

A CO-OPERATING SOLVER APPROACH TO BUILDING SIMULATION

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ABSTRACT

This paper describes the co-operating solver approach to building simulation as encapsulated within the ESP-r system. Possible adaptations are then considered to accommodate new functional requirements.

Keywords: Building performance, integrated modelling, equation solution, future requirements.

INTRODUCTION

There are three drivers for the growing uptake of integrated building simulation: the issues underlying sustainable development are too complex to be addressed by simplified design tools; simulation, where well applied, can lead to reduced design times and costs; and future legislation will call for integrated modelling in practice (e.g. the European Commission's Energy Performance of Buildings Directive).

Further, it may be expected that the demand for integrated modelling will continue to grow as appraisals of life cycle performance and impact become the norm. This will place new burdens on the methods that are presently used to solve the underlying mathematical models.

This paper details the co-operating solution methods presently employed within ESP-r to solve the conservation equations relating to the interacting technical domains: building thermal processes, inter-zone air flow, intra-zone air movement, HVAC systems and electrical power flow. Options for solver adaptation are then discussed as required to support the 'deepening' of the domain treatments to include issues such as occupant interaction and embedded renewables.

INTEGRATED SIMULATION

Within ESP-r (Clarke 2001) a building comprises a collection of interacting technical domains, each solved by exploiting the specific nature of the underlying physical and mathematical theories (linear/non-linear, sparse/compact, *etc*). Examples of important couplings include: building thermal processes and natural illuminance distribution; building/plant thermal processes and distributed fluid flow; building thermal processes and intra-room air movement; building distributed air flow

and intra-room air movement; electrical demand and embedded power systems (renewable energy based or otherwise); and construction heat and moisture flow. This section describes the core domains of building thermal, inter-zone air flow, intra-zone air movement, HVAC systems and electrical power flow in terms of the approach taken to solve the describing equations while preserving essential domain interactions.

Building thermal processes

The conductive, convective and radiative exchanges associated with the building constructions are established as a set of energy balance equations and a direct solution method applied. The approach is based on a semi-implicit scheme, which is second-order time accurate, unconditionally stable for all space and time steps and allows time dependent and/or state variable dependent boundary conditions and coefficients. Iteration is employed for the case of non-linearity where system parameters (e.g. heat transfer coefficients) depend on state variables (e.g. temperature). An optimised numerical technique is employed to solve the system equations simultaneously, while keeping the required computation to a minimum. As an example, consider the energy balance equation-set for a simple room when expressed in matrix notation:

$$\mathbf{A}\theta^{n+1} = \mathbf{B}\theta^n + \mathbf{C}$$

where \mathbf{A} and \mathbf{B} are coefficients matrices corresponding to the future ($n + 1$) and present (n) time rows respectively, θ a vector of node temperatures and flux injections and \mathbf{C} a known boundary conditions vector. Since all parameters on the right hand side are known, the equation simplifies to $\mathbf{A}\theta^{n+1} = \mathbf{D}^n$. The content of \mathbf{A} (from Clarke 2001) is shown in Figure 1 for a 6-sided room with uni-directional conduction and a single air node.

The top left corner sub-matrix corresponds to the wall 1 internal nodes, while the sub-matrix (single equation) immediately below on the diagonal corresponds to the wall 1 surface node. Similarly, there are sub-matrices corresponding to constructions 2 through 6. The last coefficient on the diagonal of \mathbf{A} corresponds to the air node within the room. The coefficients on the upper and lower off-diagonals are the radiative heat exchange coefficients connecting the inner surfaces.

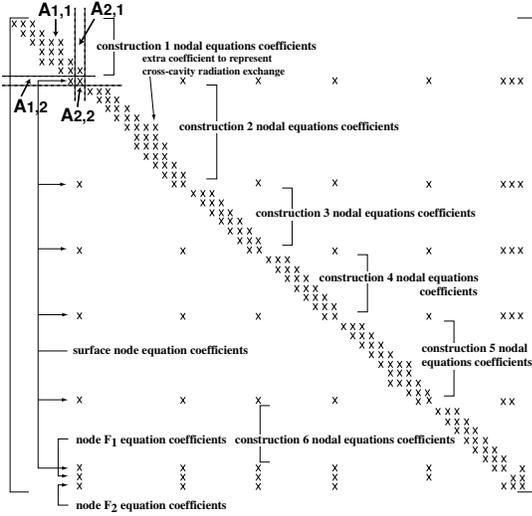


Figure 1: The future time row matrix, \mathbf{A} .

