COMPUTATIONAL FLUID DYNAMICS IN AN EQUATION-BASED MODELING ENVIRONMENT

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ABSTRACT

The simulation of the energy performance of buildings has historically been compartmentalized along the lines separating different disciplines or different analysis tools, despite their interrelations. These interrelations motivate the development of integrated analyses, which has often focused on linking pre-existing and independent simulation software together. This paper reports on initial work using a different integration strategy in which the 'pre-existing and independent software' all exist in the universe of the model description language Modelica. Specifically, the beginnings of a Modelica CFD package suitable for buildings and using the discrete-velocity Boltzmann equation is introduced.

INTRODUCTION

Basic heat transfer and fluid mechanics, along with building systems such as lights, HVAC components, and any control systems, are coupled and in general all must be treated in building performance simulations. Despite this, and with some justification, there has traditionally been a split between tools whose primary function is to simulate the energy performance of a building – energy simulation programs like DOE-2 and EnergyPlus – and tools which focus on simulating the air flow within, through, and perhaps also around the building envelope. This split can exist because each tool makes assumptions about the domain which it does not focus on. In the case of EnergyPlus, airflows are assumed to be such that temperatures are uniform throughout the space – often a good assumption – and the convective heat transfer coefficient is estimated from models (DOE, 2008).

There are situations when this is not the case however, and situations where the airflow needs to be quantified at a detail beyond what energy simulation programs can provide. For this there are three simulation approaches. The first, multizone analysis, assumes fully mixed conditions, and postulates that flow paths through a building such as ducts or other mechanical systems, cracks in the facade, or open doors between rooms are linked together at nodes which represent rooms or other spaces. The flow along these flow paths is calculated from power law equations relating volume flow rates to pressure differences between the nodes. Chemical concentrations can also be tracked in addition to flow rates (Chen, 2008, Hensen, 2003 and Axley, 2007). In a recent survey, Chen (2008) found such methods to be accepted among practitioners for whole-building airflow analysis, although their market penetration may be hindered by the user-unfriendly interfaces of the most popular multizone analysis programs, CONTAM (Walton and Dols, 2008) and COMIS (Feustel, 1998). Wetter (2006b) was able to quickly create a Modelica multizone airflow library which compared well to CONTAM.

The second method, the zonal approach, partitions a space such as a room into several – on the order of 10 – isothermal zones or cells, each with a possibly different temperature. Conservation laws are applied in each cell to determine the flows of mass and energy between the cells. This method is therefore able to coarsely treat spaces with a nonuniform temperature distribution (Megri and Haghighat, 2007). Zonal method are intended as a balance between computing time and spatial resolution, although it has been argued (Chen, 2008) that their overall utility is comparable to coarse computational fluid dynamics (CFD) methods, the third approach.

In contrast to the reduced or simplified conservation laws used by the multizone and zonal approaches, computational fluid dynamics (CFD) methods solve – or satisfy – the general mass, momentum, and energy balance laws and are the most sophisticated, detailed, and resource-intensive flow simulation techniques. As such they are reserved only for those cases and locations where their use is warranted: natural ventilation including wind- and buoyancy-driven flows, flows with high momentum, detailed studies on thermal comfort, etc. (Chen, 2008).

Thus, in addition to the split between energy simulation and airflow simulation, there is also this three-way split within airflow simulation. This latter split, however, exists for the good reason that there is no one-technique-fits-all approach to airflow simulation. Each technique has its niche. However, one simulation scenario may have more than one niche, and therefore there has been work on coupling these different airflow techniques. In some situations a multizone method may not give accurate results (Wang and Chen, 2008), and if such a situation occurs in one zone of an otherwise appropriate multizone model, then the use of a CFD model within a larger multizone model can provide a unique solution (Wang and Chen, 2007b) which improves the overall results (Wang and Chen, 2007a). Tan and Glicksman (2005) also coupled a multizone model to a CFD model and investigated the effect of choice of boundary between multizone and CFD volumes on the solution of a simulated naturally ventilated space.

