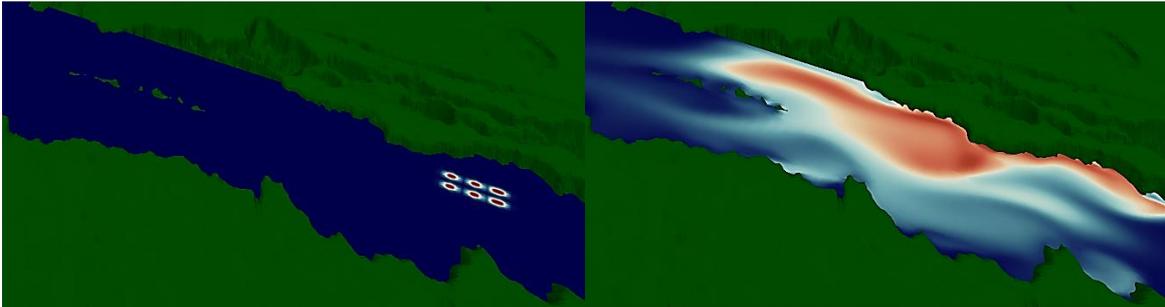


***marineFoam*: A Computational Tool for Modelling Chemical Discharge from Marine Fish Farms**

Dr Tom Scanlon BEng PhD CEng MIMechE

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Abstract

marineFoam is a new computational fluid dynamics (CFD) tool aimed at modelling the dispersion of anti-parasitic chemicals used during bath treatments to counteract sea lice in fin fish farms. The computational model has been developed within the framework of the open-source, finite volume CFD code OpenFOAM and is designed to be used either as a high-fidelity, stand-alone code or as a complementary tool to inform and improve the lower-order bath treatment models currently promoted by SEPA. An unstructured grid, non-hydrostatic approach is adopted, and the water density is calculated as a function of both salinity and temperature. Boundary conditions allow for tidal currents to be implemented and turbulence is modelled using a 2-equation, unsteady RANS approach. Arbitrary mesh refinement (AMR) is incorporated in the model together with higher order convection schemes to minimise numerical diffusion of the dispersed chemicals. *marineFoam* has been verified against the state-of-the-art, open-source community ocean model FVCOM with results comparing well with published data. Finally, *marineFoam* has been shown to produce full 3D, time-dependent solutions for chemical dispersion in a marine coastal loch with complex bathymetry. These results were determined for a physical domain of the order of ~ 1 km and the computational time involved was approximately 1 hour of CPU time per hour of tidal cycle modelled. This demonstrates that high fidelity CFD results for such scenarios are within practical engineering reach using standard, off-the-shelf PC hardware.

1. Introduction

Conventional marine aquaculture operations require chemical treatments to address the harmful effects of sea lice on salmon health. This normally consists of a topical bath treatment where the fish cage is isolated using an impermeable membrane and dosed with anti-parasitic chemicals for a short time period. Following the dosage, the enclosing envelope is removed and the chemicals are free to disperse on the back of tidal and wind-driven currents which advect and diffuse the chemical species into the local marine system. The characterisation of the fate of such chemicals is fundamental to the Environmental Quality Standards (EQS) applied by SEPA to bath treatment chemicals and these have been determined in relation to the toxicity and composition of the anti-parasitic materials used [1]. Such fate calculations allow the determination of licensed discharge quantities and can also help mitigate any site-specific environmental impact by, for example, optimum sea cage positioning and most beneficial release time in the tidal cycle for both proposed and existing fish farms.

Computer modelling is the preeminent technique currently used to predict the distribution of chemicals following a bath treatment. The current SEPA modelling suite for bath treatments consists of two relatively simple, low-order numerical approaches for short and long timescale calculations [1]. Although such unsophisticated models can produce results in comparatively quick timescales it is unclear whether they produce results with the satisfactory scientific rigour required for aquaculture siting. These approaches rely on relatively crude estimates of physical parameters such as local topology and bathymetry, multi-dimensionality, dispersion coefficients and turbulence effects.

marineFoam has thus been developed to help address the issues outlined above and provide clarity as to the efficacy of the current SEPA modelling approaches. The *marineFoam* code may be used in two ways; as a stand-alone, bespoke, high-fidelity model for chemical dispersion over several tidal cycles or as a complementary tool to inform and improve lower-order models and give enhanced confidence in their use.

2. *marineFoam*

The *marineFoam* model has been developed within the framework of the open-source computational fluid dynamics (CFD) software OpenFOAM [2]. With an estimated 10,000 users worldwide [2, 3], OpenFOAM is commonly used in the academic, research and industrial communities as a powerful, open-source alternative to commercial CFD codes [3]. It is a CFD toolbox based on the C++ programming language and the modular nature of C++ allows the user great flexibility to develop their own applications and libraries. The author has over 10-years of experience in the teaching, use and application of the OpenFOAM code.

In this way, *marineFoam* has been created to solve the unsteady conservation equations of mass, momentum, energy and species concentration in conjunction with a 2-equation Reynolds-Averaged Navier-Stokes (RANS) turbulence closure model. A thermohaline linear equation of state has been implemented where the marine water density is calculated as:

$$\rho = \rho_0 [1 - \beta_T (T - T_{ref}) + \beta_S (S - S_{ref})] \quad [1]$$

Where ρ_0 is a reference density, T is temperature and S is salinity. β_T and β_S are the coefficients of thermal expansion and saline contraction, respectively.

2.1 Code Verification

marineFoam has been verified in a test case following the work of Lai *et al* [4] who used a non-hydrostatic version of the oceanographic community code FVCOM [5]. In this numerical experiment, a "Lock-Exchange" problem is considered where a rectangular computational domain is filled half-and-half in the horizontal direction with fluids of densities 999.972 and 1000.991371 kg/ m³, respectively, as shown in Figure 1.

