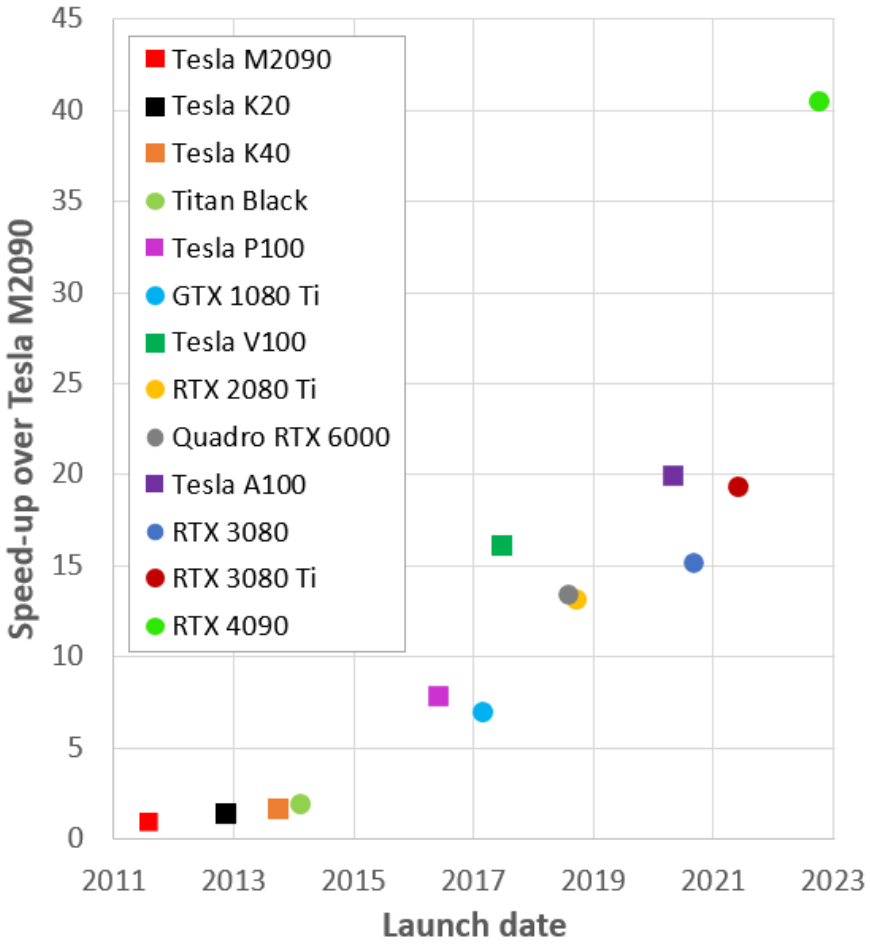
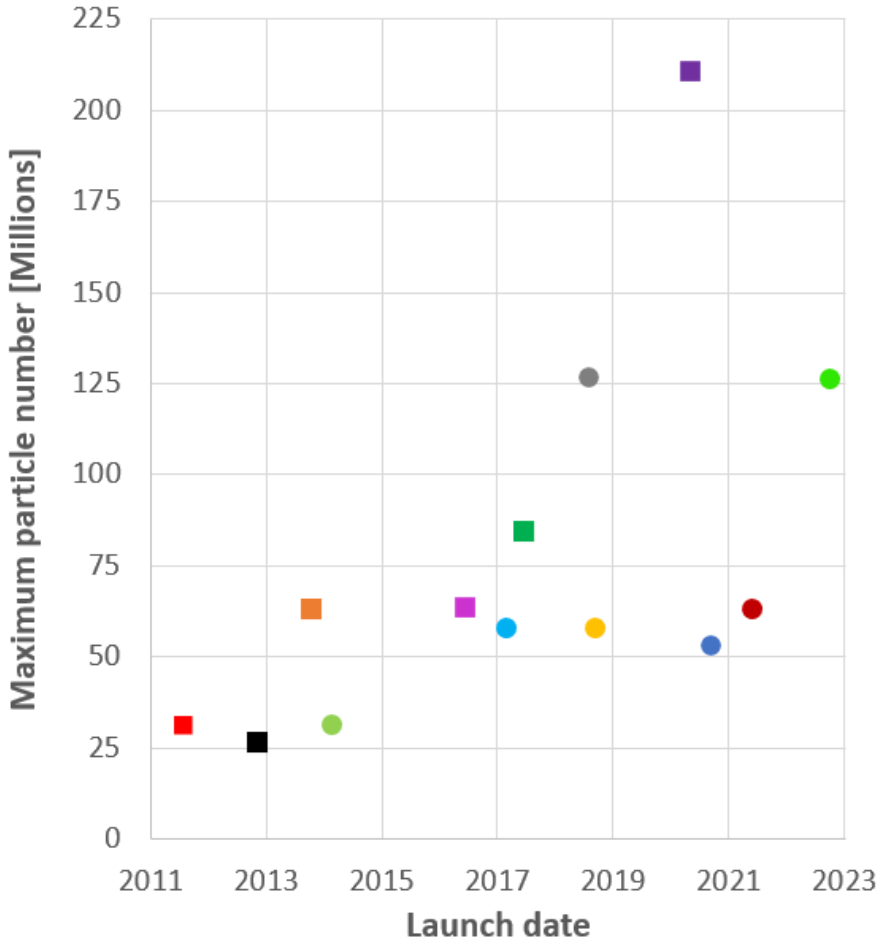
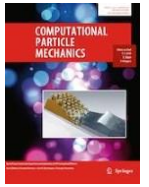
GPU improvement translated into DualSPHysics values