There has also been work in stitching the split between energy simulation and airflow modeling. Hensen (2003) gives a review, particularly in regard to coupling multizone models with energy simulation. TRYSYS incorporates a variety of methods to incorporate COMIS and CONTAM (Bradley and Kummërt, 2005), and likewise EnergyPlus has facilities for interfacing to COMIS (Crawley et al., 2001). Linking energy simulation to CFD has also received attention. The convective heat transfer coefficient h, a bridge between the two domains, can vary over several orders of magnitude (Lienhard(IV) and Lienhard(V), 2005) and is a large source of uncertainty, as is the rate of air infiltration into a building. In a study to determine the appropriateness of different energy/airflow simulation combinations, Djunaedy et al. (2004) found that depending on the design variations of a space, the uncertainty in h can cause up to a 66% deviation in the simulated maximum heating load, a 20% deviation in the simulated heating energy demand, and up to a 25% deviation in the simulated maximum cooling load. Corresponding deviations due to the uncertainty in the infiltration rate are 25%, 60%, 13%, respectively. CFD can be used to reduce these uncertainties since h can be computed as part of a CFD simulation, e.g. (Zhai and Chen, 2004), and likewise investigate the fluid-mechanical environment around a building to clarify the infiltration. The feasibility of coupling energy simulation to CFD has been demonstrated theoretically (Zhai and Chen, 2003) and in implementation (Zhai and Chen, 2005).

With the long term goal of integrating the disparate building simulation subcultures, this work reports on initial steps to build a CFD package for the Modelica model description language. The hypothesis is that the object-oriented, multidomain, and declarative nature of Modelica can be used to achieve this integration and create a more unified suite of tools that are each easily maintainable, extensible, and adaptable.

One point should perhaps be addressed. Djunaedy et al. (2005) has argued that linking energy simulation capabilities with airflow simulation capabilities should be done by interfacing pre-existing programs together, since this avoids the rewrite of code and allows each individual program to advance at its own pace and under its own mechanisms. There is merit to these points, and it may appear that what is proposed here goes against them. It does in the first case, it does not in the second. First, although this work would be a from-scratch capability, the effort is worthwhile because of the modeling possibilities and modeler benefits that Modelica can provide. Rewriting – or expressing anew – a model in Modelica is fundamentally different than rewriting a CFD algorithm within the EnergyPlus simulation kernel. Second, it is important to bear in mind that Modelica is not a solution, but a platform for solutions. Packages of Modelica models can evolve in their own domains so long as the interfaces between models remain synchronized, which is also necessary for integrating separate programs written in programming languages.

DISCRETE BOLTZMANN APPROACH

Rather than solving the Navier-Stokes and energy equations, it is proposed here to solve a discrete Boltzmann model equation. This model equation descends from the continuous Boltzmann equation describing the evolution of the single particle distribution function in a perfect gas

$$\frac{\partial f}{\partial t} + \boldsymbol{e} \cdot \frac{\partial f}{\partial \boldsymbol{x}} = \Omega_B \tag{1}$$

where $f = f(\boldsymbol{x}, \boldsymbol{e}, t)$ is the probability density function for finding a molecule (particle) of a certain momentum in a certain region of space. Ω_B is the Boltzmann collision integral, a complex nonlinear term which describes the binary collisions of particles. The term $\boldsymbol{e}$ represents the microscopic velocity of the particle. It can be shown that the continuity, Navier-Stokes, and energy equations are contained in this equation. The pressure is determined with a state equation and the macroscopic density ρ and momentum $\rho\boldsymbol{u}$ are given by

$$\begin{aligned} \rho &= \int f d\boldsymbol{e} \\ \rho\boldsymbol{u} &= \int \boldsymbol{e} f d\boldsymbol{e} \end{aligned} \tag{2}$$

(Cercignani, 1988 and Harris, 1971).

A simpler model of this equation sufficient for our purposes is the discrete Boltzmann model equation (see, e.g. Shan and He (1998); Broadwell (1964) gives an early use of such a discrete version) with the single relaxation time BGK collision operator:

$$\frac{\partial f_i}{\partial t} + \boldsymbol{e}_i \cdot \frac{\partial f_i}{\partial \boldsymbol{x}} = \frac{1}{\tau}\Big(f_i - f_i^{eq}\Big) \tag{3}$$

where the subscript i indicates a one of a finite number of directions, τ is a relaxation time, and f_i^{eq} is the single particle distribution at equilibrium. The macroscopic density ρ and momentum $\rho\boldsymbol{u}$ are given by

$$\begin{aligned} \rho &= \sum_{i=0}^{8} f_i \\ \rho\boldsymbol{u} &= \sum_{i=1}^{8} f_i \boldsymbol{e}_i \end{aligned} \tag{4}$$

(Reider and Sterling, 1995).