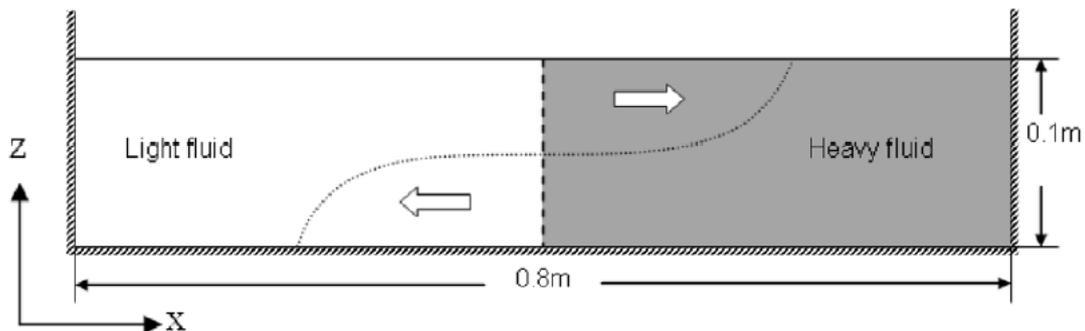
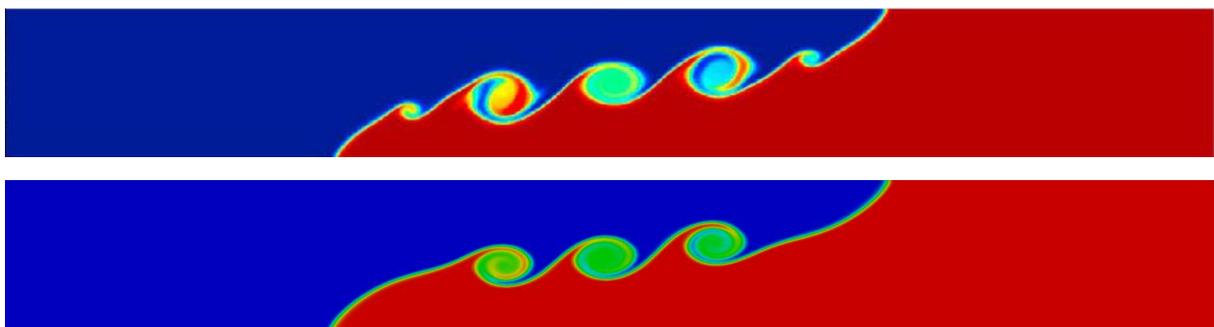


Figure 1 Geometry and initial conditions for the "Lock-Exchange" problem.

Inviscid, isothermal fluid conditions are set and gravitational force provides the impetus for fluid movement as the two fluids mix together. A linear variation in density is assumed according to equation 1 and the salinity contraction coefficient was $\beta_S = 7.5 \times 10^{-4}$. A computational mesh of 400 X by 100 Y cells was employed in a 2D solution and a time step size of 0.003 s was applied. Figure 2 shows the comparison between the *marineFoam* and FVCOM solutions. It is evident that there is a satisfactory qualitative concurrence for the gross features of the flow between the two models thus helping to verify the *marineFoam* code against a state-of-the-art model commonly used by the oceanographic community. Both models are seen to pick up the initial Kelvin-Helmholtz instabilities that occur at the density interface as the fluids begin to mix. Disparities in the results may be explained by the different discretisation schemes employed by each code.

(a)



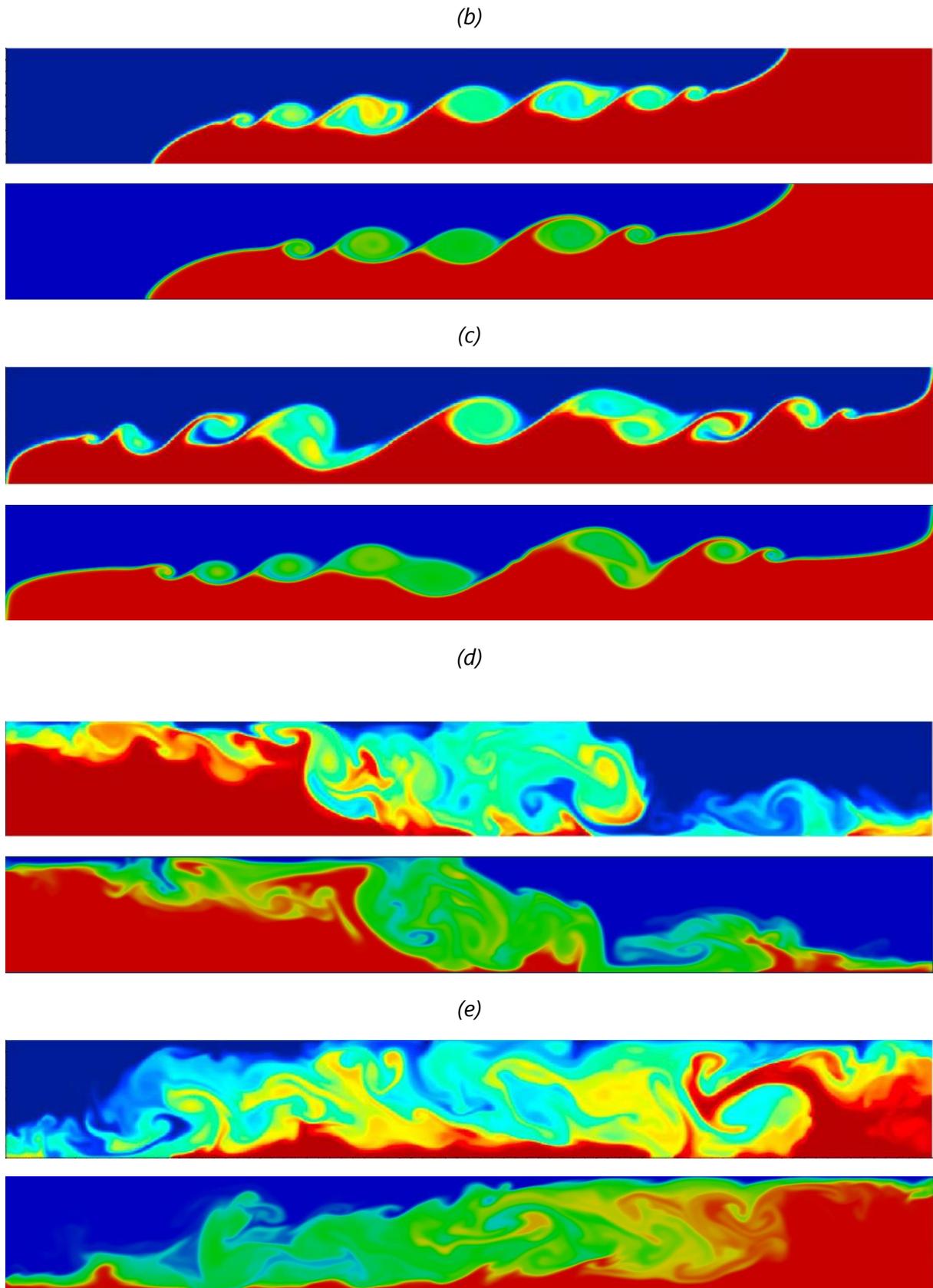
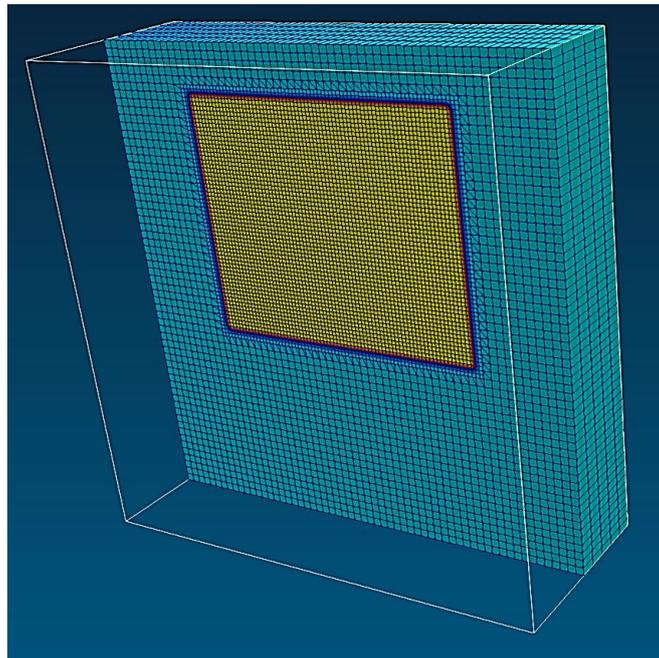


