Uncertainty Analysis and Quantification

Situation, Problem, and Need

Model Reduction, Graph Decomposition, and Uncertainty Quantification

High performance buildings are typically designed by fragmented expert teams using processes that do not scale up to large market penetration. The integration creates complex, dynamical systems from components that have been designed, in isolation, for individual high performance (i.e. component efficiency) and low cost and seldom consider their robustness to the dynamic building environment and use. Once connected into systems the components exhibit time-dependent, complicated behaviors over wide range of spatial and temporal scales, associated with building thermals, air flow, people movement, controls, computer and sensor network traffic, etc., that are difficult to predict and control. The problem is the *lack of system-level engineering design methodologies and tools that enable trading of energy, comfort, safety, and cost objectives while managing the complexity and uncertainty that is inherent in multi-scale, interconnected dynamic building systems.* Without such a capability, integration of building sub-systems will continue on an ad-hoc basis, thus leaving buildings inefficient.

The challenges of integrating heterogeneous models, managing the complexity caused by multiple time scales and their overlap, and quantifying the effect of uncertainty can be addressed with recent advances in model integrated computing and with techniques for model reduction, asynchronous co-simulation and efficient methods of computing uncertainty propagation. The key technical innovation is the simulation environment in which performance-based design of highly integrated building systems with dynamics and uncertainty can be performed rapidly with domain-specific models (such as physics-based models of energy, air, and contaminant flow, discrete-event models of communication networks, and agent-based models of people movement). Such tools will enable assessment of network design alternatives to meet reliability, fault tolerance and quality of service requirements while ensuring graceful performance degradation.

Such a capability will allow prediction of system behavior, especially component interactions, *before* the full system is built. New phenomena due to unanticipated component and subsystem interconnections can be captured and avoided by careful and rigorous application of modeling. This is crucial since sub-scale tests cannot verify robust operation in the presence of component variability or changes in operating environment, especially early in the design.

The effort will involve consideration of a broad range of external input scenarios and dynamics (weather, occupancy, indoor environment, energy prices), uncertainty in models and their inputs, and an immensely large design space. The program will enable cost-efficient and robust designs by addressing the control and communication networks in a building concurrently, and integration of energy saving control into these networks.

Model-based design obviously needs computational tools: modeling tools, analysis tools, and synthesis tools. These tools are typically expensive to build, and they are highly specialized for specific domains (e.g. CFD, dynamic system simulation, model checkers for finite transition systems, etc.) In a model-based design flow often many domains are involved, and tools are needed that address the various design activities. However, these tools need to interoperate because do-

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main models are often interrelated and interdependent. Hence, constructing such design flows necessitates the integration of models from different domains, and thus the design tools.

A further difficulty in the design of complex, heterogeneous systems is the tracking of dependencies between models and determining the impact of changes in one model on the other, dependent models. Changes in one domain may have an impact on a model of another domain, invalidating the other design. Design model management is a complex problem that cuts across domains and is very cumbersome to do manually, and infeasible for very large scale systems. Building Information Models[1] (BIM) is a popular framework being used in the buildings industry by architects, engineers, construction managers to enable accumulation and management of facility design and lifecycle information using a variety of models and databases. However, lack of consideration of the design flows mentioned above significantly reduces the potential value of concurrent design to a fragmented building design and delivery process.

Yet another complexity arises when many design variations exists for systems or subsystems. An engineering process may produce a few alternative design models for each specific (sub-)system, but when these are combined in a hierarchical way, the resulting number of possible combinations for a large design is astronomical. Designers need tools that allow managing this complexity in the model design space, and they need rapid facilities for evaluating (possibly optimizing) combinations of specific design variants.

Technical Barriers

This sub-section describes the three major technical barriers.