For this paper a two-dimensional athermal variant is implemented as an initial demonstration. In this case the discrete microscopic velocities are given by

$$\begin{aligned} \boldsymbol{e}_0 &= (0,0) \\ \boldsymbol{e}_{1,3} &= (\pm c, 0) \\ \boldsymbol{e}_{2,4} &= (0, \pm c) \\ \boldsymbol{e}_{5,6,7,8} &= (\pm c, \pm c) \end{aligned} \tag{5}$$

and the equilibrium distribution functions f_i^{eq} take the form

$$f_i^{eq}(\boldsymbol{x},t) = \rho w_i \left[1 + \frac{3}{c^2}\boldsymbol{e}_i\cdot\boldsymbol{u} + \frac{9}{2c^4}(\boldsymbol{e}_i\cdot\boldsymbol{u})^2 - \frac{3}{2c^2}(\boldsymbol{u}\cdot\boldsymbol{u})\right] \tag{6}$$

where $c = 1$ and w_i is given by

$$w_i = \begin{cases} \frac{4}{9}, & i = 0 \\ \frac{1}{9}, & i = 1,2,3,4 \\ \frac{1}{36}, & i = 5,6,7,8 \end{cases} \tag{7}$$

(He and Luo, 1997b, 1997a and Qian et al., 1992)

In place of the coupled continuity and nonlinear second order Navier-Stokes equations with nonlinear convection terms and spatial derivatives of pressure, we have a set of nonlinear first order equations with linear convection terms and pressure determined with algebra natively through a state equation. The use of these simpler Boltzmann equations is offset by the fact that there are more of them.

NUMERICAL TREATMENT

One prominent Boltzmann-based CFD scheme is the lattice-Boltzmann method, which is a particular – and somewhat crude – finite difference discretization of the discrete Boltzmann BGK equation which yields a simple algorithm in a Lagrangian framework (see, e.g. (Sterling and Chen, 1996)). It is easy to program and has been applied to CFD in buildings before(Crouse et al., 2002), but has the restriction that the spatial and temporal discretizations are bound together such that $\Delta x = \Delta t$. Here, to decouple the spatial and temporal scales and following in the vein of workers such as Reider and Sterling (1995), Cao et al. (1997) and Mei and Shyy (1998), a method of lines approach is used (Cellier and Kofman, 2006 and Schiesser, 1991), whereby the convective terms are discretized using a third order upwind weighted finite difference scheme (Hoffman, 1992), leaving the temporal derivatives to be handled within Modelica at the language level.

The basic unit in the Modelica description is the node, i.e. a grid point. The node model contains the macroscopic hydrodynamics variables, the particle distribution functions f_i and f_i^{eq}, and equations involving these variables common to other specialized nodes which inherit the basic node model. For example, the model for the interior nodes contains, in addition to the common node equations such as equation 6, the spatially discretized version of equation 3 using third order upwind weighted difference formulas. Boundary nodes contain versions of equation 3 with one-sided third order difference equations as appropriate to their location, and interfaces to boundary condition models such as a moving wall or no-slip condition. The various node models are collected into a model of the fluid domain, which mediates the connections between individual nodes and the boundary condition models. These boundary condition models specify the macroscopic velocities on the boundaries, which enter into the Boltzmann equations through the equilibrium distributions f_i^{eq}.

EXAMPLE

As an initial example of this approach, planar Couette flow is simulated using Dymola 7.1 and the default differential algebraic solver (DASSL). All units are in grid units. The kinematic viscosity ν was set to 0.0833, the top lid velocity was set to $U = 0.02604$. The size of the domain is $L = 16$ in the x (horizonal) direction, $H = 26$ in the y (vertical) direction, yielding a Reynolds number Re of 8.1. The boundary conditions were applied by specifying the macroscopic velocities u (horizontal) and v (vertical) at the top and bottom of the domain. Periodic boundary conditions were applied to the two sides of the domain.

The flow field at times $t = 20$ and $t = 2000$ are depicted in figures 1 and 2, respectively.

