Update and progress on numerical modelling in the MAGIC project

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Outdoor modelling

Summary

The outdoor simulations can be subdivided into several packages. The first is to appropriately represent the geometry of the site under consideration: this is done using Urban-Terreno, in-house software that is constantly in development to meet the requirements of the simulations. The simulations themselves are then performed using Fluidity, an open-source Computational Fluid Dynamic (CFD) software; the addition of more physics is done directly within Fluidity. The second package consists of correcting the CFD results using observed data from sensors. The third package, for operational reasons, is to deliver a model able to predict CFD results with the same accuracy but computationally faster.

Progress towards more physics

Validated against wind tunnel experiments of the LSBU test site, Fluidity simulations with more realistic physics are now undergoing testing. This includes, in addition to simulating the neutral atmospheric boundary layer, stratification effects and the prediction of heat islands. A turbulent inlet temperature profile has now been implemented in Fluidity to reproduce the behavior of the stable, unstable and neutral atmospheric boundary layer. Improvements to the representation of the wind and temperature fields near solid surfaces have been made, such as the consideration of conduction through building walls as well as through the ground; the exchange by convection between the air and solid surfaces through a Robin boundary condition and the use of a log-law wall function to estimate the proper velocity profiles near surfaces. Figure 1 shows the instantaneous temperature field around two buildings with an unstable atmospheric boundary layer taking into account conduction and convection thermal effects and assuming the buildings are concrete and the ground is asphalt. The impact of radiation on heat transfer is under-development. Figure 2 shows the shadow line in dark grey for one sun angle, depicted by the orange arrow.

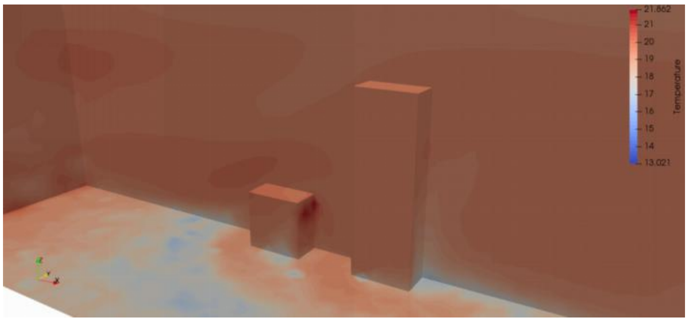


Fig 1 - Instantaneous temperature field around two buildings with an unstable atmospheric boundary layer taking into account conduction and convection thermal effect and assuming the buildings made in concrete and the ground being asphalt.

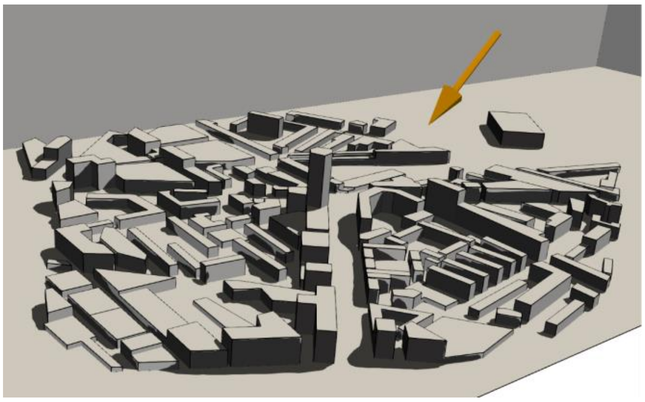


Fig 2 - Shadow lines is in dark grey. The sun angles is depicted by the orange arrow.

In parallel, a simple chemistry model for the species NO, NO_2 and O_3 is being tested as shown in Figure 3. Because the reaction rates of this chemical process are related to the amount of solar radiation, the chemistry model will be fully coupled with the heat transfer in the domain.