Heterogeneous modeling, analysis and design. The first barrier to accomplishing the proposal objectives is the difficulty in integrating heterogeneous models. The models of energy dynamics, airflow, building equipment and sensors, occupant movement, and communication networks are heterogeneous in that different modeling approaches and languages are used to represent them. However, these models are also interrelated and interdependent. State-of-the-art computational models take minutes to hours (depending on building scale) to run one energy scenario and energy performance metrics – yet to do effective and robust design, multiple scenarios would have to be evaluated with many uncertain input parameters, and in a large design space involving building topology, building equipment, sensor type and placement, and data communication network topologies. The building systems and relevant dynamics are defined by a complex interplay between a variety of components and sub-systems, with wide and overlapping time and spatial scales. The large time scales (minutes to hours) for the building comfort sensor and HVAC equipment elements have been known (Hunn, 1996) and largely responsible for fast-response dynamics of buildings being ignored. The multiple time scales issue will also be re-visited in the context “complexity and uncertainty” barrier described below.

The breadth of models includes fluid dynamics of air movement and aerosol/contaminant transport (typically using CFD or reduced order nodal models), possibly including chemical kinetics associated with a VOC (volatile organic compound) emission scenario, models of the building geometry (CAD tools), weather, HVAC equipment and system performance (typically lumped differential algebraic equations), dynamic models of occupant movement (typically agent based

[1] http://www.facilityinformationcouncil.org/bim/

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models), communications network models (stochastic or worst-case models of computation), models of the HVAC and building controls (differential equations and finite state logic), and the logic describing the HVAC system. The challenge is not to construct these models separately, but to integrate them and establish a common framework and level of abstraction in which the design decisions that are today considered separately can be co-designed in a cohesive manner.

Today designers separate these concerns because of assumed time and length scale separations. For example, it is common for the HVAC controls designer to assume the communications network is infinitely fast, and indoor air properties are uniform in a "zone." However, with IT network convergence and time scale overlap under plausible threat scenarios, these assumptions break down, implying that these heterogeneous models are interrelated and interdependent.

Complexity and Uncertainty. Complexity manifests itself in several ways. First, the presence of widely separated but coupled time and spatial scales suggest that the models will present numerically stiff equations making rapid simulation infeasible. Given millions of variables and equations involved in an airflow calculation, for example, together with several orders of magnitudes of separation between the component time scales, obtaining a single *steady-state* solution to evaluate the nominal performance can take days. Similarly, there are a huge number of possible threat scenarios to consider. Complexity also manifests itself in a very large design space, with multiple, interdependent design decisions. Managing this is a technical barrier. Establishing a common level of abstraction to facilitate these trade-offs is the key, central challenge.

A common approach for the analysis of large interconnected dynamic networks is to assemble the network model from component models as a large monolithic set of nonlinear dynamic equations. However, in the process the *structure* of the system (at this level of abstraction) is destroyed or at least ignored. *But it is precisely this structure that can be exploited to accelerate computation time and enable analyses such as model reduction and uncertainty propagation that is central to our technical approach*.

Uncertainty is pervasive in the problems we consider. Uncertainty is associated with the scenarios, boundary conditions, external factors, equipment performance, and the models themselves, which often must be simplified for computational reasons in ways that introduces uncertainty. (A good example of this is so-called nodal models of airflow in buildings.) To quantify the effects of uncertainty, models need to be simulated using probabilistic methods that describe affects of uncertainty of inputs (e.g. model uncertainty in network traffic, physics, and human behavior) and its effect on model outputs. However, traditional Monte-Carlo methods \cite{fishman1995} are infeasible in light of the complexity and breadth of these problems and could take years to simulate even if parallel computations are utilized. The analysis and robust design methods for large nonlinear dynamical systems are not yet well developed. This kind of analysis then represents a considerable technical barrier to our objective.

Proposed Approach

To overcome the above mentioned barriers, we propose addressing the model complexity and uncertainty issues including model reduction and uncertainty propagation techniques. The models (functional and non-functional) will span different domains (languages as well as tools), which is resolved using a model integration methodology mentioned in Section [Michael Wetter].

