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DualSPHysics

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Preparation for the SPH Modelling Process

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Introduction

Typical situation: You have decided to use SPH to simulate your problem and you're ready to get started!

… but …

Question: How *exactly* do you get started?

Aim of this guide: to take you through the processes you need to consider before running an SPH simulation.

- The purpose of this guide is not to teach you how to use `GenCase`, but to think about your application and SPH approach BEFORE you setup your simulations.
- How to avoid the frustration of not understanding why an SPH failed.
- Understand what is and is not possible with SPH

To address this, we are going to take you through the following topics:

1. Familiarisation with key SPH concepts
2. Planning: Key Pre-Preparation Questions
3. Geometry Preparation
4. Particle Generation
5. Physics Setup
6. Solution control with SPH & DualSPHysics
7. Post-processing: preparing your simulation to extract the data you want
8. Strategy for preparing your simulation

1. Familiarisation with key SPH concepts

The process of running SPH simulations is much easier if you can understand the key concepts of the SPH method:

- What is an SPH particle?
- What's the difference between the particle size (`dp`) and the smoothing length h?
- What is the smoothing kernel?
- Accuracy when the support of the kernel (radius of influence) overlaps with a boundary?
- How are boundaries represented in SPH?
- What SPH can and cannot do?

2. Planning: Key Pre-Preparation Questions

Before **ANYTHING**, you need to understand what you are trying simulate.

Ask yourself **KEY QUESTIONS**:

- What are the dominant physical processes you want to predict?
- What are the important length and time scales for your application?
- What dimensionless numbers characterize your application?
- Can SPH predict these length and time scales?
- Can SPH predict the dominant physical processes?
- What resolution (=particle size or `dp`) is required to capture these processes?
- Does the SPH model include the appropriate physics in its formulation?

3. Geometry Preparation

i) Sizing your domain

Bounding Box: Unless your domain is a 3-D 3-way periodic domain, your domain will likely have solid wall boundaries. Solid walls are represented by particles.
The bounding box of your domain must contain all the solid particles.

ii) What happens when my particles move?

Our particles move (of course!). What **consequences** does this have? The initial limits of our domain will need to change and this must be considered in the intial setup. In DualSPHysics, this is covered by the command `<posmax x="default" y="default" z="default + 50%" />`

iii) Inflow-outflow boundaries

Their location must be chosen carefully so that the buffer zone (if this is used) is still contained in the Bounding Box.

4. Particle Generation

i) Choosing dp

Before you run your simulation, (hopefully) you're probably thinking/asking:

"How do I choose my particle size `dp`?"

Before you can answer this question, you need to ask some important **key questions**:

(i) What are the **important length and time scales** for your application?
(ii) Can SPH predict these length and time scales?
(iii) Can SPH predict the dominant physical processes?
(iv) What resolution (=particle size) or `dp` is required to capture these processes?
(v) How are boundaries represented and how does this influence size of `dp`?
(vi) How do I check my results are converging with decreasing particle size?

ii) How are boundaries represented?

In DualSPHysics, we have 2 types of boundary conditions:
Similar to many codes or software, the boundaries are represented by particles.
Therefore, we have to choose `dp` to satisfy multiple criteria:

1. Predict the phenomena & processes we want
2. Generate the geometry & boundary
3. The number of particles `Np` is not too large for the computing device (e.g. GPU).

iii) Filling algorithms to create particles

Each SPH software will have its own way of creating the particles:

- DualSPHysics uses an initial seeding point and fills the domain until boundaries are encountered.
- DualSPHysics uses Marker values called Mk values to identify particles belonging to different components.
- Having the correct order of objects is important to avoid leakage and over writing (see later).

5. Physics Setup

In addition to understanding numerical behaviour of SPH, choosing the **right formulation and physical parameters** has a huge effect on the simulation.

Putting it simply: Choosing the wrong SPH formulation and physical parameters means your results can be nonsense.

Without the right physics, most likely your simulation will CRASH!

In DualSPHysics, the range of physics that can be simulated include:

(i) Singe-phase fluid flows with inflow-outflow boundaries
(ii) Fluid-structure interaction (FSI)
(iii) Non-Newtonian flows with multiple components
(iv) Multi-phase flows: liquid-gas

Let's look at these in turn to have an introductory understanding of how to start thinking about using this in your simulations.