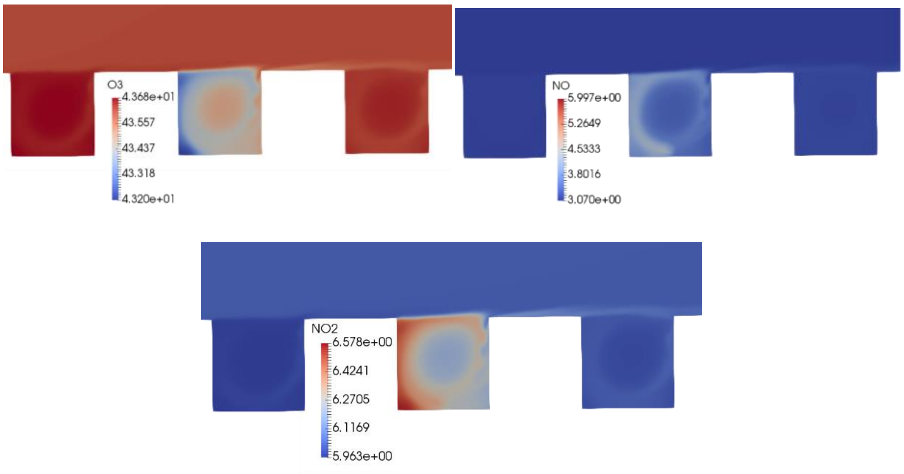


Fig 3 - NO, NO_2 and O_3 concentrations produced by a source located in a street canyon.

In addition to more physics, the numerical team is working on including in Fluidity the possibility to incorporate the influence of external features such as trees and vehicles. The trees are treated as porous material having different porosity and drag coefficients depending the type of trees, leaves and the year time (season). As shown in Figure 4, even using this simple representation, the trees can absorb a certain amount of pollutant and thus reduce the concentration downstream of them, highlighting the positive impact of adding green features in an urban environment.

Fig 4 - A passive tracer is advected from the left of the domain. A porous tree is located in the domain. The pollution is absorbed and reduction of concentration can be observed downstream the tree.

There has been significant progress on the traffic modelling side. Real emissions rates from vehicles as well as realistic driving behavior are now used. More tests are under-way but the technology is now fully operational and implemented in Fluidity as shown in Figure 5. We find that vehicles tend to entrain the emissions, carrying the pollutants along streets: the pollution generated by a vehicle is not only located behind it but can also be found upstream of it after a vehicle stops.

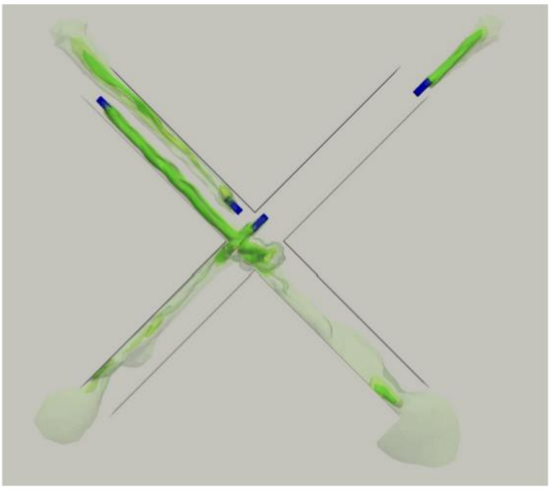
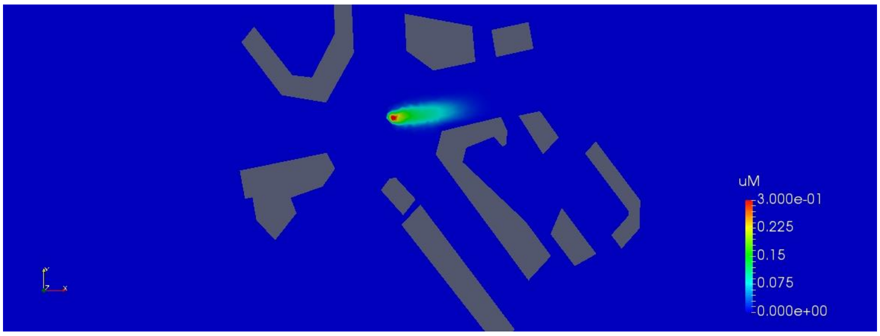


Fig 5 - Crossroads. Vehicles are in blue, while emissions are in green.

