

EXTERNAL COUPLING BETWEEN BES AND HAM PROGRAMS FOR WHOLE-BUILDING SIMULATION

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ABSTRACT

This paper discusses a procedure for the two-way run time external coupling between Building Energy Simulation (BES) and building envelope Heat, Air and Moisture (HAM) programs for enhanced wholebuilding simulation. The coupling procedure presented here involves a description of the relevant physical phenomena at the interface between the programs, domain overlaps, coupling variables, coupling strategy and types of boundary condition. The procedure is applied using the programs ESP-r and HAMFEM, where the implementation and verification issues are discussed. This work concludes that the coupling between BES and HAM programs is feasible, and it can potentially enhance the accuracy in whole-building simulation.

INTRODUCTION

Simulation of heat, air and moisture (HAM) transfer for the whole building is important for a detailed analysis of performance aspects such as condensation and mould growth risk, indoor air quality, thermal comfort and energy consumption.

Several types of buildings might benefit from wholebuilding HAM simulation. In historical buildings, for instance, it is necessary because the physical domains (heat – air – moisture) and the geometrical domains (outdoor – envelope – indoor) are closely linked. Also new low-energy high-performance buildings require detailed simulation due to the use of passive cooling, heating and integrated control strategies.

Generally, Building Performance Simulation (BPS) programs are focused on a specific geometrical domain in combination with one or more physical domains. Furthermore, they have strong capabilities, but also some particular deficiencies in terms of boundary conditions, physical models and resolution in space and time. In whole-building HAM simulation, three types of programs can be identified, Building Energy Simulation (BES) (Crawley et al., 2008), building envelope HAM transfer programs (HAM) (Hens, 1996), and finally Computational Fluid Dynamics (CFD). The first two are addressed in this paper.

BES programs, such as ESP-r and EnergyPlus, are intended to study the whole-building energy

performance and thermal comfort issues. These analyses are mainly focused on heat transfer, therefore only simplified models for moisture and air transfer in the building envelope are adopted. Contrary to this, HAM programs, such as HAMFEM, WUFI, MATCH and CHAMPS, allow detailed HAM transfer modelling. This is important for several performance indicators (Hagentoft, 1996), but it is however restricted to a single geometrical domain (a component of the building envelope) rather than the whole building.

Due to the different assumptions and simplifications present in both types of programs, the modelling uncertainty in the results of BES and HAM programs is potentially high, which could justify the efforts to combine their capabilities in a single simulation environment (Costola et al., 2008). In the present context, modelling uncertainties are those related with the assumptions and simplifications made about the physical processes involved in the problem under analysis, rather than the ones related to the input parameters (Mirsadeghi et al., 2009).

Two relevant examples of modelling uncertainty can be found in the results of the BESTEST (Judkoff and Neymark, 1995) and the IEA Annex 41 inter-model comparison for whole-building HAM simulation (Woloszyn and Rode, 2007). Those two examples are described below to highlight the importance of modelling uncertainty in whole-building HAM simulation. Figure 1 shows the results of annual cooling energy demand predicted by different BES programs for the BESTEST case 900 building. Differences up to 70% can be observed between the different programs. This is a good indication of modelling uncertainties, because the input parameters are precisely defined.



Figure 1 BESTEST case 900

A common assumption in BES programs, which is adopted in the results present in Figure 1, is the negligible effect of moisture transfer and moisture accumulation in building components. Results from Annex 41 - Subtask 1 - Common Exercise 1 (BESTEST revised) show that when moisture transfer is taken into account, the modelling uncertainty is even higher, as shown in Figure 2 (dashed line indicates the range of values from Figure 1). In the original BESTEST, the results were published after a second round of simulations, where programs with outlier results could correct some coding mistakes or assumptions in order to bring their results closer to the average. This is not the case for the results in Figure 2, which are "blind", i.e. no adjustment was performed in any program based on the overall results. Even considering this fact, the spread in the results is high (variations up to 150%), indicating the relevance of moisture transfer and accumulation in the results of this particular performance indicator and building.



Figure 2 BESTEST case 900 with moisture transfer

While moisture transfer modelling represents a major deficiency in BES programs, HAM programs model it with a very good agreement between themselves, as described in Hagentoft et al. (2004). Therefore, the combination of the capabilities of these tools is relevant and can potentially improve BPS accuracy. However, there are several ways to address this need for integration.