Table 1 SPH physical settings: FLUIDS

SPH Parameter	Effect & considerations	Typical choices
Representation of fluid & Equation of State (EoS)	3 possible options exist for fluids: (ii) **Weakly Compressible SPH (WCSPH)** – explicit 1-to-1 link of pressure & density: $p = f(\rho) \rightarrow$ easy to implement but small timestep & pressure field fluctuations (iii) **Incompressible SPH (ISPH)** – pressure Poisson equation (PPE) needs a linear algebra matrix solver → computationally expensive, but larger timestep & noise-free pressure fields (iv) **Fully Compressible SPH** where pressure $p = f(\rho, e)$ – requires 3 conservation equations: $d\rho/dt$, $d\mathbf{v}/dt$, de/dt	For WCSPH two choices are common: Tait's EoS: $\gamma = 7$ or Morris $\gamma = 1$
Speed of sound	Affects compressibility, timestep (via CFL condition), wall clock time for simulation	For WCSPH: $c_s \geq 10 \times \max v_{particle}$
Density diffusion	Controls the appearance of density (and hence pressure) fluctuations for WCSPH.	
Viscosity & turbulence	This depends on the Reynolds number of the flow.	Large-Eddy Simulation (LES) Sub-Particle Scale (SPS) turbulence model

Table 2 SPH physical settings: FLUID-STRUCTURE INTERACTION

SPH Parameter	Effect & considerations	Typical choices
SPH representation of solids	Solids objects represented by SPH particles (fluid particles with prescribed motion)	
Project Chrono	Motion and connectivity is controlled by Differential Variational Inequality	
Discrete Element Method (DEM)	Soft-contact model.	
Flexible Structures	Total Lagrangian SPH (TLSPH) for structure WCSPH for fluid	

Table 3 SPH physical settings: MULTI-PHASE LIQUID GAS

SPH Parameter	Effect & considerations	Typical choices
Speeds of sound	Each phase has a different speed of sound. Affects CFL condition.	Values depend on SPH formulation
Surface tension coefficient	Uses Continuum Surface Force (CSF) approach with gradients of colour functions.	Case dependent

Table 4 SPH physical settings: MULTI-PHASE NON-NEWTONIAN

SPH Parameter	Effect & considerations	Typical choices
SPH representation of rheology	Changes behaviour of non-Newtonian fluid.	Bingham Herschel-Bulkley-Papanastasiou
CFL number	This will be different to Newtonian fluids since non-Newtonian flows have different diffusion characteristics.	Case dependent

6. Solution control with SPH & DualSPHysics

When we run a simulation, there are many solution parameters that we can set.

We can group these Solution Control Parameters into 2 categories:

(i) SPH **numerical parameters** that control how the SPH solver behaves
(ii) Typical SPH **software-specific parameters** that control how the simulation runs

Let's look at these in turn.

(We won't consider the choice and control of hardware here)

Table 5 Solution Control 1: SPH numerical parameters

SPH Parameter	Effect & considerations	Typical choices
h/dp ratio	Controls radius of kernel relative to particle size. A larger *h*/dp means more neighbours inside each kernel, more particle-particle interactions and longer simulations but probably smoother results.	1.2 – 3.0
CFL number	Controls stability of explicit timestepping calculation. Larger CFL means larger timesteps, but less stability.	0.1 – 0.3
Choice of TimeStepping	Controls stability, dissipation, diffusion and conservation of energy & momentum over time. Must be second order or higher since the particles move!	Velocity Verlet Symplectic
Choice of Boundary Condition	Depends on BC theory implement in code. DualSPHysics example: - Dynamic Boundary Condition (DBC) → very fast simulation - Modified DBC → better velocity profiles near boundary, but more computationally expensive & time to set up	
Choice of Kernel	Cubic spline (3rd order approximation to a Gaussian) Wendland (5th-order), less clumping and greater stability	Wendland
Particle Shifting	Applies a tiny shift (or movement) particles at end of timestep to keep particles regularly spaced → reduces instability & noise	Fluid particles only Shifting coefficient = -2

Table 6 Solution Control 2: Software-specific parameters

DualSPHysics Software Parameter	Effect & considerations	Typical choices
TimeOut	Max physical time (s) of simulation	
TimeMax	Time (s) between each output frame e.g. time (s) between PART0001 to PART0002	TimeOut/100 → 100 frames (PART files)
RhopOutMin RhopOutMax	Min and Max values of particle density (rhop) before particle is removed from simulation (to prevent instability and particle clumping)	700 kg/m^3 1300 kg/m^3
DtIni	Initial timestep. Having too large a timestep initially can render the simulation unstable from the start.	Case specific
PartsOutMax	Percentage (%) of particles allowed to leave the simulation before simulation is stopped (not including open boundaries!).	1%

There are many other parameters in DualSPHysics (see <parameters> section of case XML file)

7. Post-processing: preparing your simulation to extract the data you want

If we want to plot the force on a specific surface (for example the right wall of a dam break in a 2-D rectangular tank), how do we do this?

The right-wall needs to have its own specific marker. In DualSPHysics this can be achieved using Mk values specifically for that wall.

So, before running the simulation, think about what data you want to extract and where you want to extract it.

8. Strategy for preparing your simulation

In addition to the previous points we have covered, I have some standard advice worth repeating.

Many test cases are **very complex**.

Be realistic. Don't try to set up the entire complex simulation and expect it to work immediately.

Build your simulation in stages adding & checking each element of complexity one by one:

1. Start from a working example.
2. Change one thing at a time.
3. Check each change does not “break” your setup or your simulation.
4. Repeat until you reach the setup you want.