Such a system of equations can be solved efficiently by partitioning and reordering: Figure 2 shows the outcome when applied to the coefficient matrix of Figure 1. Note that null matrices are not shown; sub-matrices in the even rows and the last row are single equations; and T_i , T_{is} and T_a correspond to the temperatures of the intra-construction, surface and air nodes respectively.

The sub-matrices may be rearranged by changing rows such that the vectors corresponding to the intra-construction nodes are moved to the upper part of the system matrix, and the vectors (single equations) corresponding to the surface nodes are moved to the lower part. This gives rise to the matrix of Figure 3 from which it may be observed that:

1. the block matrix at the top left corner consists of sub-matrices of internal construction nodes, and is block tri-diagonal;
2. the block at the lower right corner is a full block matrix, comprising surface nodes and the air node; and
3. the block matrices at the top right and lower left corners represent the connections between the innermost construction nodes and the corresponding surface node.

The lower left block matrix can be eliminated (as shown below) and thus the internal construction nodes and the surface nodes are decoupled. Therefore, only $m + 1$ equations need be solved simultaneously to obtain the nodal temperatures of the wall surfaces and the air within the room (where m denotes the number of constructions bounding the room).

Once the temperatures of the wall surfaces and the air are obtained, the temperatures of the internal construction nodes may be obtained using backward substitution. This is done by taking into

account the particular features of the equation-set, i.e. the sub-matrices on the diagonal with odd number ($A_{1,1}$, $A_{3,3}$, ...) are tri-diagonal, while even numbers are single equations; most of the off-diagonal sub-matrices have only a single coefficient.

Without losing generality, the notion of matrix inversion is used. However, here the inversion requires only the elimination of the lower-diagonal coefficients in the first pass. Consider the system of equations:

$$\begin{aligned}
 A_{1,1}T_1 + A_{1,2}T_{1s} &= D_1 \\
 A_{2,1}T_1 + A_{2,2}T_{1s} + A_{2,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 &\quad + A_{2,10}T_{5s} + A_{2,12}T_{6s} = D_{1s} \\
 A_{3,3}T_2 + A_{3,4}T_{2s} &= D_2 \\
 A_{4,2}T_{1s} + A_{4,3}T_2 + A_{4,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 &\quad + A_{2,10}T_{5s} + A_{2,12}T_{6s} = D_{2s} \\
 \dots
 \end{aligned}$$

To eliminate T_1 from the 2nd equation, T_2 from the 4th equation, and so on, it is assumed that inverse matrices, \mathbf{A}^{-1} , exist such that

$$\begin{aligned}
 T_1 &= A_{1,1}^{-1}(D_1 - A_{1,2}T_{1s}) \\
 A_{2,1}T_1 + A_{2,2}T_{1s} + A_{2,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 &\quad + A_{2,10}T_{5s} + A_{2,12}T_{6s} = D_{1s} \\
 T_2 &= A_{3,3}^{-1}(D_2 - A_{3,4}T_{2s}) \\
 A_{4,2}T_{1s} + A_{4,3}T_2 + A_{4,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 &\quad + A_{2,10}T_{5s} + A_{2,12}T_{6s} = D_{2s} \\
 \dots
 \end{aligned}$$

Substituting the 1st equation into the 2nd, the 3rd into the 4th, and so on, gives

$$\begin{aligned}
 Sch(A_{2,2})T_{1s} + A_{2,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 + A_{2,10}T_{5s} + A_{2,12}T_{6s} &= D_{1s} - A_{2,1}A_{1,1}^{-1}D_1 \\
 A_{4,2}T_{1s} + Sch(A_{4,4})T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} \\
 + A_{2,10}T_{5s} + A_{2,12}T_{6s} &= D_{2s} - A_{4,3}A_{3,3}^{-1}D_2 \\
 \dots \\
 A_{4,2}T_{1s} + A_{4,4}T_{2s} + A_{2,6}T_{3s} + A_{2,8}T_{4s} + A_{2,10}T_{5s} \\
 + Sch(A_{2,12})T_{6s} &= D_{6s} - A_{6,5}A_{5,5}^{-1}D_6
 \end{aligned}$$

where $Sch(A_{2,2})$ is the Schur complement for $A_{2,2}$:

$$Sch(A_{2,2}) = A_{2,2} - A_{2,1}A_{1,1}^{-1}A_{1,2}$$

This results in 7 equations, with a full coefficient complement, to be solved simultaneously. The solution gives the temperatures of the air and surface nodes; back substituting the nodal temperatures of the surface nodes gives the temperatures of the internal construction nodes. Taken together, this procedure gives the simultaneous solution of the complete matrix equation for the room.