In the past, several projects were carried out in order to include moisture transfer in BES programs, e.g. the research by Nakhi (1995) on the program ESP-r, or to extend HAM programs to perform wholebuilding simulation, e.g. the programs WUFI-Plus and CHAMPS-BES (Nicolai, 2007). In these cases, internal coupling was used, with the usual drawbacks of this software development strategy. As a result, most of those programs might not provide some state of the art models or are still missing some features that have become standard in new and/or other programs. This can be exemplified by the exclusion of liquid water boundary conditions in the "BESTEST revised" because many whole-building simulation programs could not handle this input. However, liquid load is a standard feature in many HAM programs.

In this sense, external coupling presents a suitable approach to address the combination of BES and HAM programs capabilities (Trcka et al., 2006a; Trcka et al., 2006b).

One-way external coupling is a straightforward technique for a first investigation of the coupling between these two programs, where one program performs a stand-alone simulation and its results are used to provide boundary conditions to the other program with no interaction on time step bases. This alternative was investigated by Costola et al. (2008) and will not be addressed here.

This paper deals with two-way external coupling between BES and HAM programs, i.e. the programs exchange data during run-time. It provides a theoretical framework and a procedure for this purpose. The proposed procedure is implemented in the BES program ESP-r (Clarke, 2001) and in the HAM program HAMFEM (Janssen et al., 2007), and the changes in each code are briefly discussed, followed by verification issues in the implementation. Finally, general conclusions about the coupling procedure are presented.

COUPLING FEATURES

Domain overlap

The first issue in the coupling between BES and HAM programs is the domain overlap between those programs, i.e. both are dedicated to the calculation of the temperature distribution inside the wall, using however different sets of equations. While in BES only the 1D Fourier equation is solved, the HAM programs solves the more comprehensive set of coupled equations for the 1D, 2D or 3D transfer of heat, air and moisture. Here, two possible approaches to solve the domain overlap problem are introduced: suppression of the overlapped domain in the BES program, or the synchronization of both programs in the overlapped domain.

Figure 3 schematically represents the suppression of the overlapped domain in BES. It is simple in nature, but complex concerning the implementation because it involves deep modifications in the problem description in the program. The definition of a few interface nodes at the surfaces is an advantage, because the programs only need to exchange information for these nodes.



Figure 3 Suppression of the overlapped domain Figure 4 schematically represents the synchronization of domains. It aims to keep both programs

calculating the temperature distribution inside the wall, exchanging data for all these nodes. In this case, the heat transfer equations in the BES program should be modified to include moisture related terms, such as heat storage, changes in the thermal conductivity and sink/source terms for latent heat. Although possible, synchronization presents no major benefits because, as the suppression, it requires deep modifications in the problem description in the program. The number of interface nodes is much higher when compared with the suppression approach, and stability and convergence problems can be expected due to the strong interaction between the BES and HAM programs.



Figure 4 Synchronization of the overlapped domains

In this paper, the suppression of the overlapped domain in the BES program is adopted, and the implications of this approach are discussed in the section about modifications in the BES code.

Geometrical features and 1D versus 2D-3D simulation

Most BES programs calculate heat transfer through building components in only one dimension, while many HAM programs can provide also 2D or 3D calculations. The difference in dimensions in BES and HAM programs do not represent a problem, because it is possible to run a 1D simulation in most of the HAM programs, so the problem description is done in the same level in both programs.

However, two issues should be highlighted concerning this topic.

Firstly, the relevance of air transfer modelling in 1D is highly reduced for lightweight constructions, which is exactly where the air transfer is more relevant due to the high number of joins and potential leakage in this type of construction. It happens, among other reasons, because the buoyant flow inside the wall cannot be reproduced by the 1D model. Li et al. (2007), provide a good example of the importance of 2D effects in air transfer in the building envelope. Therefore, in spite of this recognized importance (Hagentoft, 1996), air transfer is often neglected in 1D calculations. In the present paper, this is also done when 1D simulations are performed by the HAM program.