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- Energy dynamics models can be described by discretized partial differential equations (i.e. a set of coupled nonlinear ordinary differential equations) and tools such as Energy Plus, Matlab/Simulink or Dymola will be used to describe these.
- Airflow dynamics model can be obtained by Galerkin projection of Navier-Stokes or Businesq models onto reduced set of modes (POD is one option) and represented in Matlab/Simulink or Dymola.

The Model Management engine is the module that facilitates the integration of the different domains and has to assure that the correct properties are maintained across domain boundaries. This can be done either through mapping the domains to a common (semantic) domain or through co-simulation where this model now fulfills the role of translator during run-time.

As an outcome of the model management module are several "analysis" tools. All these tools operate at the system level and hence will provide methods to quantify the system behavior, including situation where there is tight coupling, e.g. through time-scales. The analysis tools include the following:

- Simulation engine. This will provide a high accuracy simulation of the integrated system. This simulation can be used to validate the levels of abstraction that are chosen during the modeling phase, as well as provide a mechanism for trade studies to investigate the effect of parametric changes (e.g. physical layer, network speed, network protocol, routing or connectivity changes, traffic from other sources)
- Analysis engine. This will provide a formal framework to determine specific system level properties without the need for Monte Carlo simulation of the entire system.

Enablers

Robust Uncertainty Management methods and tools

In addressing complexity and uncertainty, a number of important foundational approaches and tools for the problem of analyzing and designing dynamic systems robust to uncertainty were developed under DARPA-DSO funding (F49620-03-C-0035 and FA9550-07-C-0024). This work created a novel approach to analysis, simulations, and design of robust dynamic systems by *exploiting* rather than ignoring the *relative time scale differences of component dynamics* as well as the *interconnection structure*. For example, it was demonstrated that one is able to *design* systems that develop coherent structures when it is important to mitigate uncertainty through dynamics. The approaches developed with this DARPA funding will be extended and applied to complex models for energy and airflow transport, and for building phenomena models such as for people occupancy dynamics. Application of these methods to moderate complexity problems, involving 40000 states are already in progress for molecular dynamics problems and will be demonstrated by September 2008.

Reduced Order Models for Building Dynamics

The integration of building systems is creating large, complex, dynamic, inter-connected systems. The models will capture these characteristics of building physics, equipment and sensors, and communication networks. Recently, UTRC has investigated and developed the following types of models for building system and dynamic phenomena encountered in buildings: building

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topology models; building occupant models; air transport and smoke propagation models; building security system models; models of real-time situational awareness systems involving information fusion from sensor infrastructure belonging to the security and life safety systems; and system level dynamic models of HVAC, building energy flow and control systems. Some of the relevant models are described briefly below.

Building occupant models: The state-of-the-art in traffic simulation is "agent-based models". These fine-grained models (see example in 2-floor building in Figure 1.1.6) can be used to compute the motion of individual occupants using parameters that dictate the source and destination of the occupants, their speed and behavior (such as in the vicinity of other occupants). These simulations can be accurate with careful choice of the parameters but have very poor scaling properties: the computations scale as N^2 (N – number of agents). For large buildings and complexes, the problem of simulating occupant motion can become computationally intractable. The UTRC team in collaboration with researchers in University of California (Santa Barbara) and University of Illinois (Urbana-Champaign) developed a novel approach to represent the agent dynamics on a graph and utilized graph decomposition methods (described later) to extract reduced-order models by identifying weakly coupled sub-systems in the graph. The resulting models (such as illustrated with a 5-node graph in Figure 1.1.6) can be computed much faster and are scalable, making them suited to use in design (such as proposed for the proposed effort) and even during building operations.