Considering the dimensions of $A_{1,1}$, $A_{3,3}$, ..., and assuming each is approximately 10x10, the complete matrix \mathbf{A} will be 67x67. Given that the method outlined above solves only 7 simultaneous equations per zone, the computational saving is substantial.

where \dot{m}_k is the mass flow rate along the k th connection to node i and N is the total number of connections linked to node i . These residuals are used to determine nodal pressures corrections, \mathbf{P}^* , for application to the current pressure field, \mathbf{P} :

$$\mathbf{P}^* = \mathbf{P} - \mathbf{C}$$

where \mathbf{C} is a pressure correction vector. The process, which is equivalent to a Newton-Raphson technique, iterates until convergence is achieved. \mathbf{C} is determined from

$$\mathbf{C} = \mathbf{J}^{-1} \mathbf{R}$$

where \mathbf{R} is the vector of nodal mass flow residuals and \mathbf{J}^{-1} is the inverse of the square Jacobian matrix whose diagonal elements are given by

$$J_{n,n} = \sum_{i=1}^L \left(\frac{\partial \dot{m}}{\partial \Delta P} \right)_i$$

where L is the total number of connections linked to node n . This summation is equivalent to the rate of change of the node n residual with respect to the node pressure change between each iteration.

The off-diagonal elements of \mathbf{J} are the rate of change of the individual component flows with respect to the change in the pressure difference across the component (at successive iterations):

$$J_{n,m} = \sum_{i=1}^M - \left(\frac{\partial \dot{m}}{\partial \Delta P} \right)_i \quad ; n \neq m$$

where M is the number of connections between node n and node m .

To address the sparsity of \mathbf{J} , its solution is achieved by LU decomposition with implicit pivoting—known as Crout's method with partial pivoting (Press *et al* 1986).

Conservation considerations applied to each node then provide the convergence criterion: $\sum \dot{m} \rightarrow 0$ at all internal nodes. As noted by Walton (1982), there may be occasional instances of low convergence with oscillating pressure corrections required at successive iterations. A relaxation factor is therefore applied using a process similar to Steffensen Iteration (Conte and De Boor 1972).

Intra-zone air movement

ESP-r employs a built-in CFD model by which a flow domain (room) is represented by a set of time-averaged conservation equations for the three spatial velocities (U , V , W), temperature (θ) and concentration (C) and, where the $k - \varepsilon$ model is active, the turbulence intensity (k) and its rate of dissipation (ε). As with the building thermal domain, these conservation equations are discretised by the finite volume method (Negrao 1995,

Versteeg and Malalasekera 1995) to obtain a set of linear equations of the form

$$a_p \phi_p = \sum_i a_i \phi_i + b$$

where ϕ is the relevant variable of state, p designates a cell of interest, i designates the neighbouring cells, b relates to the source terms applied at p , and a_p , a_i are the self- and cross-coupling coefficients respectively.

Because these equations are strongly coupled and highly non-linear, they are solved iteratively for a given set of boundary conditions. The SIM-PLEC method is employed (Patankar 1980, Van Doormal and Raithby 1984) in which the pressure of each cell is linked to the velocities connecting with surrounding cells in a manner that conserves continuity. The method accounts for the absence of an equation for pressure by establishing a modified form of the continuity equation to represent the pressure correction that would be required to ensure that the velocity components determined from the momentum equations move the solution toward continuity. This is done by using a guessed pressure field to solve the momentum equations for intermediate velocity components U , V and W . These velocities are then used to estimate the required pressure field correction from the modified continuity equation. The energy equation, and any other scalar equations (e.g. for concentration), are then solved and the process iterates until convergence is attained. To avoid numerical divergence, under-relaxation is applied to the pressure correction terms.

The solution of the discretised flow equations is achieved using the tri-diagonal matrix algorithm favoured because of its modest storage requirements and computational speed.

HVAC systems

As a general rule, the plant-side matrix equation is substantially smaller than its building-side counterpart. For example, within ESP-r the total number of equations for a domestic central heating system is approximately 150, while a building-side model for an average-sized house will require approximately 1000 equations. It is therefore possible to process the plant model as single equation-sets for energy and mass balance (up to two phases are permitted) without the application of partitioning to accommodate sparsity. These equation-sets appear as additional sub-matrices in the \mathbf{A} matrix shown in Figure 1.