Secondly, BES programs usually treat the building components as a single entity, i.e. the whole wall is considered as a single element, with uniform state and boundary conditions over the whole surface. This approach compromises the analysis of local problems such as mould growth and condensation in spots near edges and corners. Although it presents a limitation, the discretization of the building components in several co-planar 1D elements, the so called surface discretization as presented in Figure 5, does not necessarily improve the resolution of the model. The problem in the surface discretization in BES is related to the empirical algorithms used to estimate the surface averaged convective heat transfer coefficients, which often requires the length of the surface as an input. When the length of the surface is reduced by the discretization, BES wrongly calculates the transfer coefficient, and potential improvements in the accuracy of the results can become compromised. consequently Coupling between BES and CFD can overcome this limitation and it could make the surface discretization a useful strategy when coupling BES-CFD with HAM programs.



Figure 5 Surface discretization in BES

In the present work, no CFD simulation is included, but it clearly represents the next step in order to improve the accuracy and resolution of HAM wholebuilding simulation. The BES-HAM-CFD coupling could also be used to simulate 2D or 3D details, as presented in Figure 6, where the difference in the length of the building component is exemplified. In this case, coupling variables representing fluxes should not be described in terms of absolute values, e.g. W, but as function of the surface are, e.g., W/m². This approach is expected to reduce the importance of the difference in the component length/surface for most of the cases.



Figure 6 Geometrical differences when simulating 2D details

Coupling variables

As described in the previous section, the surface of building components is defined as the interface between the BES and HAM programs. In the HAM program, the boundary condition (bc) can usually be defined in two forms, as a state (Dirichlet bc) or a flux (Neumann bc). While both forms are possible, the use of Neumann bc for the HAM program presents a clear advantage concerning the coupling with BES programs: it allows the HAM program, which has more a comprehensive model of the building envelope, to calculate the state at the surface node. After that, the BES program can use the states calculated by the HAM program as boundary condition, and perform the calculation to obtain the fluxes of each quantity at the surface. This structure is schematically presented in Figure 7 and is adopted in this paper.



Figure 7 Coupling variables

The flux bc could be imposed in two different ways, as an integrated value or as a function of the surface node state which is the option described in Figure 7.

The integrated value consists of the sum of all fluxes at the surface, as exemplified in Figure 8. Using the state calculated by the HAM program as a boundary condition, BES solves all the unknown states of the nodes in the model, and afterwards calculates the various fluxes at that boundary.



Figure 8 Scheme representing the integrate flux

For the heat flux, the integrated value to be delivered to the HAM program is:

$$Q^{t+1} = Q^{t}_{SW} + Q^{t}_{cg} + Q^{t}_{hvac} + Q^{t}_{Conv} + Q^{t}_{LW}$$
 [1]

where Q_{SW}^t , Q_{cg}^t and Q_{hvac}^t are respectively the gains due to shortwave radiation, casual gains due to occupancy, equipments and lighting, and the radiant fraction of the HVAC system, being those terms independent of the surface temperature (T_s). In fact, Q_{hvac}^t depends on T_s, but it is not taken into account in the present work. The terms Q_{Conv}^t and Q_{LW}^t are the gains due to convection and longwave radiation, respectively, which are dependant on T_s. In this case, Q_{Conv}^t and Q_{LW}^t are calculated using data known at time t, T_s^t.

Obtaining the integrated flux is straightforward, because many BES programs provide postprocessing facilities to calculate the heat flux at a given node. However, the use of integrated values in HAM programs present two drawbacks. The first is the delay due to the use of flux values based on the state at the previous time step. The second, and more important, is the adoption of the "Newton-Raphson" scheme by some HAM programs, e.g. HAMFEM. This scheme improves the convergence of the highly non-linear coupled equations of heat, air and moisture transfer in the building component, but it requires knowledge about the derivatives of the flux at the boundary regarding the node state. In this case, it is necessary to have the boundary condition in the flux equation form.

The flux equation describes the total flux as a function of the surface temperature, so additional parameters are required, as represented for the case of the heat flux in Figure 9:



Figure 9 Scheme representing the some parameter of the flux equation

Some additional values required are the convective heat transfer coefficient (h_c), air temperature (T_{air}), all surface temperatures (T_{s-n}) and the view factors (f_n). The heat flux equation is described below:

$$Q^{t+1} = Q^{t}_{SW} + Q^{t}_{cg} + Q^{t}_{hvac} + Q^{t}_{Conv}(T^{t+1}_{s}) + Q^{t}_{LW}(T^{t+1}_{s})$$

where T_s^{t+1} is unknown and will be calculated by the HAM program.