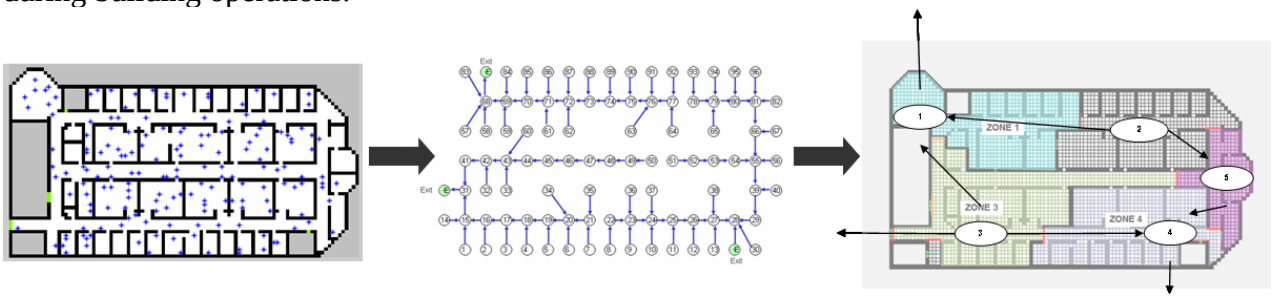

Figure. Building occupant dynamics, showing fine-grained agent based models at the left, graph-based representation of dynamics in the center, and "coarsened" representation on the right.

Building air and contaminant transport models

The state-of-the-art in airflow modeling is "computational fluid dynamics" (CFD). These simulations are used to simulate the evolution of airflow and other contaminants transported by airflow by discretizing the Navier Stokes or Businesq nonlinear partial differential equations on a fine grid (see example of smoke propagation dynamics during a fire breakout in a building in Figure 1.1.7). The simulations can be accurate but are computationally intensive due to the detailed discretization required. A 2 minute long simulation of smoke propagation from a fire in a small (2-floor) building shown in Figure 1.1.7 can take up to 2 days to run on a state-of-the-art workstation using best available commercial software (e.g., Fluent[2]). The UTRC team has developed an innovative approach to simulating threat propagation, capable of running 3 orders of magnitude faster that the fine-grained simulations (see illustration in Figure 1.1.7), making them suited to design iterations (needed for the proposed effort).

[2] http://www.fluent.com/

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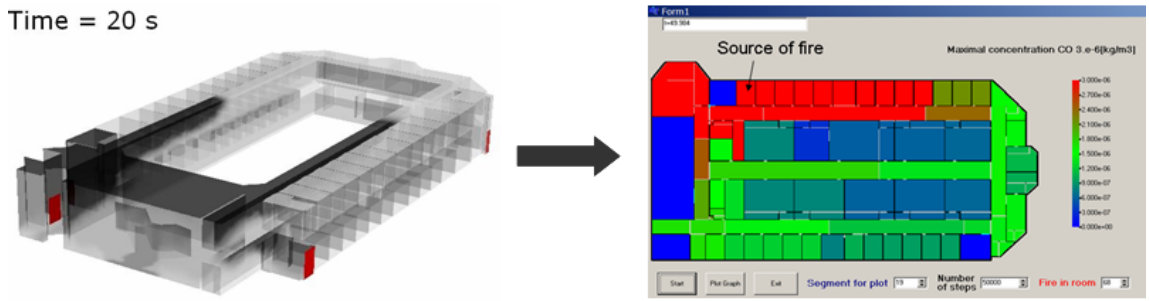

Figure. Smoke threat propagation dynamics modeled using detailed simulation methodology on left and UTRC model on the right showing coarser representation but with much faster computational turnaround.

Two problems arise when such diverse, static, dynamic, spatially distributed, continuous and discrete models are integrated: 1) the coupled simulation and analysis of these models becomes extremely computational complex, 2) the appropriate technique for propagation of uncertainty from input parameters to output metrics is not known.

To address these problems, UTRC will leverage technology being developed under the DARPA contract "Dynamic Network Analysis for Robust Uncertainty Management," for building systems. The essence of the approach is the following: a large system or network of dynamical components is decomposed into components using spectral graph theory (Varigonda et al. 2004). Operator theory and geometric dynamics methods are used to reduce component models and analyze propagation of probability measures in components.