Electrical power flow

The approach to network air flow, as elaborated previously, can also be applied to resolve electrical power flows where transient effects are

unimportant (Kelly 1998). The electrical circuit is conceived as a network of nodes representing the junctions between conducting elements and locations where power is extracted to feed loads or added from the supply network or embedded renewable energy components.

Application of Kirchoff's current law to some arbitrary node, i , with N connected nodes, forms the basis for the network power flow solution:

$$\sum_{j=1}^N \tilde{I}_{i,j} = 0.$$

The actual solution procedure is identical to that employed for inter-zone air flow except that here the state variable is voltage, not pressure, and two equation-sets must be solved corresponding to real and reactive power flows.

Linking domains

The whole system problem can now be stated as the co-ordinated solution of the domain equations under control action that links certain model parameters (e.g. room air temperature to the mass flow rate induced by a fan). Figure 4 summarises the ESP-r procedure, which is based on the iterative solution of nested domains. Given that the building time constants are generally greater than those related to the plant, the approach taken is to process the plant system at the same, or greater, frequency than the domains associated with the building. In this way, the plant equations may be solved for small time steps, to accurately represent the effect of control action, while the more slowly evolving building may be solved less frequently. Where required, the processing frequencies may be matched and/or increased.

At each building-side time step, and for a given climate boundary condition, the air/liquid flow networks corresponding to the building and plant are established, control considerations imposed and the equations solved. Solution of these networks give the air and working fluid flow rates throughout the building and within the plant system respectively.

The electrical power flow network representing building-side entities (e.g. lighting, small power, photovoltaic facades *etc*) and plant components (e.g. fans, pumps, CHP plant *etc*) is established, constrained by control action and the equations solved. The facility may be used to impose demand side actions on load consuming systems. (This network model and the preceding one for air/liquid flow may also be invoked at higher frequency from within the HVAC solution loop.)

The building-side, multi-zone matrix equation is then established using the latest estimates of the fluid/power flows and plant induced flux

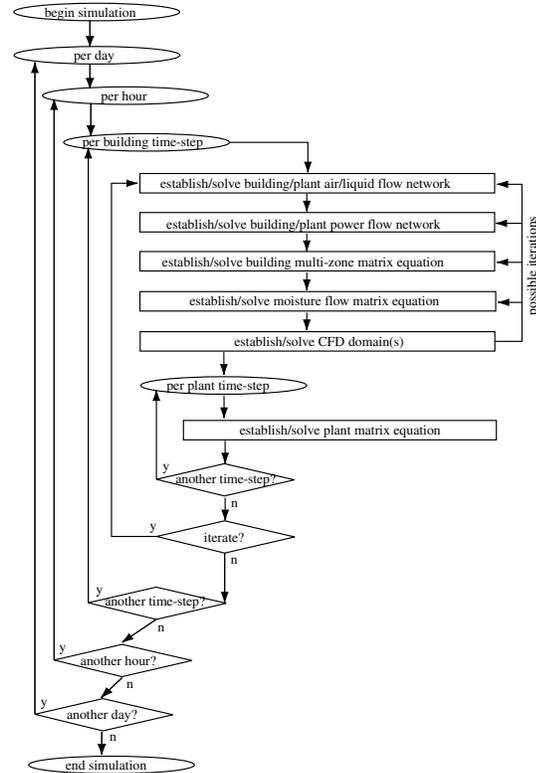


Figure 4: Iterative solution of nested domains.

injections/extractions. Equation solution is achieved as described previously to obtain the building's temperatures and heat flows.

Using the newly computed intra-construction temperatures, the construction moisture flow matrix equation is established and solved. This gives the moisture distribution within the building fabric.

Using the building temperatures and air flow rates as boundary conditions, the CFD model is established and solved. This gives the intra-zone distribution of temperature, velocity, pressure and contaminants.

The building temperatures and air/liquid flow rates are then used, along with relevant control loops, to establish and solve the plant heat and mass flow matrix equations. Solution of these equations gives the plant temperatures and flow rates.

To orchestrate the process, domain-aware conflation controllers are imposed on the different iterations. Consider, for example, the linking of the building thermal, network air flow and CFD models. This employs a controller that ensures that the CFD model is appropriately configured at each time-step (Beausoleil-Morrison 2001).