Figure 2 Density field comparison between FVCOM (top) and marineFoam (bottom) at times (a) 12, (b) 18, (c) 27, (d) 78 and (e) 144 s after the vertical barrier is lifted in the inviscid, non-hydrostatic simulation.

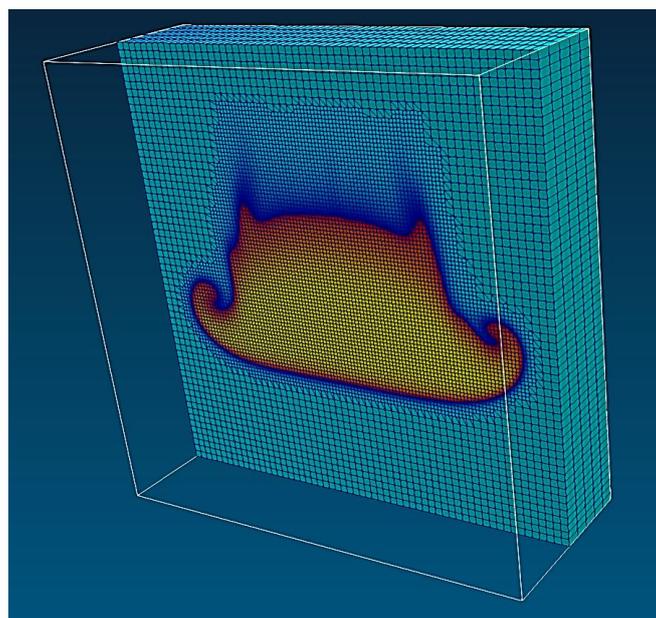
3. Arbitrary Mesh Refinement (AMR)

In order to minimise the effects of numerical diffusion on the transport of the chemical species arbitrary mesh refinement (AMR) has been incorporated into the *marineFoam* code. AMR allows local mesh refinement to take place in regions where the species concentration level is evident, subsequently increasing the accuracy of the advection-diffusion process within the scalar transport equation for chemical species. Figure 3 shows the transient progress of a parcel of heavy fluid (yellow) as it falls into a lighter fluid (light blue) driven by gravitational force. The AMR is shown to increase the mesh density in the regions where the chemical species is being advected.

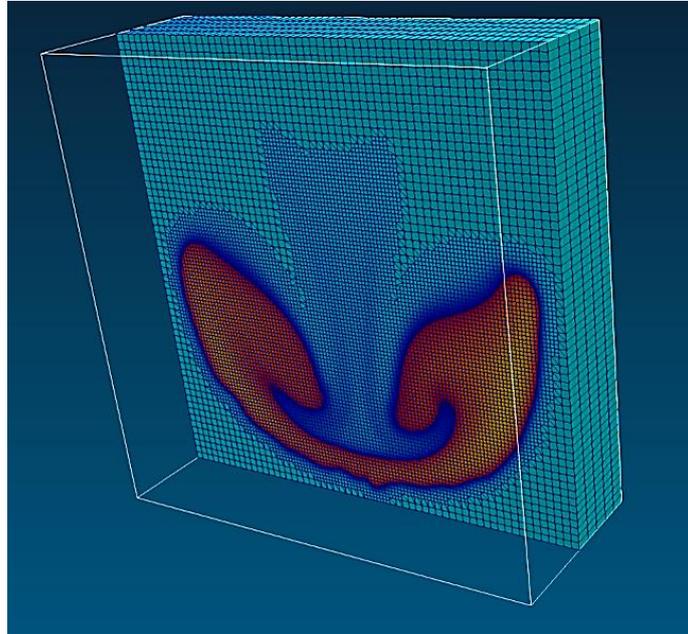
0 s



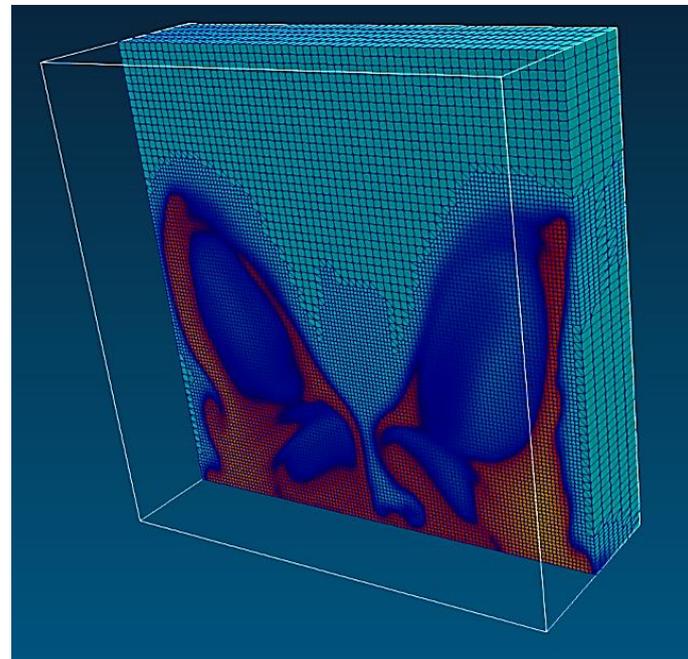
10 s



20 s



30 s



40 s

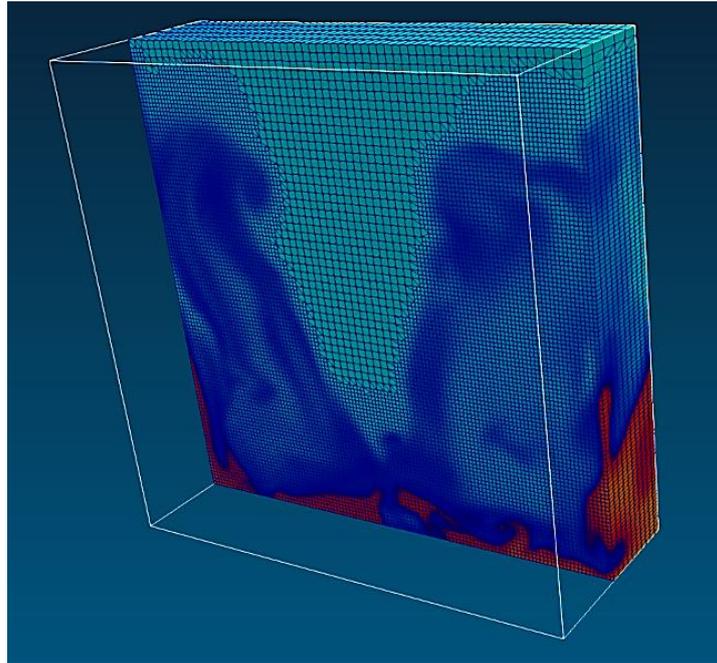


Figure 3 Transient advection of a heavy parcel of fluid showing Arbitrary Mesh Refinement (AMR) on the species concentration field.