Model reduction

We will begin with the choice of spatial coarse variables and then compute a temporal evolution operator for the coarse variables (Froyland 2001). The choice of coarse variables shall include the scales that determine the metric of performance of the building and the scales that couple with other components (Mehta et al. 2006). The coarse variables shall be determined by physical considerations or by post-processing data from resolved simulations (Holmes et al. 1996) and diffusion coordinates (Coifman et al. 2004, Lafon 2004, Coifman 2004). Reduced order model of temporal dynamics for airflow and energy can be extracted by analytic Galerkin projection of equations of motion (Holmes et al. 1996) onto modes (POD, sensitivity, etc.) while reduced order description of occupancy dynamics can be accomplished by extraction of Markov Models (Froyland 2001) from simulations of agent-based models (if available). Moreover, coarse temporal integration (Equation-Free) methods (Xiu et al. 2002) shall be used to simulate slow variables in the components of multiscale simulations. Parametric low order ODEs can be then obtained by system identification techniques. These shall in turn be used to complete the reduced-order models for the building occupant motion and airflow transport for state estimation and Model-Predictive Control.

Graph Decomposition

The main objectives in this section approach are to: (i) develop a mathematical framework based on Markov chains for obtaining and translating between hierarchical spatial scales (from fine to

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coarse) for the building domain models; (ii) implement a computational tool for constructing Markov chains on graph from the problem description using numerically efficient set-oriented methods; (iii) demonstrate multilevel graph partitioning algorithms based on *spectral analysis* of Markov chains: (iv) obtain consistent (across scales) reduced order building domain models; and (v) relate the spatial decomposition to analysis timescales (performance quantification).

To illustrate the use of graph decomposition based analytical techniques for model reduction a transport phenomenon relevant to building fire safety is discussed. Such phenomena are modeled by a convection diffusion partial differential equation. The proposed approach recasts the transport dynamics from this nonlinear partial differential equation as a Markov chain on graphs (Figure 1.1.9 illustrates the idea). At the finest scale, the graph is a representation of the high-fidelity CFD simulation with nodes representing the CFD grid, and the arrows representing the transport between nodes. At the coarsest scale (and large times), the entire building is represented as a single node capturing the fact that any initial condition in concentration will diffuse uniformly. The contaminant concentration is represented as a distribution over nodes of the graph. Dynamics is represented as time evolution of uncertainty in initial condition, propagated by a Markov chain.

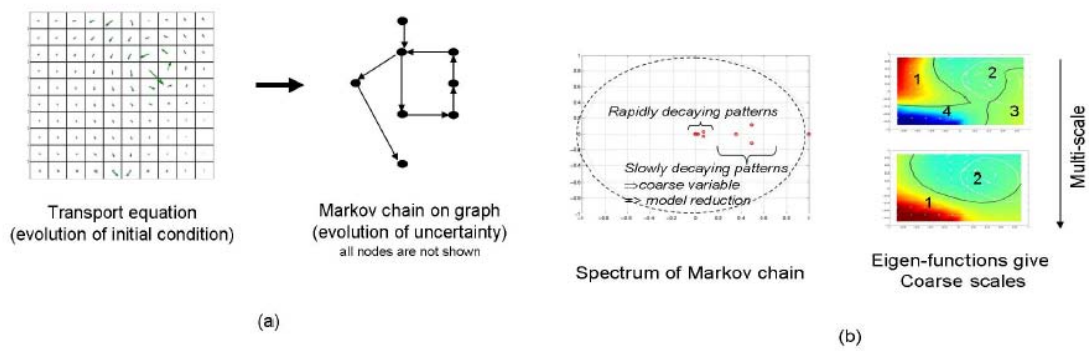

Figure. Airflow dynamics modeling problem transformed into a Markov chain on graph. (b) Spectral analysis of the Markov chain to obtain a multi-scale decomposition of the graph and associated dynamics

