AWS HPC Blog

Three-dimensional simulation of a dam break flow over an obstacle with WINTS on AWS

by Georges Halim Atallah, Benoît Trouette and Stéphane Vincent | on DD MMM 2022 | in link, link, link | Permalink |
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This post was contributed by Steve Messenger, function, Gilles Tourpes, function.

WINTS is a **W**eb **INT**erface for **S**imulation in fluid mechanics and heat/mass transfer. It was born from an assumption: the need for enterprises to design ever more innovative services or products quickly, with limited cost and risk. This cost and risk are explained by the fact that most "classic" product or system design processes systematically involve physical prototypes. In many cases, these prototypes involve complex physical phenomena that appear in a wide variety of sectors of industry, aeronautics, automobile, or even computer science, etc. Among these physical phenomena, we can mention fluid mechanics which can easily be identified as being present in a very wide spectrum of industrial applications (environment, energy, nuclear, wind, naval, meteorology, health, security, agriculture, etc.).

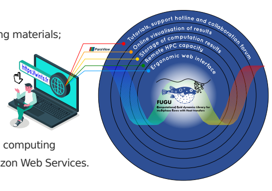
Fluid mechanics is the study of the movement of liquids and gases. It is a complex science, so much so that it is now a common practice to use the computational power of hundreds of processors (high performance parallel computing) to solve problems involving fluids with numerical simulations. Using software that contains advanced algorithms for solving the equations of motion of fluids, we model the physics we wish to solve, then we simulate the associated phenomenon by running the software code on computational infrastructure.

The numerical simulation is a tool for design, decision-making and control. It gives access to data that cannot be directly measured experimentally and allows significant savings in money, time and raw materials. It also allows to reduce risk, to increase the freedom of innovation, to study and test many variants of the same prototype, to optimize the designed solutions and to limit failure : this is the framework of digital twins that is covered by WINTS. However, the access to such a technology remains difficult, because it requires expensive computer hardware as well as numerical simulation software that must be skilled.

The aim of WINTS

The main idea of WINTS is to unify everything necessary to perform numerical simulations of fluid flows in heterogeneous media (flows involving two phases such as air and water but also fluid/structure interactions) via a web platform at your fingertips. It includes:

- The numerical simulation software named Fugu;
- An ergonomic user interface for access to non-specialists with training materials;
- The computing resources for its exploitation (Amazon EC2);
- Data storage (Amazon S3);
- Online visualisation of results (NiceDCV and Appstream);
- Expertise, a hotline and an open science collaborative forum.



In short, WINTS attempt to remove the need to invest in expensive parallel computing hardware by providing HPC capacity with the help of partners such as Amazon Web Services.

In this blog, we show how the combination of the WINTS solution and AWS allows users to perform complex computational fluid dynamics simulations in a very easy way. Some features of the Fugu simulator are also presented through the simulation of a three-dimensional dam break flow over an obstacle.

The WINTS solution, a simple way to perform complex CFD simulations

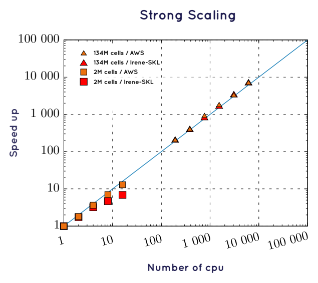
In this section, we present the WINTS solution and how it works with the different AWS services used such as Amazon ParallelCluster, Amazon EC2, Fsx for Lustre or Amazon S3.

An all-in-one Software as a Service solution to easily perform numerical simulations

The structure of WINTS works like a funnel. The first action required from the user is to create a simulation project. Once this project is open, you can create simulations in which you configure the numerical and physical parameters (size of the computational domain, increment of the spatial and temporal discretizations, configuration of the properties of the fluid(s), writing frequency of the visualization files, etc.). Note that you can work in teams with the possibility of associating several members of your account to the same project.

In general, with traditional CFD software, users set up their simulation without being able to check if they have made errors, leading to simulator crashes when the job is run. WINTS has safeguards that allow the user to verify whether or not they have made errors. If so, WINTS will indicate where the error is and how to correct it before launching your job.