DualSPHysics performance



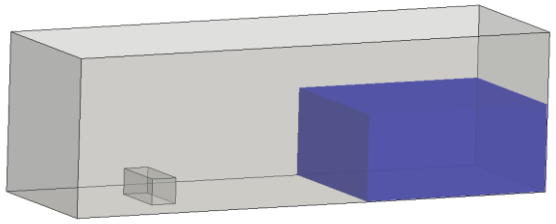
J.M. Domínguez, G. Fourtakas, C. Altomare, R.B. Canelas, A. Tafuni, O. García-Feal, I. Martínez-Estévez, A. Mokos, R. Vacondio, A.J.C. Crespo, B.D. Rogers, P.K. Stansby, M. Gómez-Gesteira. 2022. **DualSPHysics: from fluid dynamics to multiphysics problems.** Computational Particle Mechanics. 9(5): 867-895. doi:10.1007/s40571-021-00404-2

cpu gpu

DualSPHysics

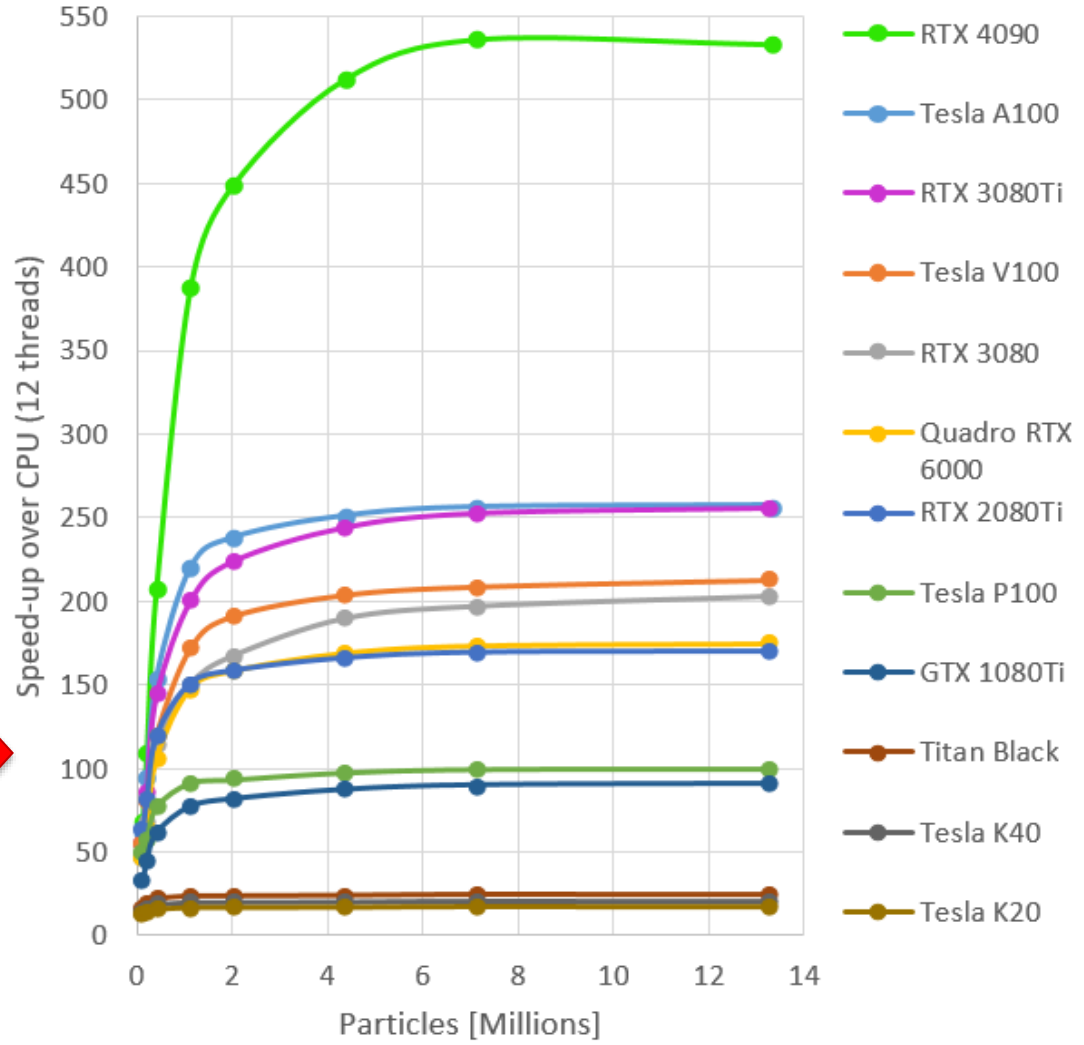
Testcase for performance test

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

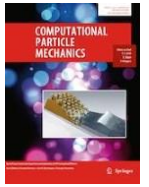


Speed-up: 533x on **RTX 4090**
257x on Tesla A100
255x on RTX 3080Ti
over
CPU Intel Core i7-8700K
(12 threads)

SPH HIGHLY PARALLELISED



DualSPHysics performance



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cpu gpu

DualSPHysics

200M particles on **professional GPU** Tesla A100 (40 GB)
&
More than **120M** particles on ***gamer* GPUs** (24 GB)