From the discussion above, it is clear that obtaining the flux equation requires more information, and consequently more efforts for its implementation. The final equation however is very simple, because all terms in Eq. [2] are linear or can be casted into the linearied format, so independent and dependent terms can be grouped, resulting in:

$$Q^{t+1} = a \cdot T_s^{t+1} + b$$
 [3]

In Figures 8 and 9, only the internal surface is represented, but in reality, one equation is calculated for each surface, for each time step in BES.

In this paper, the flux equation form is adopted, due to its applicability to a wider range of HAM programs.

Coupling strategy

Several previous works on coupling demonstrate the computational benefits of using the loose coupling strategy, even with the short time step value required to avoid large errors and instability. Assuming the loose coupling strategy, it is necessary to define a convenient data exchange rate to preserve stability and accuracy.

In BES programs, the time step length is often defined based on previous case studies, rather than in time step independence tests for each model. Clarke (2001) exemplifies that 1 hour is a good trade-off between accuracy and computational effort in BES simulation. It is known that the accuracy of BES simulation depends on the wall composition and node distribution, and implicit schemes mask the discretization errors in time and space. However, using adaptative time steps is not common in BES.

In HAM programs, the use of an adaptative time step is more common, particularly due to the necessity of convergence between the coupled system of equations for HAM transfer. The time step can vary from one hour to a few seconds depending on the boundary conditions, particularly when liquid water boundary conditions is present.

Considering the limitation of BES programs in terms of time step independency, the definition of the data exchange rate in BES-HAM coupled simulations cannot be performed based on general rules. However, values obtained from case studies can be considered as an initial indication for the definition of data exchange rate in other simulations. The best practice is to test the sensitivity of the simulation results to the data exchange rate value.

In this paper, the time step in BES (Δt^{BES}) is defined arbitrarily to be 15 minutes, while the time step in the HAM program is adaptative, so the different programs work in different rates (multi-rate). The data exchange rate is equal to the higher time step, in this case the BES one. Programs run in parallel after data exchange. Figure 10 shows schematically the coupling strategy, time steps and data exchange rate used in this paper.



Inter-process communication (IPC)

IPC is a purely computational issue in coupled simulations, however its importance goes from basic aspects such as the time expended in the simulations to more general aspects, such as the popularization of coupled simulations. Previous studies about coupling used mainly platform-dependant IPC with coding specifically adapted for the model under analysis (Djunaedy, 2005; Trcka, 2008). These codes are hard to reuse for others, therefore they are rarely included in new versions of the programs. In order to avoid this situation, a platform-independent IPC with low possibilities of hardcoding should be adopted in the current project.

An alternative in IPC is the Building Controls Virtual Test Bed (BCVTB) (Wetter and Haves, 2008), which "modular, extensible, open-source software is platform that allows designers, engineers and researchers of building energy and control systems to interface different simulation programs." While introducing relevant improvements the in dissemination of coupled simulations, the BCVTB concentrates in the hands of one developer the tasks of learning the programs, their codes, and also the BCVTB. In spite of using sockets, which is a multiplatform IPC, BCVTB is currently designed for use on a single computer, which should run all programs.

Due to these reasons, it was decided to adopt a more traditional approach in the present work, using a small TCP/IP sockets library written in "C", which is compiled with each program, and allows their communication during the simulation. This approach allows multiple users to run each of the programs involved in the simulation from different computers. Once the coupling procedure is defined, as described in the previous sections, different developers with different expertises can implement the necessary modifications in their codes to perform the coupled simulation.

PROTOTYPE FEATURES

Based on the coupling procedure described in the previous section, a prototype program was developed using the BES program ESP-r and the HAM program HAMFEM. In this section, the main changes in each code are discussed.