To demonstrate the approach, a simple, symmetric problem of two interconnected rooms in a building with a two-dimensional heterogeneous velocity field and homogeneous diffusivity is considered (Mehta et al. 2006). The initial complex graph was taken to be over a 10x10 computational grid for each room for a total of 200 graph nodes. The spectrum of the Markov chain, shown in Figure below, is expected to be typical to many Markov chains arising in building applications (e.g. for occupant motion, energy and comfort network models). The presence of relatively few dominant eigenvalues implies that a graph with fewer nodes is in fact sufficient to describe the dynamics, providing a methodology for model reduction. The corresponding eigenfunctions can be used to separate (and evaluate separately, speeding up computations) the building regions that interact on different timescales.

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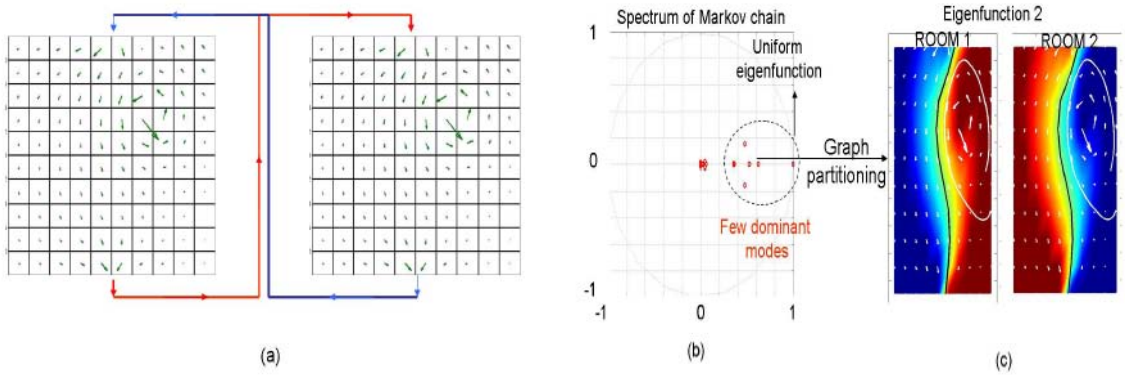

Figure. Example building two-room problem results: a) convection-diffusion problem defined over a 200-node computational domain, b) spectrum of Markov chain, and c) reduced-order 2-node graph obtained using the 2nd eigenfunction of the Markov chain.

Efficient Quantification of Uncertainty

Once system decomposition into subcomponents has been achieved, efficient methods for Uncertainty Quantification in such sub-components (Varigonda et al. 2004) will be used. Several options for the choice of stochastic basis including Polynomial Chaos expansion \cite{ wiener1938} with coefficients fitted using evaluating using the Collocation method \cite{ xiu2005c, xiu2002, xiu2007, loeven2007, prempraneerach2007, wan2005}, or Stochastic Finite Element methods \cite{ghanem1991, lovett2004, }, Stochastic Response Surface \cite{isukapalli1999 }, and equation-free \cite{xiu2005, xiu2005b} Uncertainty Quantification methods, and Quasi MC methods (Analytical Systems Engineering, DARPA final report, […]) will be pursued. Depending on the required accuracy of approximation of the mean and variance (or higher stochastic moments), these methods typically offer several orders of magnitude acceleration over Monte Carlo.

The action of the uncertainty propagation for the models of interconnected homogeneous or heterogeneous components will be done by iterative procedures using Wave-Form Relaxation techniques. The Jacobian Graph decomposition technique (Varigonda et al. 2004) shall be used to identify weak connections in the system. Iterative, multi-scale methods for interconnected system simulation using graph decomposition and asynchronous co-simulation, and uncertainty quantification (Varigonda 2004) based on Wave-Form Relaxation (Lelarasmee et al. 1982) and Multi-Grid methods (Brandt 2001) shall be implemented. Prior work (Varigonda 2004) has proved the point-wise convergence of the iterative procedure used in the density mapping method (Huzmezan & Kalmar-Nagy 2004).

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