Testcase for performance test

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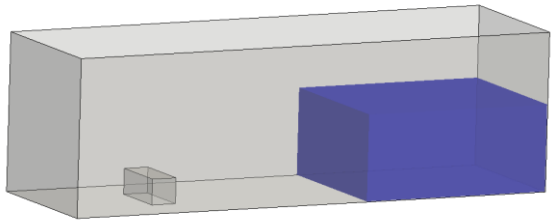
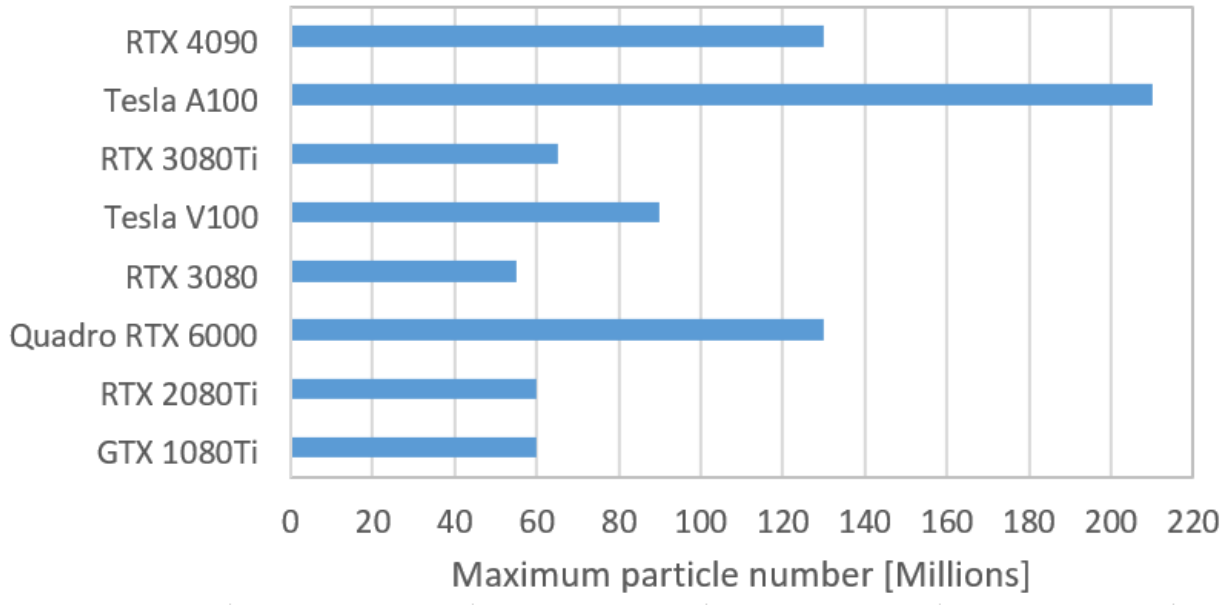
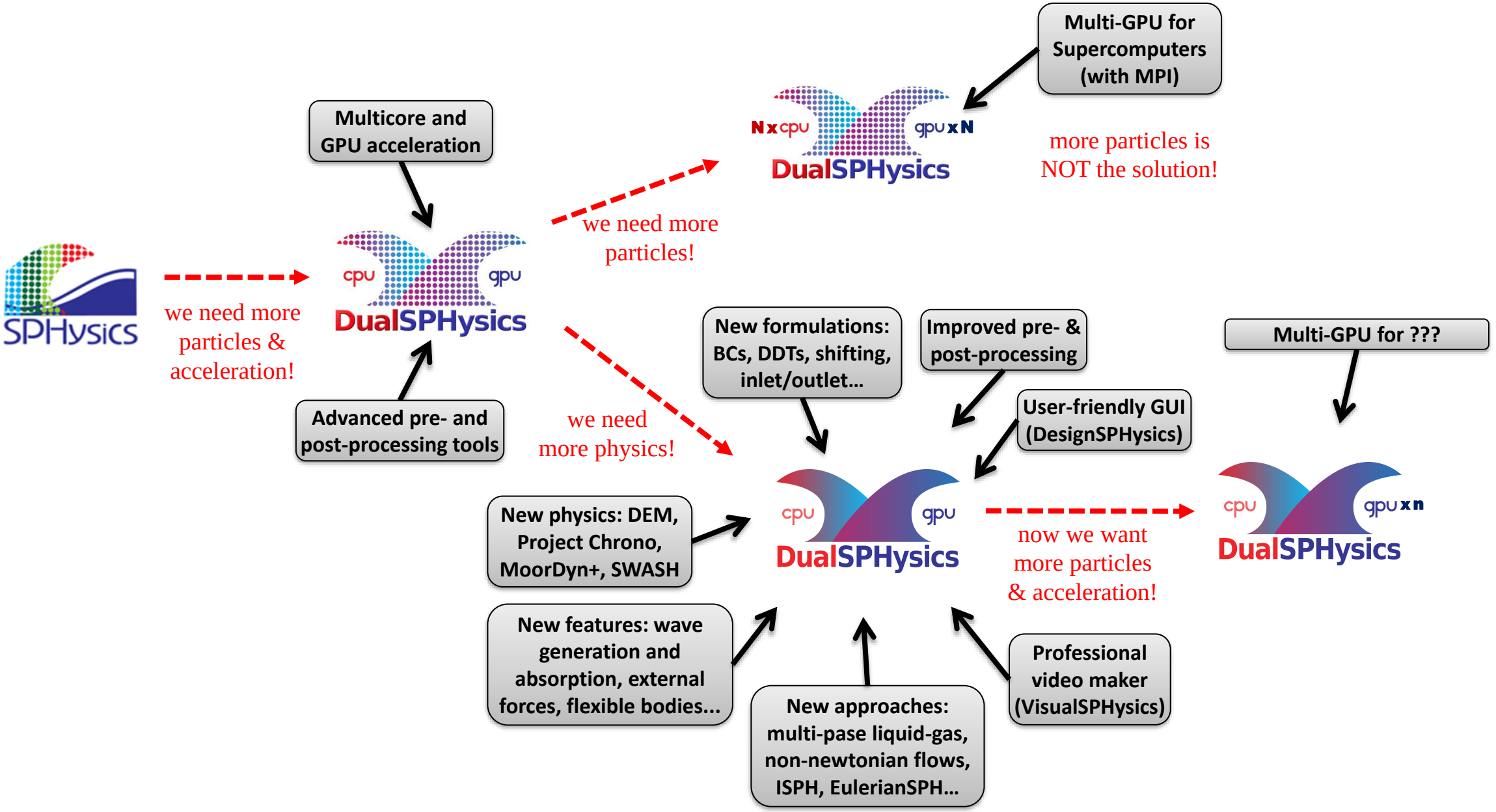
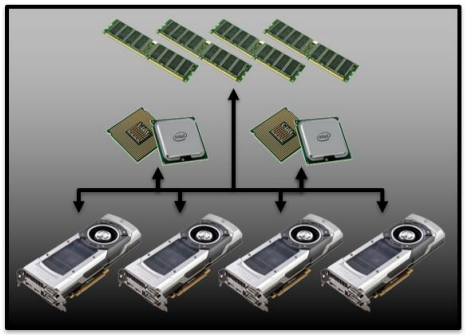