Modifications in HAMFEM

HAMFEM is a 3D HAM program developed at the K.U. Leuven using the finite element method. As many academic codes, the program is written in Fortran 90, has no graphical interface and no control over the quality of the input data. One important feature is the high level of hardcoded information in the program, e.g. the boundary conditions are implemented directly in the code for each model/simulation. This feature represents a serious concern when quality assurance aspects are considered, but it facilitates the coupling with other programs because the coding process for boundary condition implementation is well documented and straightforward. In HAMFEM, the main modifications were focused on the implementation of the bc provided by ESP-r. As discussed in the previous section, HAMFEM uses Neumann bc during the coupled simulations, with the fluxes obtained from ESP-r as flux equations, such as Eq. 3. Due to the iterative solution process of the coupled equation of heat, air and moisture transfer by HAMFEM, the boundary condition is recalculated for each iteration for each equation.

Considering the boundary condition for the moisture balance calculation, the flux equation obtained from ESP-r is modified in HAMFEM to include the winddriven rain term (Blocken and Carmeliet 2004). This approach was adopted because ESP-r has no database for catch ratios, while HAMFEM includes detailed data concerning this parameter (Blocken and Carmeliet 2004).

Modifications in ESP-r

While in HAMFEM the modifications are small and simple, in ESP-r code the modifications affect the core of the program. The complexity and extension of modifications necessary to perform a coupled simulation seems to be proportional to the code size and history. ESP-r is a code with more than 3 decades of continuous development, it has a graphic interface, extensive quality assurance procedures, and other features that can make the learning curve for users and developers rather unattractive. A positive point in ESP-r structure is its modularity, so the code related to air flow network or HVAC systems is completely separate from the core module, responsible for the building heat balance. The modifications described here applies only to the bps module.

Two major modifications were implemented in ESPr: (1) extraction of the flux equation for the surfaces of each coupled building component; (2) suppression of nodes from the ESP-r matrix corresponding to the coupled building components. Each modification is briefly discussed in the paragraphs below.

1. Obtaining the heat flux parameter described in Figure 9 is simple due to the availability of all necessary data in a single subroutine responsible for the post processing in each time step. The flux equation, obtained in this way, considers the heat balance in the time step, and is based on calculated states of all nodes for that time step. The flux equation can be used in the two-way coupling, which is the aim or the present paper, but it can also be exported from a stand-alone ESP-r calculation, using the trace facilities, for posterior use as boundary conditions in one-way coupling with any HAM program.

2. As discussed in a previous section, the domain overlap between BES and HAM programs can be overcome by the suppression of overlapped nodes from one program. ESP-r is very suitable for this purpose, due to the procedure adopted to form and solve the heat balance matrix of each zone. In ESP-r, the zone matrix is partitioned for each building component, which means that suppression of one building element does not affect the others. The building component matrices are coupled with the matrix for the air and surfaces nodes. In this matrix, the surface temperature of the coupled building component is known, so its equation should be removed from the matrix. Some terms related to the heat exchange between the coupled surface and the surrounding can also be calculated by multiplying the known temperature with the corresponding coefficients in the matrix, where the result is transported to the right-hand side of the matrix.

Figure 11 schematically shows the air and surface nodes matrix, at time equal to t+1. Assuming that the first line represents the coupled building component, this line is suppressed from the matrix, as well as the columns with the cross-coupling coefficients relative to this building component, resulting in the matrix indicated in dark gray (magenta). For each one of the remaining nodes, the cross-coupling coefficients relative to the coupled building component are multiplied by the surface temperature at time equal to t, as calculated by HAMFEM, and transported to the right-hand side of the equation.



Figure 11 Scheme of ESP-r surface nodes matrix (after Clarke, 2001)

Concerning the moisture terms, the modifications are much smaller. The only relevant modification is the inclusion of the flux from/to the building component into the air node moisture balance.

One important limitation of the current implementation is the impossibility of placing control/sensor nodes in the coupled building component. Concrete core activation and other techniques were there is heat injection/extraction inside the building component cannot be simulated using this coupling procedure.

Another important, but rather philosophical aspect of the current implementation is the disassembling of the ESP-r core. In the case where all the building components are coupled with HAMFEM, the only node remaining in ESP-r calculation is the air node. One might argue that in this case, ESP-r is reduced to a sophisticated pre and post processor for the HAM program. In fact, many of the ESP-r qualities are based in pre and post, and also in the integration with other domains, such as AFN, HVAC system, CFD, renewable energies, etc. In this sense, much of ESP-r is preserved in the present coupling procedure. It is clear that ESP-r stand-alone is highly optimized for 1D calculations of heat transfer in building components, and the current prototype cannot compete in terms of computational efficiency for problems involving only heat transfer.