4. *marineFoam* Practical Application

In order to test a practical application of *marineFoam* the dispersion of bath treatment chemicals from a salmon farm consisting of 6 cages in a generic sea loch of ~1 km length has been simulated. This case highlights the ability of *marineFoam* to handle complex 3D bathymetry and Figure 4 shows a section of the modelled sea bed with computational mesh.

A sinusoidal boundary condition for velocity has been implemented to mimic the tidal stream currents (real tidal data may also be input in tabulated form). Isothermal conditions were assumed and the density variation with salinity is set following Eq. 1. The initial salinity conditions for the 6 sea cage baths were set such that the cage water had a density of $1000.991371 \text{ kg/ m}^3$ while that of the surrounding marine environment was 999.972 kg/ m^3 . A computational mesh of ~350,000 cells was employed and a time-step size of 1 s was adopted in conjunction with the AMR treatment described in section 3

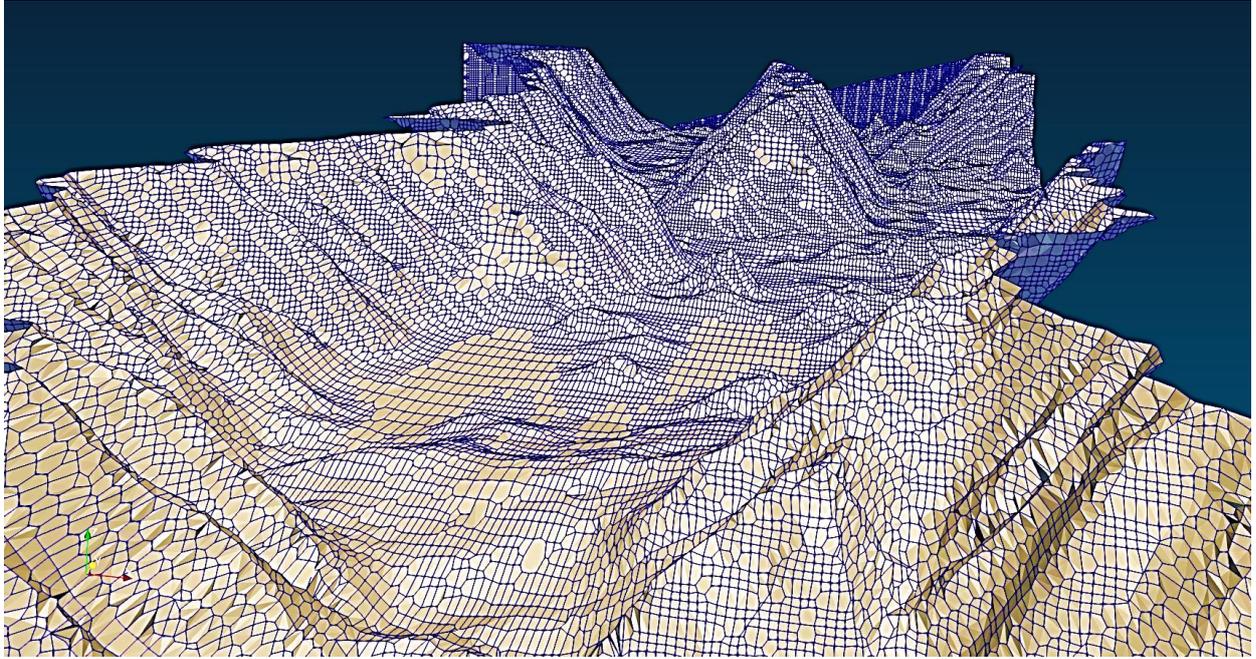
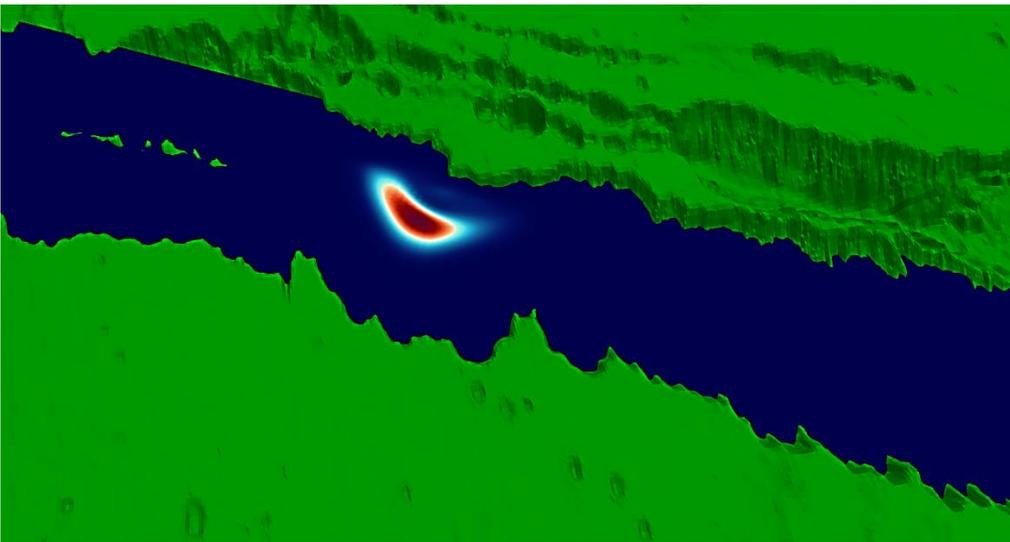
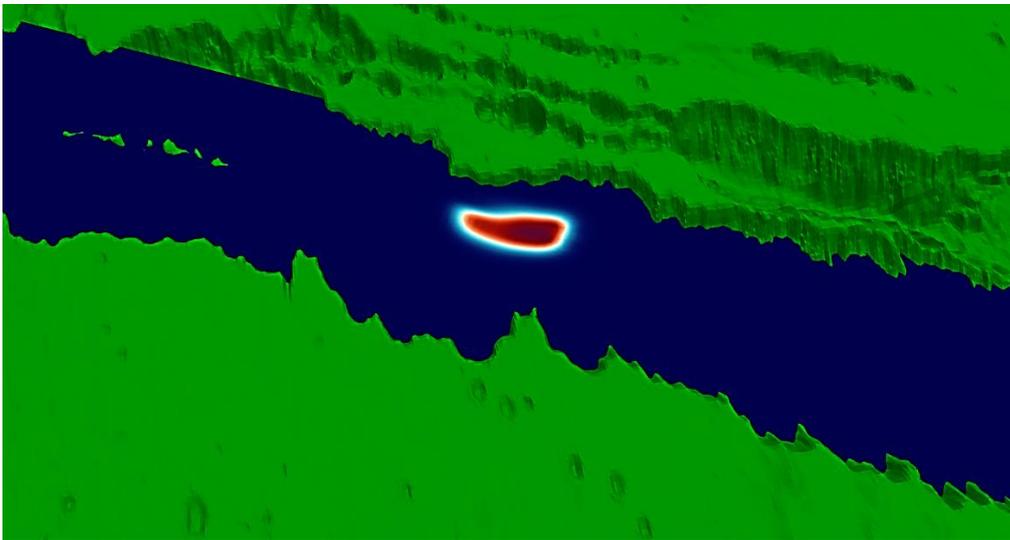
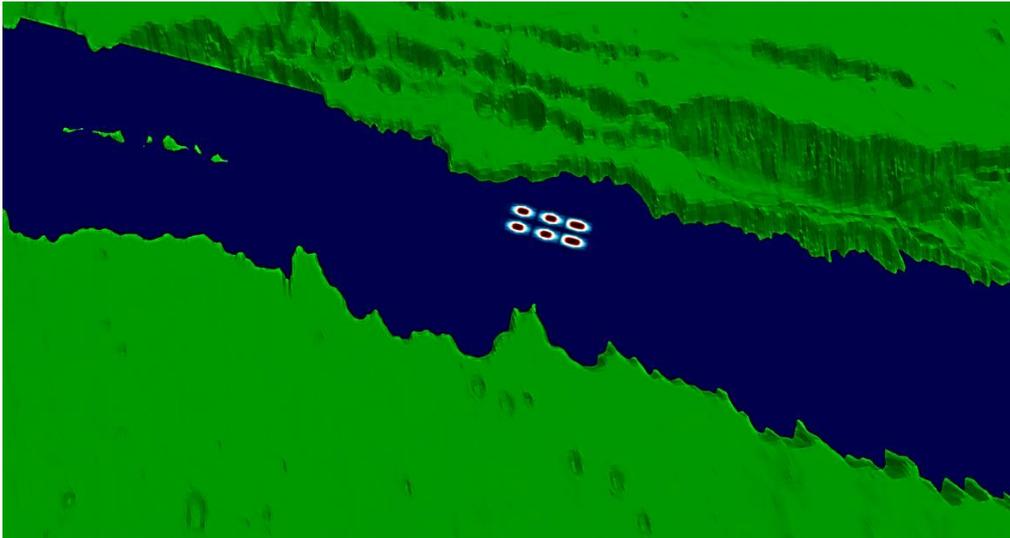
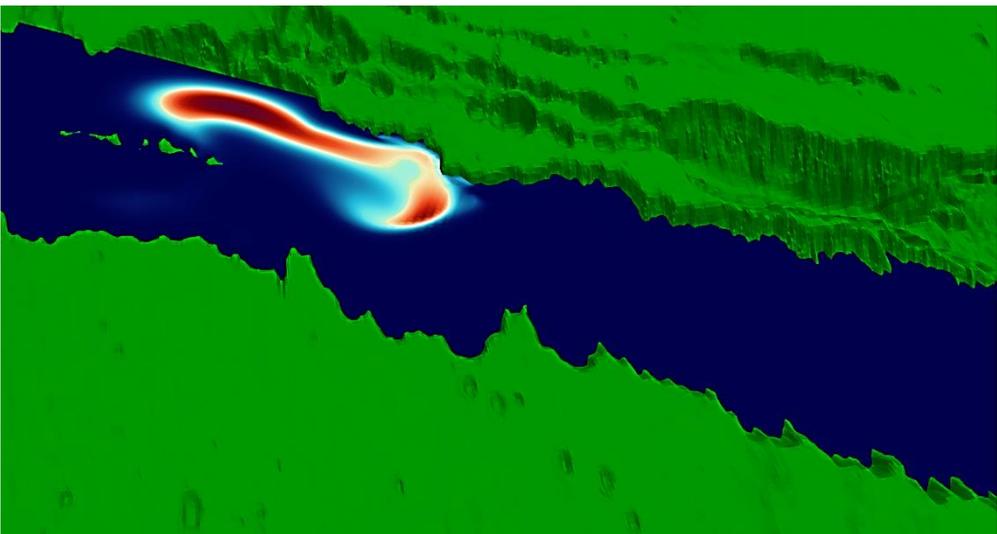
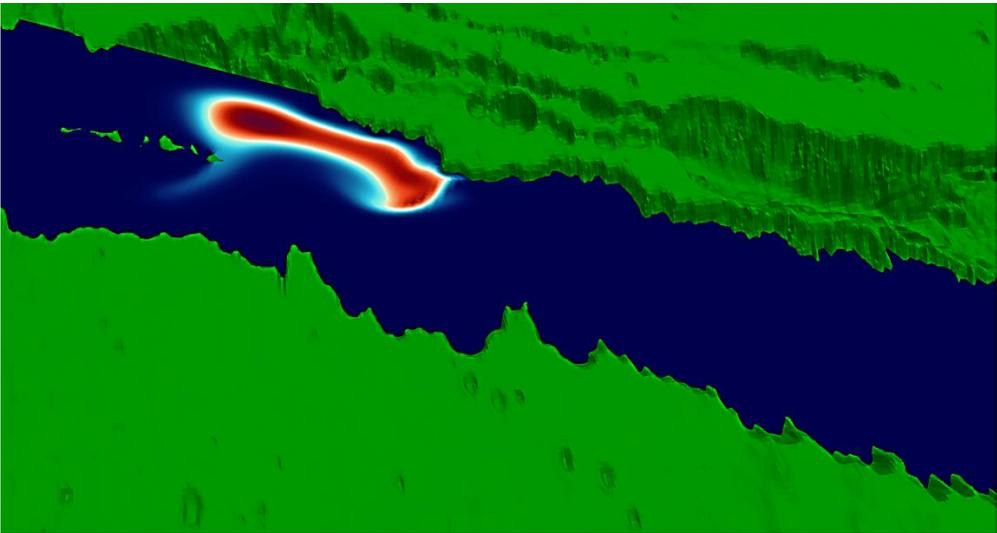
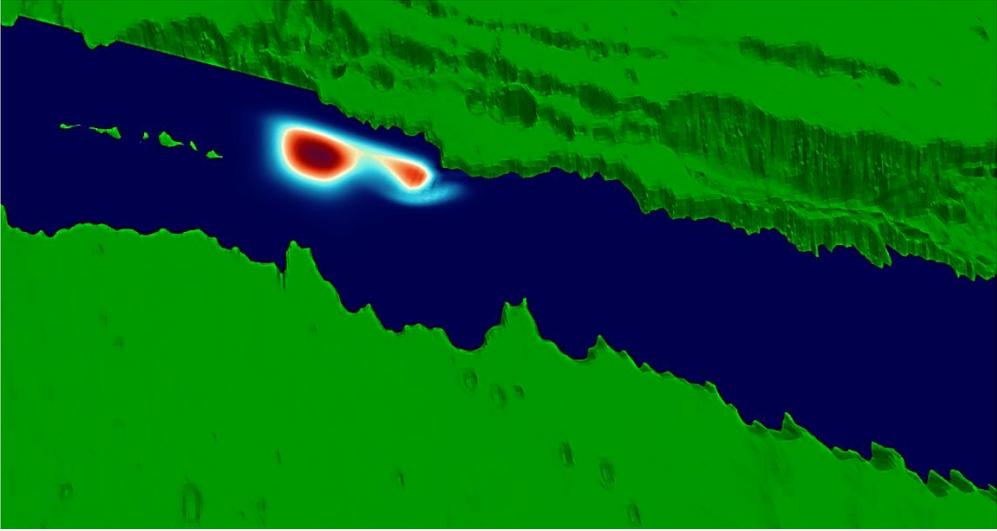
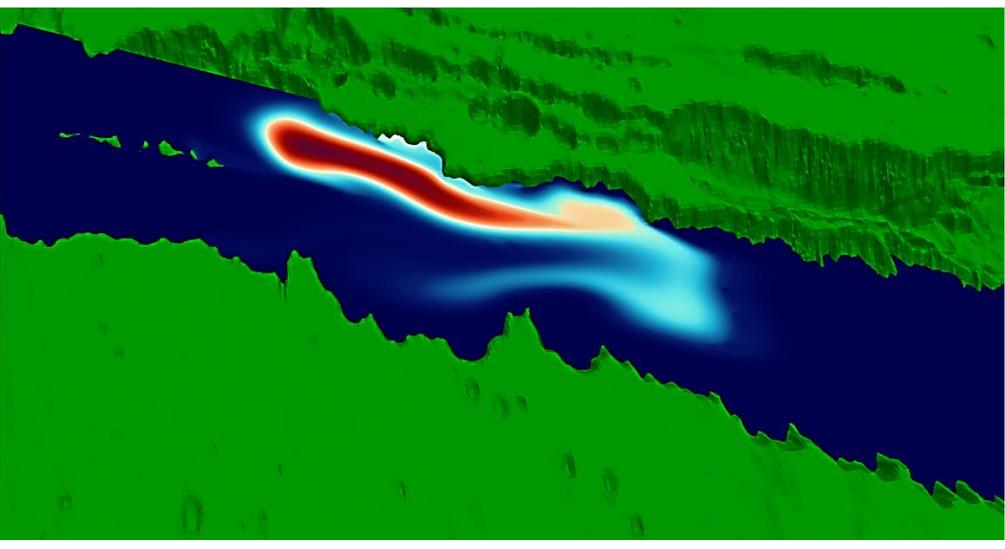
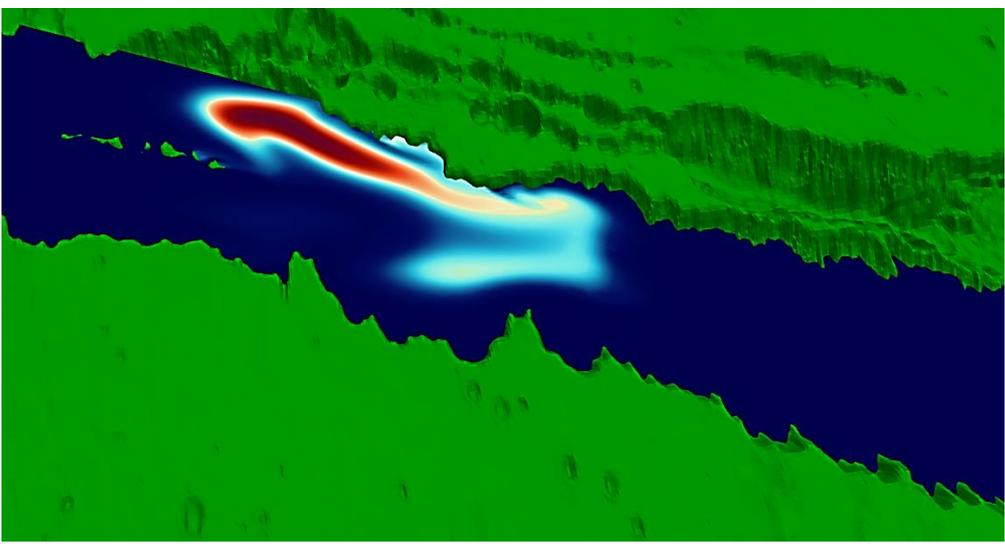
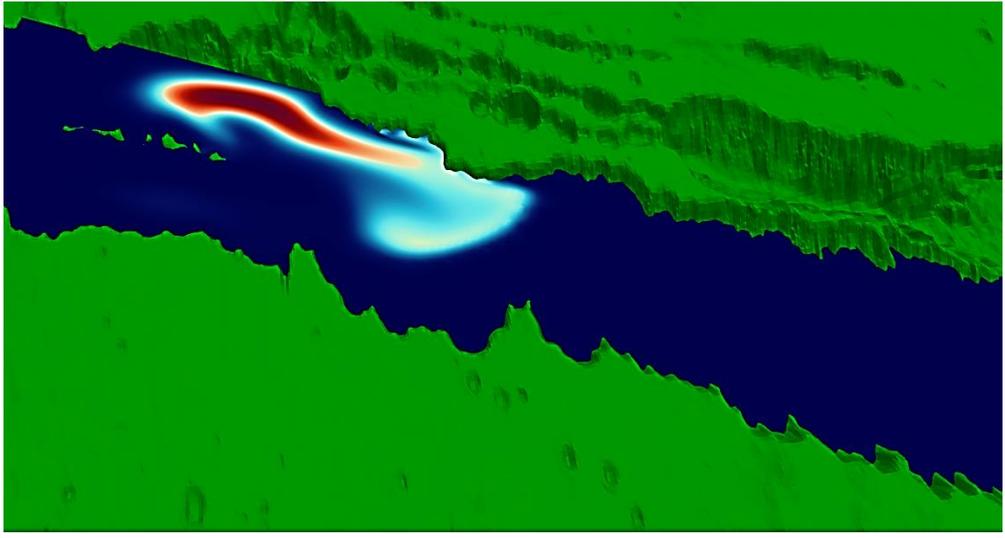