Finally, the impact of roof-shape is under study experimentally in the EnFlo wind tunnel at Surrey University, and also numerically using Fluidity. The change in the flow pattern and the dispersion of pollution is investigated to estimate the level of detail needed, in term of roof height and shape, to accurately assess the external condition of a target building.

Progress towards more accurate and faster models

Data assimilation (DA) consists of incorporating observational data, from sensors for example, into an existing model in order to improve accuracy of the results and reduce the error. DA algorithm, used in the context of the MAGIC project, is based on the 3D-Var method and has been fully developed to be as generic as possible but also suitable to answer air pollution problems. DA technology needs to estimate which errors are intrinsically related to the full model, here Fluidity, for computing the so-called background error covariance matrix. As this matrix is usually big (several hundred-thousand nodes times several hundred simulated time-steps), a truncated matrix is used instead. The choice of the optimal truncation parameter requires an a-priori sensitivity analysis. For the first time in DA, it has been shown that this optimal parameter can be found using a mathematical relationship, thus saving significant effort and excluding user misjudgment.



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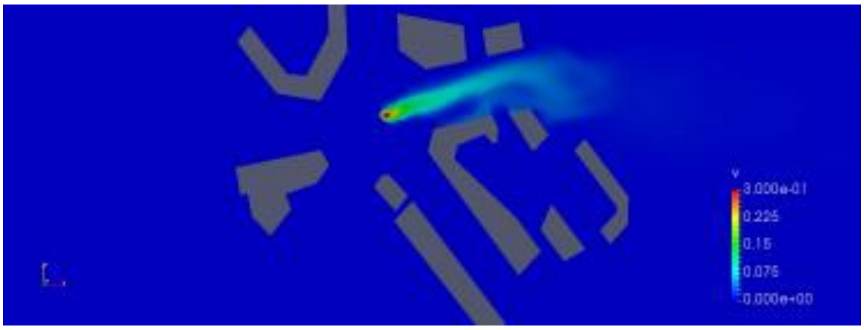

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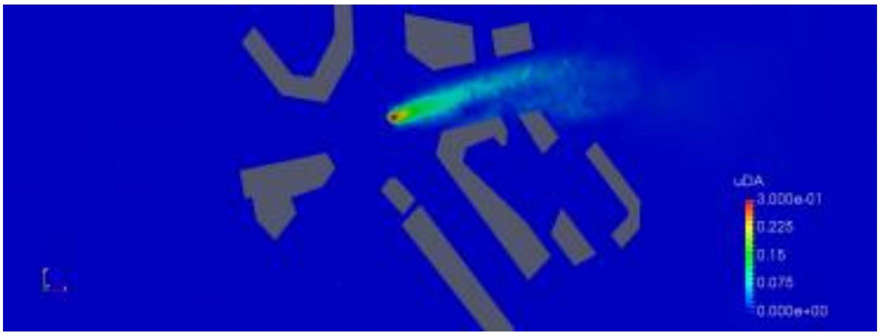
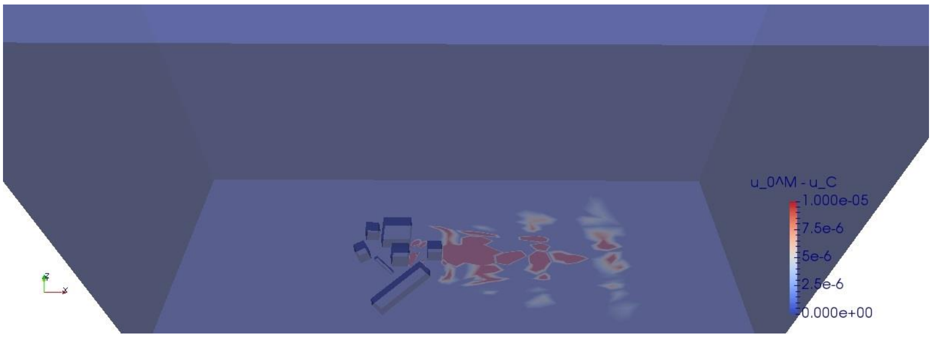


c)

Fig 6 - Dispersion of a passive tracer in LSBU area. a) Fluidity results, b) observed data and c) corrected results using data assimilation.

