# Applied & Computational Mathematics
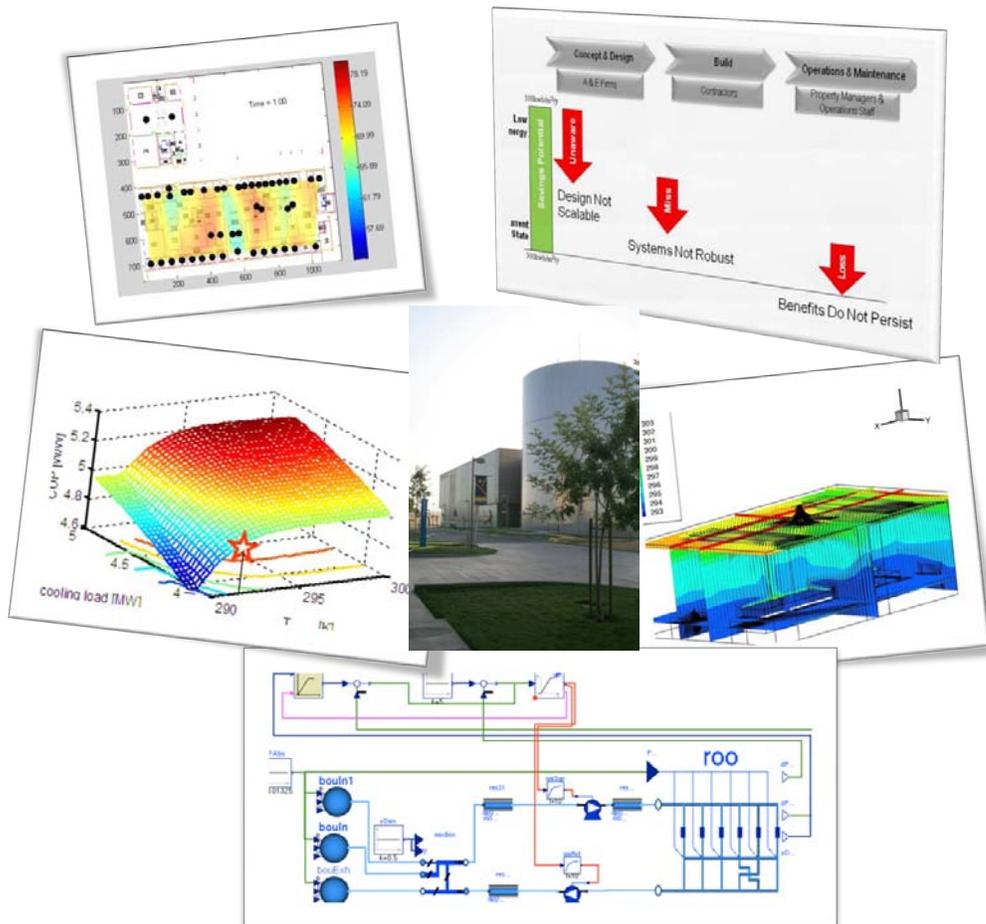# Challenges for The Design and Control of Dynamic Energy Systems

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# Contents

# I  Summary

The Energy Independence and Security Act of 2007 (EISA) was passed with the goal *"to move the United States toward greater energy independence and security."* Energy security and independence cannot be achieved unless the United States addresses the issue of energy consumption in the building sector and significantly reduces energy consumption in buildings. Commercial and residential buildings account for approximately 40% of the U.S. energy consumption and emit 50% of $CO_2$ emissions in the U.S. which is more than twice the total energy consumption of the entire U.S. automobile and light truck fleet. A 50%–80% improvement in building energy efficiency in both new construction and in retrofitting existing buildings could significantly reduce U.S. energy consumption and mitigate climate change.