Depending on the configuration of parameters that the user has entered, WINTS will analyze it (especially the number of cells) to propose to launch a job with the optimal number of processors to use, taking into account the architecture of Amazon EC2 instances and the parallel scaling behavior of the Fugu simulator.



To manage the job execution with EC2 instances and associated HPC clusters, WINTS combines the SLURM tool with the Amazon ParallelCluster service.

Once the job is started, the simulator will generate visualization data files containing the flow velocity fields, pressure, its eventual different phases, turbulent viscosity, etc. according to the writing frequency the user specified in the configuration parameters. These data can be visualized directly on WINTS using Paraview, which is an open-source data analysis and visualization application. It is also possible to download them to visualize them locally. For I/O data management and storage, WINS has chosen to use technologies from FSx for Lustre and Amazon S3 services.

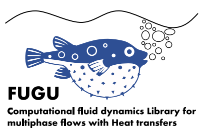
FSx is a high-performance, parallelized shared file system dedicated to HPC. Depending on the simulation you are performing, it is possible that the Fugu simulator generates large files with high writing frequency. In this case, FSx for Lustre is very well suited for intensive I/O. FSx will only be used for writing and eventually reading data from the simulator. When a job ends, the data that was written to the FSx shared file system is automatically moved to an Amazon S3 bucket in a fully transparent way for users.

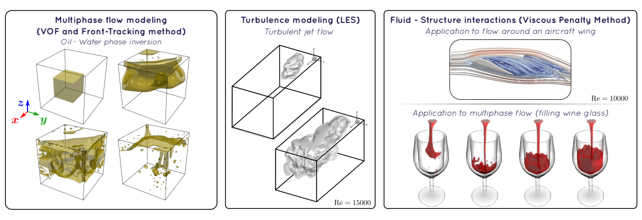
If you use the WINTS solution intensively, with several members running jobs on the same account, an interesting feature that is offered is the monitoring of the use of computing resources (EC2) and data storage (S3). This will help you not to overuse resources and to manage your data serenely.

Overview of the Fugu simulator through the simulation of a three-dimensional dam break flow with a solid obstacle

In this section, we present a use case of the Fugu simulator through the simulation of a three-dimensional dam break flow over an obstacle.

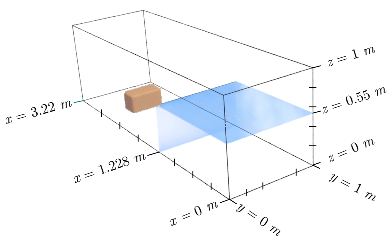
Fugu is a home-made Fortran simulation software for fluid mechanics and heat/mass transfer. It is developed by the Heat and Mass Transfer team of the MSME laboratory from Gustave Eiffel University in France and this is the core technology of WINTS. Fugu is dedicated to the multi-scale modelling of complex mass and energy transfer configurations, including flows in heterogeneous media, namely, flows involving two phases such as air and water but also fluid/structure interactions. The simulator is parallelized according to the MPI standard for high performance computing and the conservation equations are solved with a finite volume method on a staggered Cartesian grid. Some illustrations are given below:





Description of the case

We consider here the three-dimensional dam break flow over an obstacle to handle real three-dimensional free-surface flows. This configuration is interesting as the unsteady behavior of the free-surface flow is characterized by interface ruptures and coalescences with the effect of the presence of an obstacle. The fluids considered here are water and air and the dimensions of the computational domain are 3.22 m × 1 m × 1 m. The initial water reserve dimensions are 1.228 m × 1 m × 0.55 m. The figure below shows the initial state of the flow before the dam break.

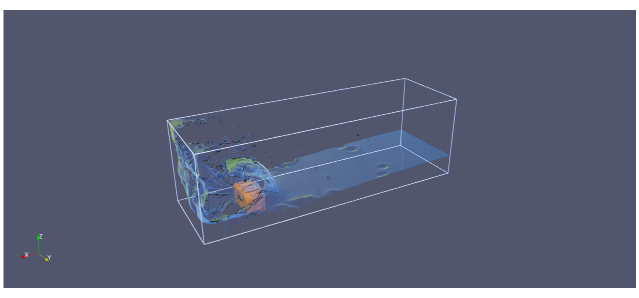


Two probes H_1 and H_2 are used to compute the numerical time evolution of the free-surface elevation respectively at (x_1, y_1) = (0.614 m, 0.5 m) and at (x_2, y_2) = (1.726 m, 0.5 m). Others probes pressure points P_1 and P_2 are used to compute the time evolution of the pressure in the front side of the obstacle respectively at (x_1, y_1, z_1) = (2.42 m, 0.5 m, 0.04 m) and (x_2, y_2, z_2) = (2.42 m, 0.5 m, 0.08 m). This quantities are then compared with experimental data [1].