VERIFICATION

Several measures were adopted to verify the implementation of the coupling procedure described in the previous sections.

Considering the complexity involved in any kind of coupling, it is advisable to perform the implementation and verification in steps.

The first step in the implementation was the facility to export the flux equation from ESP-r. This implementation is easily verified confronting exported data with the values obtained from the standard ESP-r output. Using the surface temperature and the flux equation, it is possible to calculate the integrated heat flux at the surface for each time step, and this value can be compared with the hourly values for the flux at the surface, also obtained using ESP-r graphic interface.

The second step in the implementation was the facility to suppress building components from ESP-r calculation. Based on a stand-alone ESP-r simulation, the surface temperature of the suppressed building component is obtained. Then, the modified version is tested using this surface temperature as the one that would be provided by the HAM program in the final prototype. In both simulations, the overall ESP-r results are almost the same, and the implementation is considered verified for this part.

The approach used in the previously discussed verifications can be described as self-coupling, because it aims to reproduce results from the program itself. This technique proved to be valuable during the implementation of modifications aiming coupled simulations.

The verification in the IPC functions is straightforward, because it consists only of the comparison of three values: the original ones calculated by the program, the sent values by the IPC function and the received values by the other program. For this purpose, ESP-r and HAMFEM were tested separately, and small programs emulate the behaviour of the program that was not under test. The values agree completely and the IPC is considered verified.

Concerning HAMFEM, two major verifications procedures were adopted.

Firstly, part of the HAMSTAD exercises (Hagentoft et al., 2004) were reproduced, in order to assure that the present code complies with the previous versions which complied with the HAMSTAD results.

Secondly, the program was tested using one-way coupling based on the flux equation obtained from ESP-r stand-alone simulations, using the facility to export "surface flux to HAM model". The same material properties, spatial and temporal discretizations were used in ESP-r and in HAMFEM, and only heat transfer is considered. Using the flux equation from ESP-r, HAMFEM should be able to reproduce the surface temperatures calculated by ESP-r stand-alone. Result are obtained from simulations of the west wall of the BESTEST case 600 building. Figure 12 shows the comparison of HAMFEM and ESP-r results, in the form of a probability density plot of the differences found between their calculated internal surface temperature. As expected, the difference is negligible for most of the cases, but some larger differences occur, probably due to the difference in the numerical methods and the coarse grid used in the simulations, i.e. the ESP-r default grid. The comparison is considered successful.



Figure 12. Comparing ESP-r and HAMFEM results

CONCLUSION

This paper concludes that:

- 1. the external coupling between BES and HAM programs is viable and feasible,
- 2. it can potentially improve the accuracy of wholebuilding performance simulation,
- 3. the suppression of the overlapped domain in the BES program presents the best cost-benefit ratio to solve the domain overlap problem,
- 4. 1D heat and moisture calculations proves to be the simplest approach to perform BES-HAM coupled simulations,
- 5. 2D and 3D simulations in the HAM program coupled with BES depend, among other factors, on improvements of the convective transfer coefficients in BES, and the most suitable approach for this seems to be BES-CFD coupling,
- 6. the use of surface discretization to improve the geometrical resolution in stand-alone BES programs presents drawbacks related to the empirical relations for transfer coefficient calculation, and should therefore be avoided,

- 7. concerning the coupling variables, the HAM program should be responsible for the calculation of the states of the boundary nodes, so Neumann bc should be used in the HAM program, and Dirichlet bc in the BES program,
- 8. based on literature review and the physical phenomena involved, multi-rate loose coupling with parallel execution seems to be the most suitable coupling strategy,
- 9. IPC using "C" socket libraries proves to be easily implemented and flexible in its application,
- 10. HAMFEM and ESP-r proved to be suitable codes for BES-HAM coupling, and some of the implemented facilities, such as exporting "surface flux to HAM model", can be readily used with any HAM code,
- 11. self-coupling proved to be a valuable technique for verification, particularly is in BES,
- 12. one-way coupling proved to be a useful technique for verification purposes.

Future work should concentrate on the validation of the prototype and on a coupling necessity decision procedure.

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