Fluidity has been fully coupled with DA, highlighting that DA is able to reduce the error of the prediction of pollutant transport to up to one order of magnitude while being computationally efficient and accurate, see Figure 6. This technology has been applied using sensor data from the wind tunnel experiments to improve the numerical predictions produced by Fluidity. Figure 7 (a) shows the misfit between the data provided by the wind tunnel experiments and the numerical results. DA is used to reduce this misfit in order to increase the physical meaning of the numerical predictions. Figure 7 (b) shows the misfit after the assimilation process.



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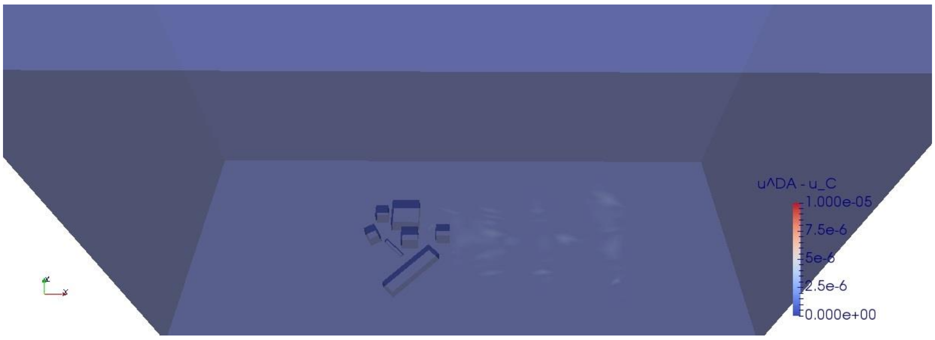
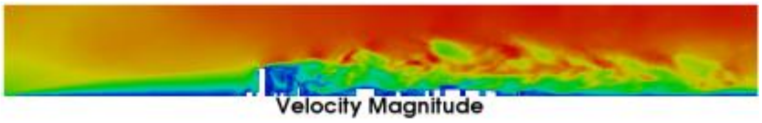


b)

Fig 7 - misfit between the data provided by the wind tunnel experiments and the numerical results from Fluidity before (a) and after (b) the assimilation process.

The DA code has also been modified to be able to run in parallel for a bigger urban environment test case using a domain decomposition approach. The efficiency and the scaling of the paralleled version of the DA code is currently being tested.

Fluidity simulations are based on an LES approach that not only captures the average wind pattern, but also the instantaneous fluctuating behavior of the flow. This approach is very accurate but also computationally expensive. Therefore, a reduced order model has been developed to simulate the wind pattern with the same accuracy but much faster (in a few seconds instead of a few days). The approach adopted in MAGIC is based on a non-intrusive version of a reduced order model (NIROM), meaning that the NIROM model still needs the full model (Fluidity results) for computing the appropriate basis function to run. It has been shown that the NIROM is able to reproduce Fluidity results with good agreement: the greater the number of basis functions, the more the dynamics of the flow are captured, as shown in Figure 8. Subsequently, DA has been coupled with NIROM in order to further reduce the errors in the model. NIROM was then successfully coupled with a neural network (NN) technology, and the NIROM coupled with NN can not only reproduce known Fluidity results, but also is able to predict Fluidity results that were not used to compute the basis functions and train the NN. Finally, NIROM was recently modified to incorporate domain decomposition technology to compute different sets of basis functions in different domains: in regions where there are lot of dynamics (related to high values of Reynolds stresses) more basis functions are used than in domains with less dynamics. This approach allows us to reduce the computational time even more.



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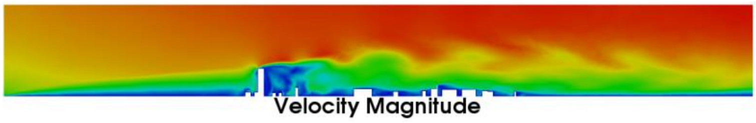

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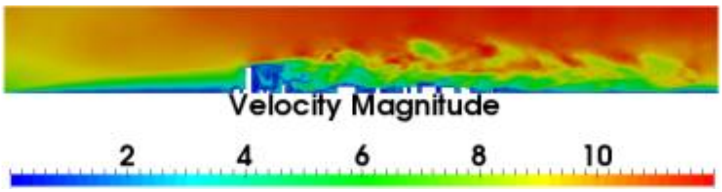

c)

Fig 8 - a) Fluidity results, b) NIROM results using 24 basis function and c) using 382 basis function.