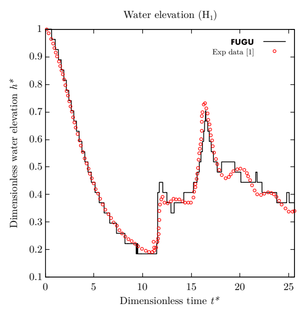
The computational Cartesian grid used here contains 161 × 50 × 50 (405 500 cells) and we use a adaptative temporal increment according to a CFL equal to 0.5.

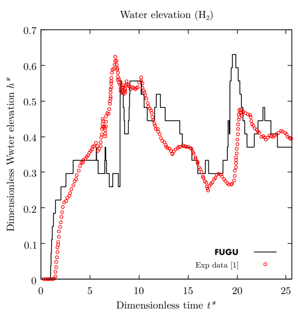
The parallelepiped obstacle of dimension 0.1 m x 0.2 m x 0.2 m is numerically modeled by a fictitious domain approach and a penalty method [2,3]. Concerning the resolution of the flow, a one-fluid formulation is adopted here to model the two-phase flow with a conservative VOF method. In practice, this means solving the motion of a single fluid whose physical characteristics such as density varies between that of air and water. Furthermore, the surface tension forces between air and water have also been considered. Finally, a fully coupled method for velocity-pressure coupling is used here to solve the two-phase flow with high density and viscosity ratio between the two phases [4, 5].

The evolution of the two-phase flow over the parallelepipedic obstacle can be watched in the video (or figure) below:



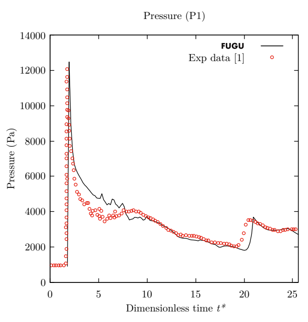
Let's now look at the ability of the simulator to reproduce the correct real physical behaviour by comparing the numerical results (free surface elevation and pressure in the front side of the obstacle) with the experiment [1]. The time evolution of the free-surface elevation values of probes H_1 and H_2 are presented in figure (xx):

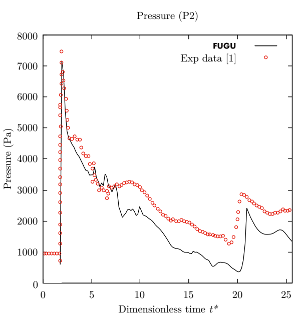




We can notice a very good global agreement between the measurements and the simulations. Here the main discrepancy concerns the H2 probe with the water elevation slightly in advance compared to the experiment as well as an overestimation of the water elevation peak at t^* =19.5.

In the figure xx are presented the comparison of the numerically and experimentally obtained pressure values in the front side of the obstacle





In the same way as the water elevation, the numerical pressure probes provide values very close to the experimental values. However, one difference is that the numerical pressure is underestimated compared to the experimental one on the P2 probe.

Conclusion

WINTS, associated with an ergonomic interface and its FUGU simulator, tends to facilitate access to a high-tech numerical simulation tool without the need for specific skills. In addition to this, there are the hardware requirements (computing power) that we manage to remove without too much effort thanks to partners such as AWS, which provides the most recent hardware. It is also the services offered by AWS that allow us to meet the technical requirements of WINTS and make it reach its objective. Amazon EC2 and its scalability allows WINTS to run its entire workload, regardless of its size. The FSx file system allows the FUGU simulator to perform very low latency I/O and all generated data is stored, secured and available in S3 buckets. Such a strategy will save WINTS users time and money.

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