At the start of a time-step, the zero-equation turbulence model of Chen and Xu (1998) is employed in investigative mode to determine the likely flow regimes at each surface (forced,

buoyant, fixed, fully turbulent or weakly turbulent). This information is then used to select appropriate surface boundary conditions, while the estimated eddy viscosity distribution is used to initialise the k and ε fields. A second CFD simulation is then initiated for the same time-step.

On the basis of the investigative simulation, the nature of the flow at each surface is evaluated from the local Grashof (Gr) and Reynolds (Re) Numbers, which indicate "how buoyant" and "how forced" is the flow respectively:

$Gr/Re^2 \ll 1$; forced convection effects overwhelm free convection

$Gr/Re^2 \gg 1$; free convection effects dominate

$Gr \approx Re^2$; both forced and free convection effects are significant

Where buoyancy forces are insignificant, the buoyancy term in the z-momentum equation is discarded to improve solution convergence.

Where free convection predominates, the log-law wall functions are replaced by the Yuan *et al* (1993) wall functions and constant boundary conditions imposed where the surface is vertical; otherwise a convection coefficient correlation is prescribed (this means that the thermal domain will influence the flow domain but not the reverse). Where convection is mixed, the log-law wall functions are replaced by a prescribed convection coefficient boundary condition.

Where forced convection predominates, the ratio of the eddy viscosity to the molecular viscosity (μ_t/μ), as determined from the investigative simulation, is examined to determine how turbulent the flow is locally:

$\mu_t/\mu \leq 30$:- the flow is weakly turbulent; the log-law wall functions are replaced by a prescribed convection coefficient;

$\mu_t/\mu > 30$:- retain the log-law wall functions.

The iterative solution of the flow equations is re-initiated for the current time-step. For surfaces where h_c correlations are active, these are shared with the building thermal model to impose the surface heat flux on the CFD solution. Where such correlations are not active, the CFD-derived convection coefficients are inserted into the building thermal model's surface energy balance.

Where an air flow network is active, the node representing the room is removed and new connection(s) added to effect a coupling with the appropriate domain cell(s) (Negrao 1995, Clarke *et al* 1995). A technique by Denev (1995) is employed to ensure the accurate representation of both mass and momentum exchange in the situation where CFD cells and network flow components are of dissimilar size.

Similar conflation mechanisms exist to enact informed 'hand-shaking' between the other domain pairings.

FUTURE REQUIREMENTS

User interface aspects aside, the ESP-r approach to integrated building simulation is able to accommodate many of the issues that underpin energy conscious building design. While the Open Source (www.opensource.org) nature of ESP-r should ensure that it continues to evolve in the light of new research findings, the real issue is whether the underlying approach is able to accommodate future user requirements. In some respects this is assured: a new method will only require the implementation of a new source term, the adjustment of existing equation coefficients or incorporating both together through a control function. Examples include the detailed modelling of ventilated facades, internal shading devices and time/location dependent heat injections. In other cases an entirely new domain model may be required so that the issue becomes the ease with which the new model can be integrated.

This section identifies some upcoming modelling issues and considers how the ESP-r solution approach may be evolved to accommodate them.

Domain solution developments

Building thermal processes

The ESP-r model has proved to be resilient when applied to a range of problems over two decades. Recent work has focused on the implementation of phase change materials, while ongoing work is addressing the nuances of double skin facade modelling. In both cases no solver adaptations were required.

The system is also well adapted to the modelling of innovative components such as light sensitive shading devices and hybrid photovoltaics, requiring enhancements to the resolution of existing models to allow, for example, slat angle adjustment in the former case and heat transfer surface geometry modelling in the latter.

An area where solver adaptation would be required relates to the extension of construction moisture flow modelling from 1D to 3D. Such an extension impacts upon the treatment of surface (de)absorption in the presence of an active CFD domain. This will require extensions to the conflation controller linking the building thermal/moisture and CFD domains to handle the possible gridding cases: 1D/3D, 2D/3D and 3D/3D.

Inter-zone air flow

At the present time ESP-r's network air flow model is based on the steady-state line integration of the Navier-Stokes equation. When coupled with the building, oscillation problems may occur due to the numerical error. This issue can be resolved in two ways: by introducing a pressure capacity term into the mass balance equations; and by introducing transport delay terms to the network connections. Additionally, the modelling of contaminant concentration distribution can be carried out in parallel and/or coupled with the network air flow and building thermal models. Since it is a diffusive type system, with the convective terms predicted by the network air flow model, contaminant distribution may be evaluated as a scalar quantity and therefore the solution is straightforward.