Improvements of Urban-Terreno

Urban-Terreno is a tool developed in the context of the MAGIC project, able to automatically generate a 3D unstructured mesh of a complex urban environment. In order to address the changes to Fluidity from the addition of more physics and the need for a bigger domain to test the paralleled version of DA, Urban-Terreno was recently modified. First, to be able to apply a proper boundary condition for heat transfer in cities, Urban-Terreno has been improved for assigning different boundary identifications to different types of materials and/or land as long as they are provided on a 2D map. Hence, roads, blue spaces, green spaces and buildings can now be identified separately and automatically as shown in Figure 9. Moreover, the code has also been modified to be able to run in parallel to generate a bigger domain faster (see Figure 10). The scaling of the paralleled version is currently being tested using the bigger test case generated for the paralleled version of DA.

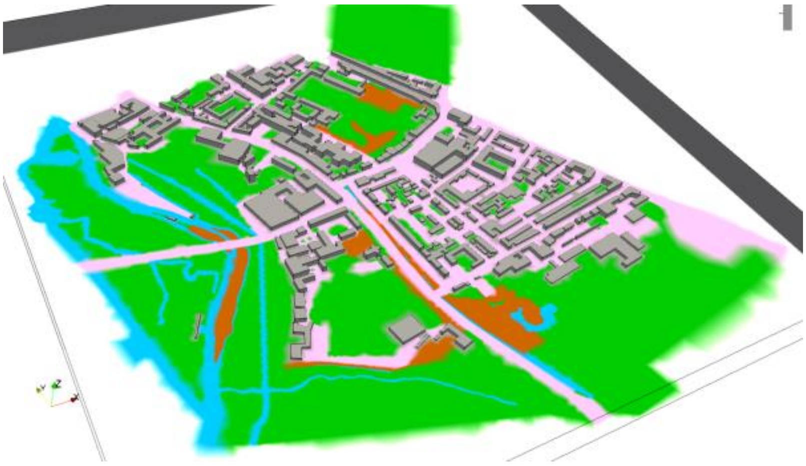

Fig 9 - Cambridge test site. Green denotes green areas, blue denotes blue areas, brown denotes woods area, pink denotes roads and grey the buildings.

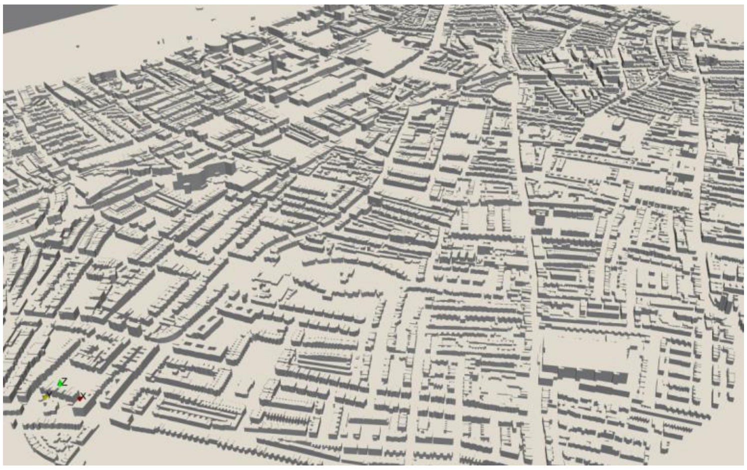

Fig 10 - Bigger area computed with the parallel version of Urban-Terreno

Fluidity Manual

In addition to this work, the numerical team have written a manual to explain how to use Fluidity for indoor-outdoor and urban environment simulations. This manual includes lot of tricks and user experience advice and any beginner with Fluidity can use it to quickly learn how to run a simulation.