DualSPHysics evolution



New Multi-GPU approach for single-node



multi-GPU machine

Implementation based on C++ threads and CUDA streams (not MPI)

The target is…

- Multi-GPU **useful for researchers** using DualSPHysics (not computer engineers)
- **Full support** of all current DualSPHysics functionalities
- Aimed at **100-200M** particle simulations **without extra user effort**
- Multi-GPU to run on a workstation or computing node with 4-8 GPUs
- **Accessible hardaware** for research groups with limited financial resources

Advantages:

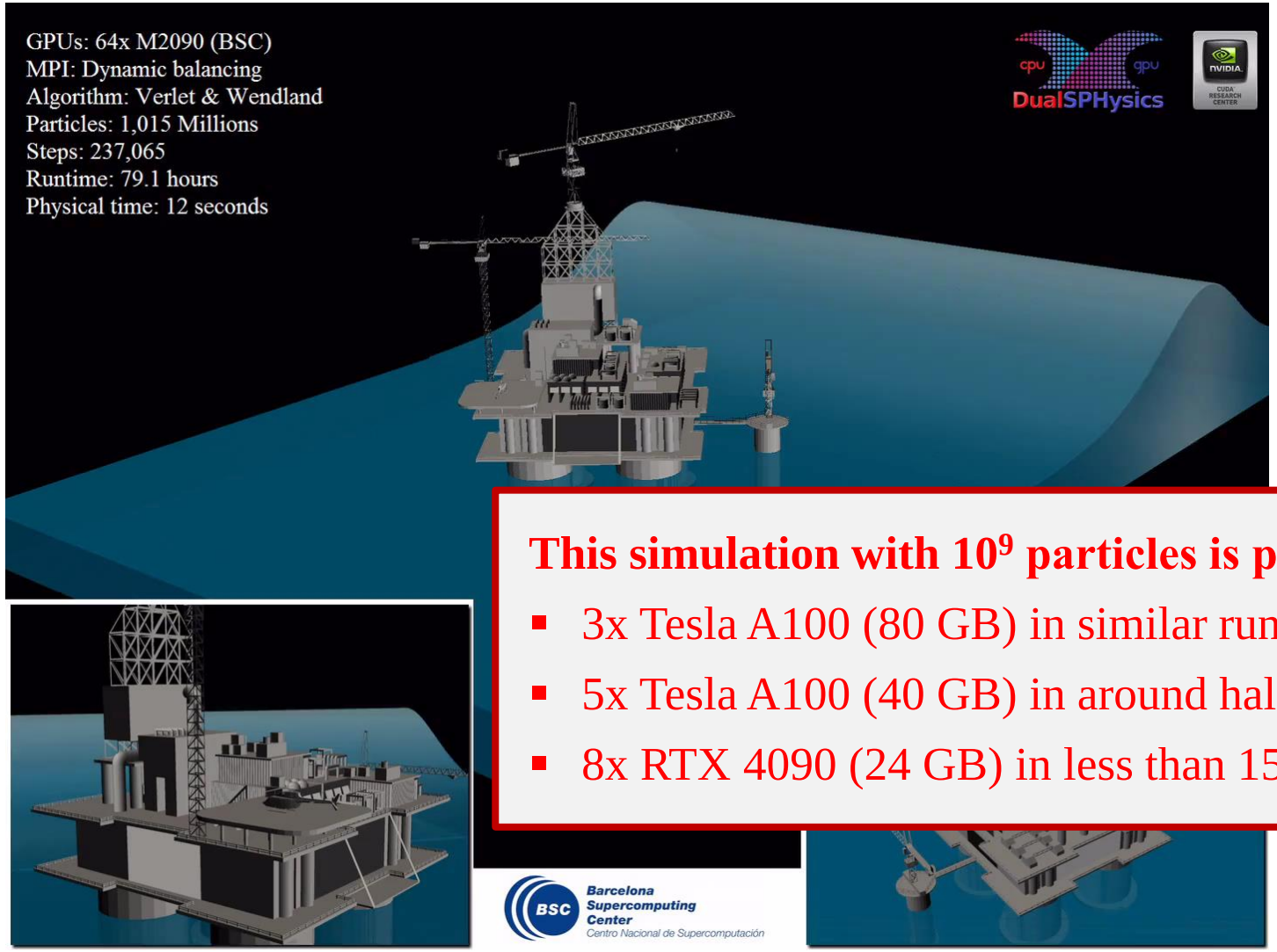
- More portable and easy to use in Linux & Windows
- Simpler code using shared CPU memory for main program data
- More efficient communication. MPI overhead was removed.
- Not special pre-processing and post-processing tools required