The current theory may also be readily extended to handle higher level systems such as district heating, and problematic issues such as 'water hammer' (via the introduction of a pressure capacity term).

Intra-zone air movement

Several developments may be readily applied to the CFD model: tunnel-type fans, as used in indoor car parks, can be modelled as free-standing supply or extract points; while dampers and diffusers can be modelled by the imposition of a pressure boundary within a space. Such devices may be implemented through relatively simple coding modifications without the need to significantly modify the underlying solution procedure.

Other developments will require additional equations and so will impact upon the solution procedure. For example, the CFD technique is presently incapable of modelling small solid particulates that have weight transport within the main air stream. Two particle dispersion/deposition modelling methods are being considered for implementation: treating the particles as a continuum or particle tracing using Lagrange coordinate.

The modelling of fire/smoke requires that extra equations be added to handle combustion reactions and the transport of combustion products (e.g. via the implementation of mixture fraction or grey gas radiation transport models). Such adjustments can be readily implemented within the existing code since the governing equations are of diffusive type and so can be treated in the same way as the energy and species diffusion equations. In conjunction with the network flow model, the transient distribution of fire and smoke may then be applied as a boundary condition for the prediction of the movement of occupants during a fire.

HVAC systems

The HVAC domain comprises models for each plant component, which may be based on the same or dissimilar theories. In this sense, the extensibility of the approach is unlimited: new modelling methods may be implemented as new products emerge.

The major issue confronting ESP-r is the generation of the component models in the first place and the combination of the selected components to form a working HVAC system. To this end, two issues need to be addressed: the synthesis of component models from basic heat transfer/flow elements and the automatic linking of the resulting models. The former issue is addressed by the Primitive Part technique (Chow *et al* 1998) whereby component models may be synthesised as and when required; while the latter issue might build upon previous research into object oriented HVAC (Tang 1996).

Further developments are also required in relation to the connection of HVAC and CFD domains, especially where the former impose complex flow patterns on the latter.

Domain interaction developments

Occupancy interactions

It is well known that the effects of occupancy can vastly increase energy use. These effects arise from two avenues: behaviour (e.g. the occupants' response to window opening) and attitude (e.g. the rejection of facilities on other than performance grounds). There is a need to explicitly model such behaviour and, in the context of ESP-r, two approaches are possible: 'typical' interactions may be included within a controller that has authority to adapt the parameters of the affected domain models prior to solution; or, more realistically, an occupancy response model may be introduced by which the response to stimulus is explicitly represented. In both cases the aim is to address the distributed impacts of occupant actions (e.g. the impact on the network flow, CFD, thermal and lighting domains of window opening).

Micro-grids

The future is likely to be characterised by a significant utilisation of renewable energy delivered through the public electricity network (distributed generation) and by local schemes serving to complement the grid (embedded generation). In the latter case, it will prove beneficial to group building types so that the aggregate load profile is favourable in relation to the power variations associated with the renewable energy supplies. Modelling such micro-grids will require the development of demand management algorithms

that may be applied to switch certain loads within the context of renewable power trading. Such a facility will primarily interact with the building thermal, HVAC and electrical domains by acting to reschedule heating/cooling system set-point temperatures, and withholding/releasing power consuming appliances where acceptable.

Next generation

In the long term, additional solver developments may be implemented to bring about computational efficiencies and thereby assist with the translation of simulation to the early design stage. For example:

1. additional, context-aware solution accelerators may be embedded within the solvers to control their appropriate invocation;
2. parallelism may be introduced to allow the different domains to be established and solved in tandem to reduce simulation times; and
3. network computing might be exploited to allow different aspects of the same problem to be pursued at different locations as an aid to team working.

Such developments might well be built upon entirely new methods such as 'intelligent matrix patching' whereby the coupling information between domain models are stored in a 'patch matrix' allowing the numerical model of the coupling components to be activated only when the actual coupling takes place. Further, a greater level of coefficients management may be introduced to ensure that the matrix coefficients are only updated when required and otherwise never reprocessed. Such devices would lead to significant reductions in computing times.

CONCLUSIONS

This paper has summarised the distributed approach to domain solution as employed within the ESP-r system. Several possible technical developments were then outlined as required by new user demands that imply a need to extend and deepen the analysis scope.

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