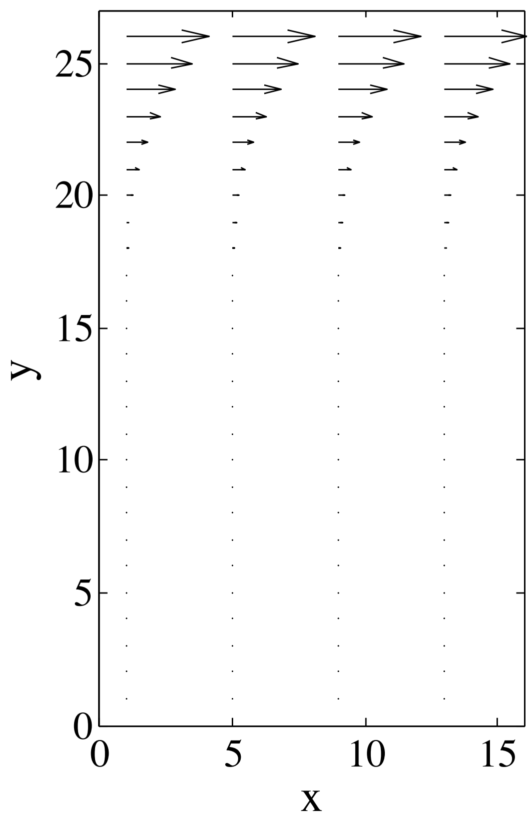

Figure 1 The flowfield at t = 20

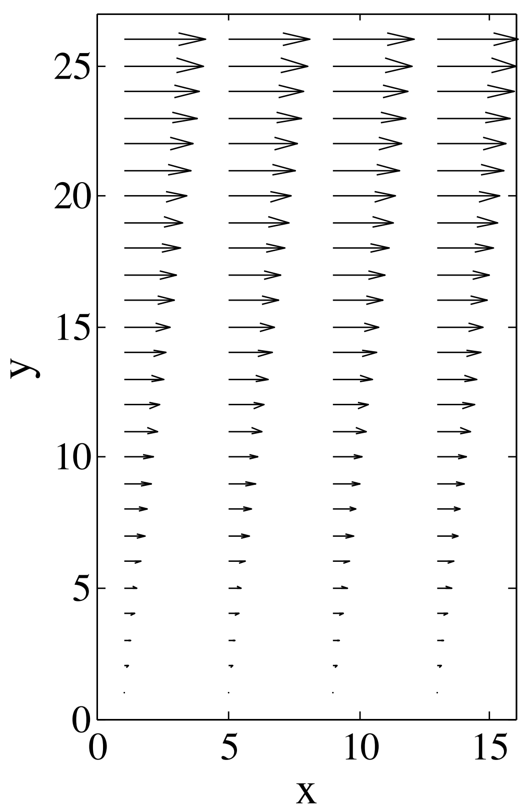

Figure 2 The flowfield at t = 2000

Comparisons with the exact solution

$$u^{exact} = U\left[\frac{y}{H} + 2\sum_{k=0}^{\infty}\frac{(-1)^k}{\zeta_k H}e^{-\nu\zeta_k^2 t}sin(\zeta_k y)\right] \quad (8)$$

where $\zeta_k = k\pi/H$ at times $t = 20, 100, 200, 400, 800,$ and 1600 are shown in figure 3. It can be seen that velocities are slightly under-predicted at early times and over-predicted at later times.

CONCLUSION

The practice of building simulation is fractured. The split between energy, multizone airflow, CFD airflow, and controls analysis, and analysis tools, are the fault lines of this fractured state. Previous attempts to integrate these analyses and tools have focused on linking pre-existing tools together. Our work takes a different approach, hypothesizing that an integration using the object-oriented/component-based, equation-based, multi-domain model description language Modelica as the underlying platform is fundamentally suited to analysis integration. The combination of object orientation with declarative, acausal modeling will enable greater code reuse and lower overhead in the modeling process by allowing modelers to simply state what the problem is rather than specifying how to solve it, leading to rapid creation of comprehensive multi-domain models and greater modeling flexibility.

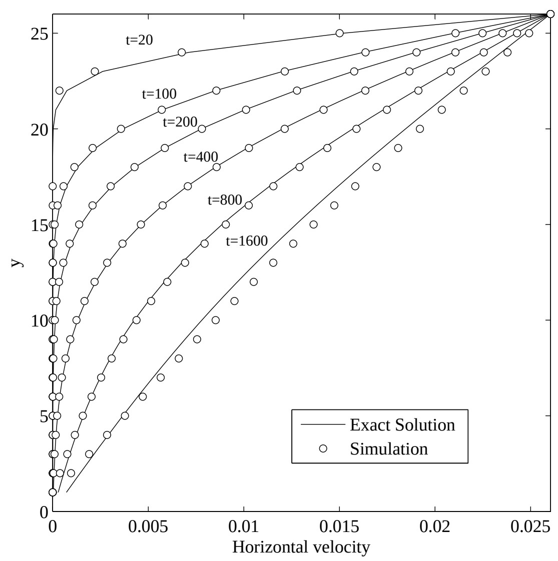

Figure 3 Comparison to the exact solution

The long-term goal of the present work is to provide an initial CFD capability in Modelica which is suitable for building simulations which incorporate energy, airflow, and controls. We hasten to add that this capability is intended only for integrated, multi-domain modeling and is not meant to compete with standalone CFD solutions. This work is a small initial step in that direction. Ongoing work includes analysis of numerical consistency and stability, extension to thermal flows, and incorporation of turbulence modeling. Interfacing to other aspects of building simulation, in particular the coupling between CFD and thermal energy flows through the building, is being investigated as a high priority.

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