Drawbacks:

- Limited number of GPUs (2-8 GPUs)
- Does not work in distributed systems
- Limited size of the simulations?

Multi-GPU for supercomputers using MPI

Largest full SPH free-surface fluid simulation in 2013. More than 1 billion particles!!



- Large wave interaction with oil rig using **10^9 particles**.
- More than 237,000 simulation steps to simulate **12 physical seconds**.
- **79.1 hours** using **64 GPUs** Tesla M2090.
- **Huge complexity** for pre-processing, simulation and post-processing.

This simulation with 10^9 particles is possible with…

- 3x Tesla A100 (80 GB) in similar runtime
- 5x Tesla A100 (40 GB) in around half runtime
- 8x RTX 4090 (24 GB) in less than 15 hours (5 times less)

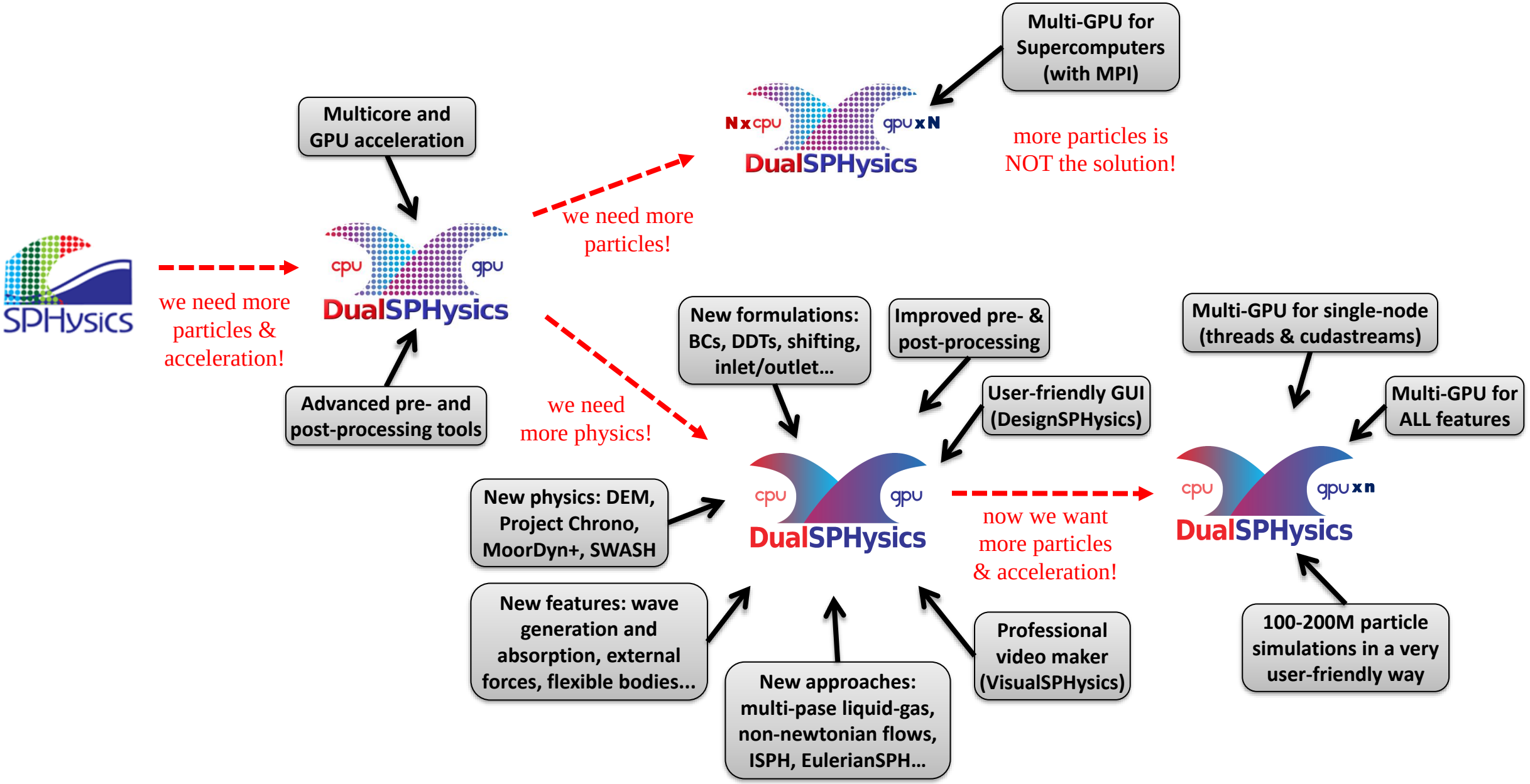
llenge but not very

mputer is required.

practical use.

ot allow modelling of involving different physical phenomena.