Figure 4 Section of the *marineFoam* mesh and sea bed structure in the generic sea loch.

Figure 5 shows the time evolution of the surface plume of chemicals released into the marine environment from the 6 salmon cages during part of a simulated tidal cycle.







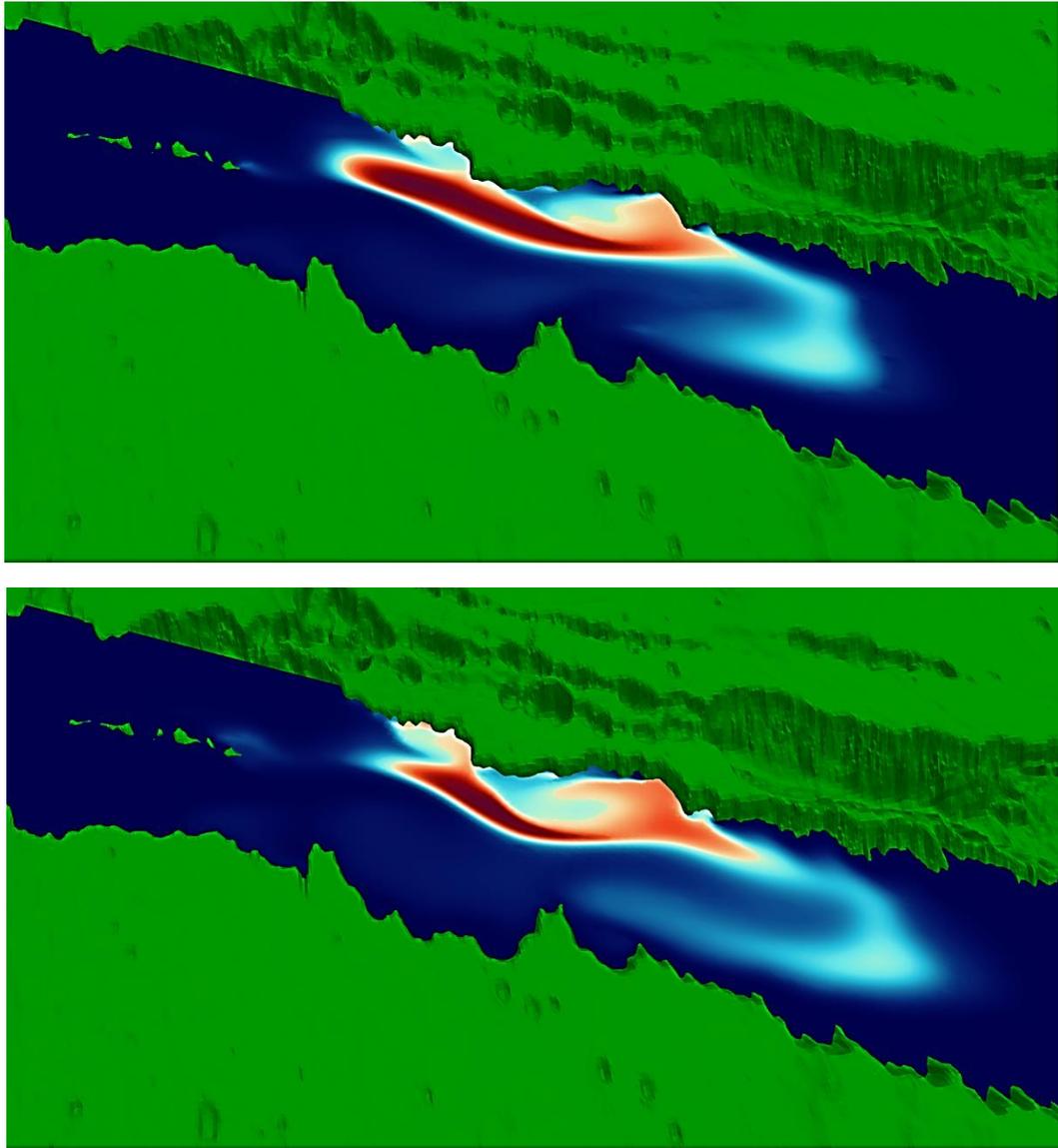


Figure 5 *Time evolution of the surface plume of bath treatment chemicals during part of the tidal cycle.*

Figure 6 highlights the automatic remeshing procedure as the *marineFoam* solution adapts to the species concentration field using AMR. Figure 7 shows the surface velocity contours with accompanying surface streamlines and, finally, Figure 8 shows iso-contours of species concentration highlighting the three-dimensional nature of the chemical plume and its penetration towards the sea bed.

In terms of computational resources, the simulation for the generic sea loch case was executed on a single core of a standard desktop PC with an Intel i7-7820-HK CPU @ 2.90 GHz and 32.0 Gb RAM. The computational time involved was approximately 1 hour of CPU time per hour of tidal cycle modelled and it is noted that this performance can be significantly improved by using the unlimited parallel processing capabilities of OpenFOAM.