DualSPHysics evolution



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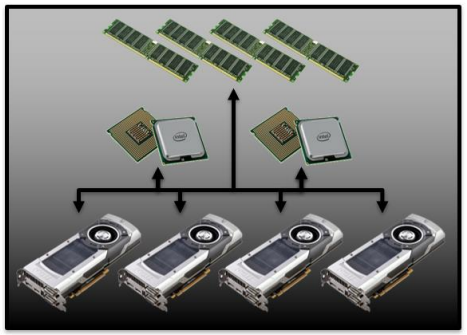

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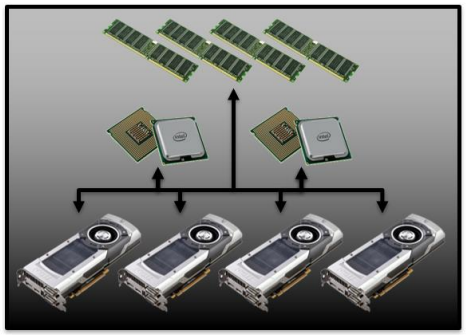
- **Accessible hardaware** for research groups with limited financial resources

The challenges are…

- DualSPHysics includes a lot of functionalities and options (**full support is not easy**)
- **Refactoring of many parts** (floating bodies, gauges, inlet/outlet…) is mandatory to minimise communication and synchronisation points
- The pre-processing tool can generate up to 500M particles (upgrade is necessary)
- GPU acceleration may be required for some post-processing tools (e.g. IsoSurface)
- More post-processing options in the DualSPHysics solver are necessary to minimise the size of the output files (7.7GB per output file of 100M particles)

New Multi-GPU approach for single-node

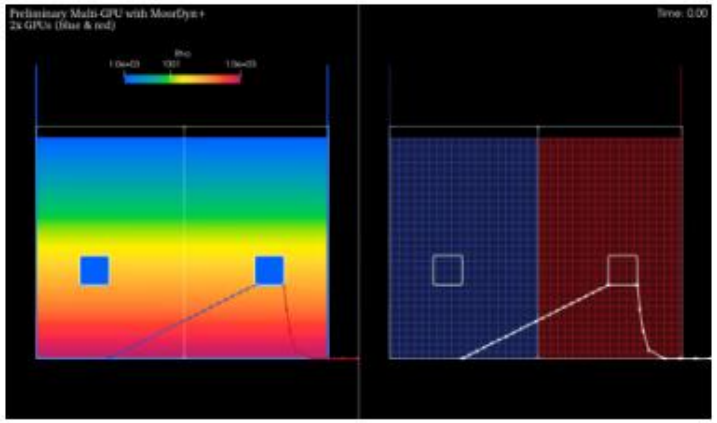


multi-GPU machine

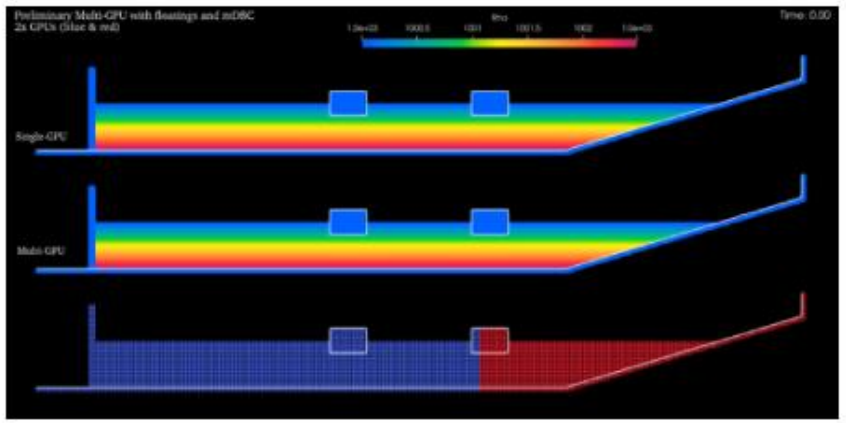
Implementation based on C++ threads and CUDA streams (not MPI)

Work in progress…

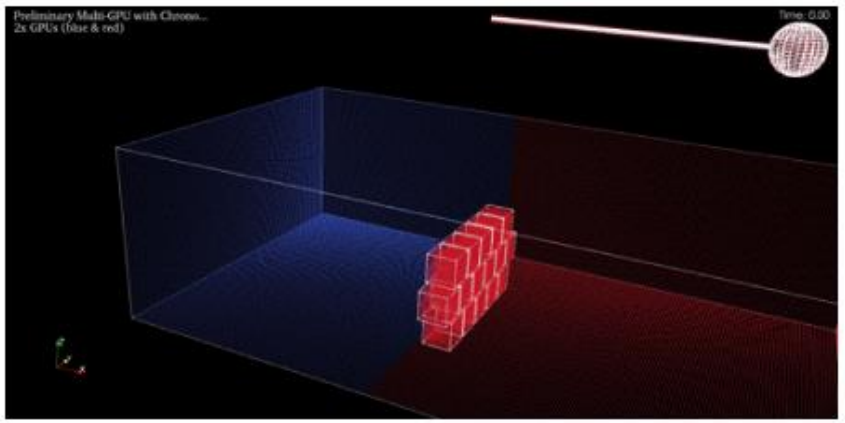
- All formulations are finished, but some significant functionalities are missing
- 74% of the example cases included in the release package (more than 100) already support multi-GPU
- Preliminary results are very promising
- **New multi-GPU release expected in 2025!!**



Moored floating bodies on multi-GPU



Floating bodies between 2 GPUs using mDBC



Project Chrono simulation on multi-GPU