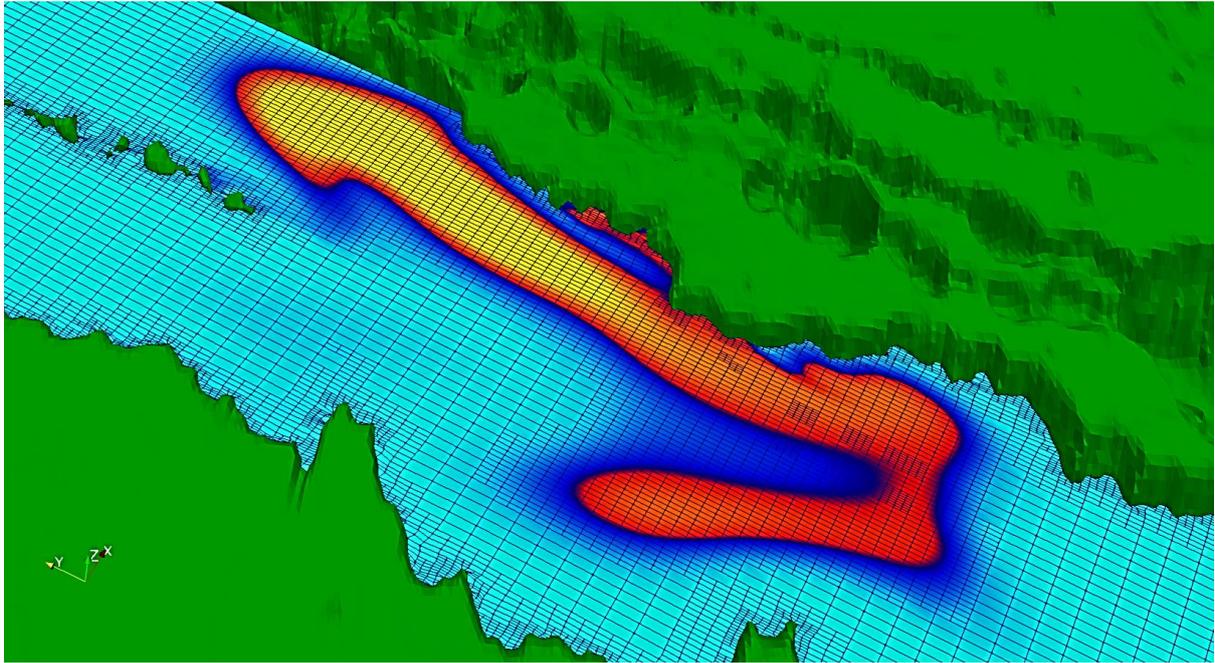


Figure 6 *Automatic remeshing procedure during AMR.*

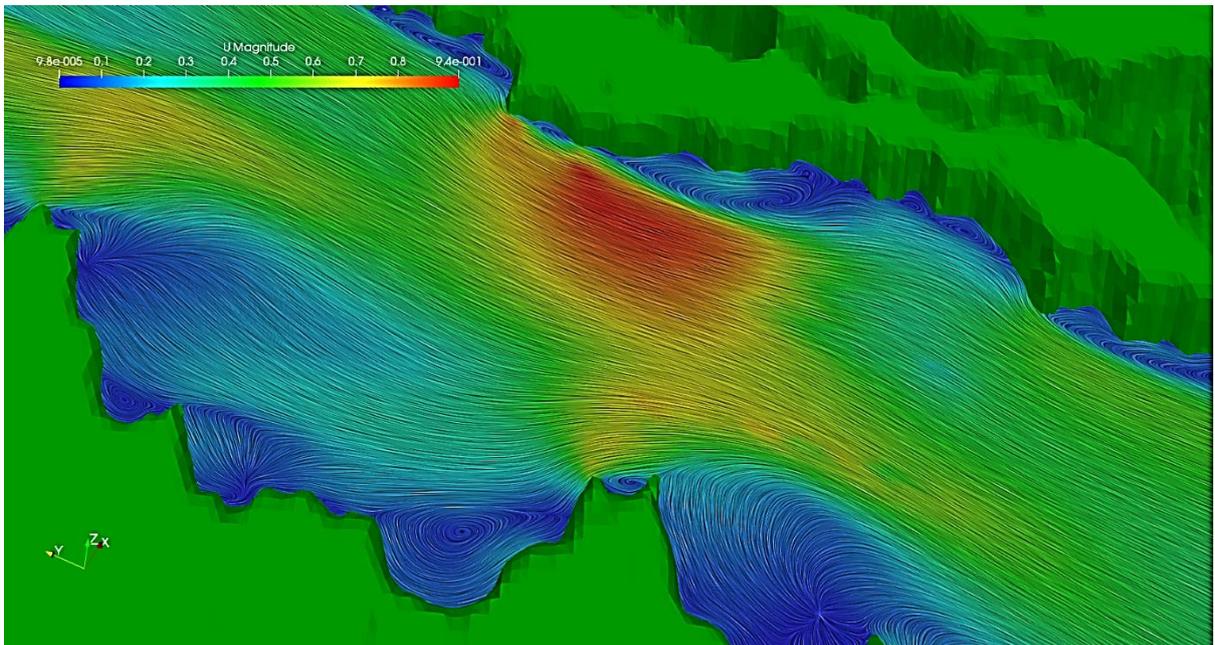


Figure 7 *Surface velocity contours and streamlines.*

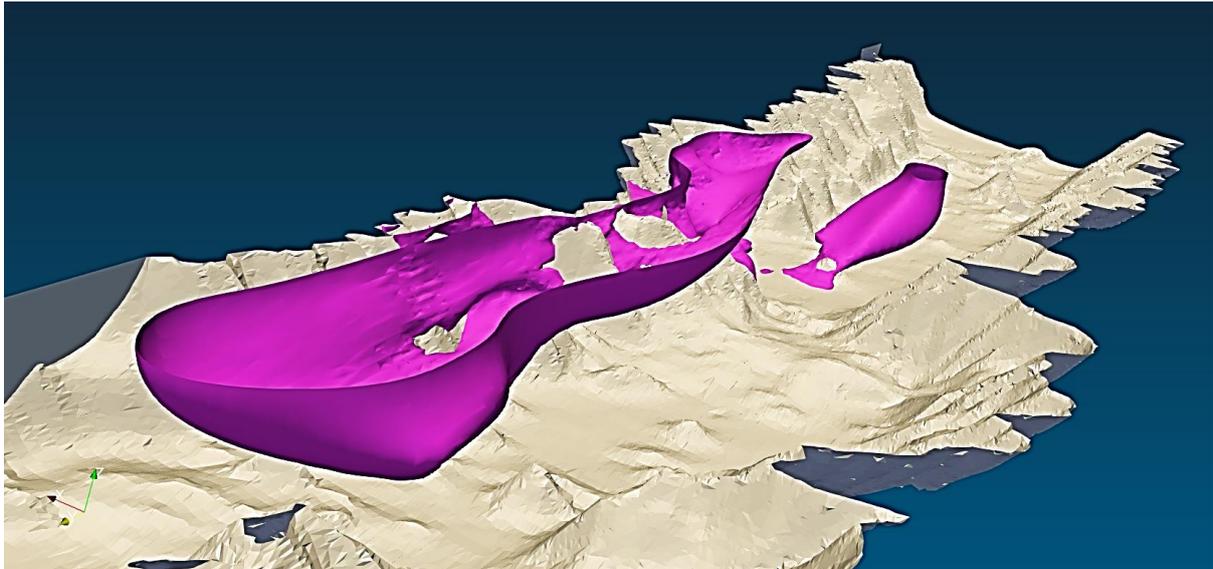


Figure 8 Iso-contours of species concentration highlight the 3D nature of the plume.

5. Conclusions and Perspectives.

A new computational tool called *marineFoam* has been developed for the study of chemical dispersion from bath treatments in salmon farms. The new model is designed to act as either a stand-alone simulator or to inform and improve current lower order models. *marineFoam* has been verified against the conventional oceanographic model FVCOM and can model the transient advection of chemical species in a complex topographical environment within practical timescales on a standard desktop PC. Future work could include the use of enhanced turbulence models such as LES/DES, the adaption of *marineFoam* to study tidal stream generator devices using actuator disk models and a Lagrangian model to consider the distribution of solid organic waste.

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