Reaching these aggressive building efficiency goals will not happen without significant Federal investments in areas of computational and mathematical sciences. Applied and computational mathematics are required to enable the development of algorithms and tools to design, control and optimize energy efficient buildings. The challenge has been issued by the U.S. Secretary of Energy, Dr. Steven Chu (emphasis added): *"We need to do more transformational research at DOE ... including **c**omputer design tools for commercial and residential buildings that enable reductions in energy consumption of up to 80 percent with investments that will pay for themselves in less than 10 years."*[1]

On July 8 – 9, 2010 a team of technical experts from industry, government and academia were assembled in Arlington, Virginia to identify the challenges associated with developing and deploying new computational methodologies and tools that will address building energy efficiency. These experts concluded that investments in fundamental applied and computational mathematics will be required to build enabling technology that can be used to realize the target of 80% reductions in energy consumption. In addition the finding was that there are tools and technologies that can be assembled and deployed in the short term — the next 3–5 years — that can be used to significantly reduce the cost and time effective delivery of *moderate* energy savings in the U.S. building stock. Simulation tools, which are a core strength of current DOE computational research programs, provide only a part of the answer by providing a basis for simulation enabled design. New investments will be required within a broad dynamics and control research agenda which must focus on dynamics, control, optimization and simulation of multi-scale energy systems during design and operation. U.S. investments in high performance and high productivity computing (HP2C) should be leveraged and coupled with advances in dynamics and control to impact both the existing building stock through retrofits and also new construction. The essential R&D areas requiring investment are:

1. Characterizing the Dynamics of Multi-scale Energy Systems;

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[1] Secretary of Energy Dr. Steven Chu, House Science Committee Testimony, March 17, 2009.

2. Control and Optimization Methodologies of Multi-scale Energy Systems Under Uncertainty;

3. Multiscale Modeling and Simulation Enabled Design and Operation.

The concept of using design and control specific computational tools is a new idea for the building industry. The potential payoffs in terms of accelerated design cycle times, performance optimization and optimal supervisory control to obtain and maintain energy savings are huge. Recent advances in computational power, computer science, and mathematical algorithms offer the foundations to address the control problems presented by the complex dynamics of whole building systems. The key areas for focus and associated metrics with targets for establishing competitiveness in energy efficient building design and operation are:

- **Scalability.** Current methodology and tools can provide design guidance for very low energy buildings in weeks to months; what is needed is hours to days. A 50X improvement is needed.

- **Installation and commissioning.** Current methodology and tools can target a three month window for commissioning of building subsystems; what is needed is one week. A 10X improvement is needed.

- **Quality.** Current design tools can achieve 30% accuracy; what is needed to make design decisions is 5% with quantification of uncertainty. A 5X improvement is needed.

These challenges cannot be overcome by raw computational power alone and require the development of new algorithms. Here algorithms mean much more than simulating the building physics but need to be inclusive of a better understanding of the building and the control systems associated with the building and to capture the entire set of dynamics. The algorithms must represent computationally new mathematical approaches to modeling, simulation, optimization and control of large multi-scale dynamic systems and bringing these elements to bear on industry in simulation enabled design approaches. These barriers may be overcome by investing in an aggressive research program in applied and computational mathematics.

Dynamics and control is the underlying science and technology focus for this report. This area has not received attention in the building community nor in the fundamental mathematics and science areas of relevant funding agencies. There is an urgent need to have sustained attention to develop and to deploy technology to DoD/GSA/DOE buildings that fully utilize advances in controls in the short run but also develop underlying math & science base.

## II  The Mathematics of Dynamics & Control in Energy Efficiency

### II.1   Issues and Needs

Figure II.1 illustrates the opportunities for increasing energy efficiency in buildings across the design, construction and operation portions of the lifecycle. This figure is of course only a schematic and much more detail needs to be added, however, it gives a good map of how to target investments to reduce energy consumption in buildings. The scale is based on $100\,\text{kWh/m}^2$/year site energy usage which includes heating, cooling and lighting loads and which is an EU and Asia target — it should be noted that the U.S. current average is well above $600\,\text{kWh/m}^2$/year!

Focus for applied mathematics needs to be placed on the dynamics and control of multi-scale energy systems. This focus is driven by the observation that a building is a complex energy system because:

- Buildings have complicated dynamics that are critical to understand and shape to impact energy consumption, moreover, building systems are composed of heterogeneous components that do not have mathematically similar structures and which involve different scales in both time and space.
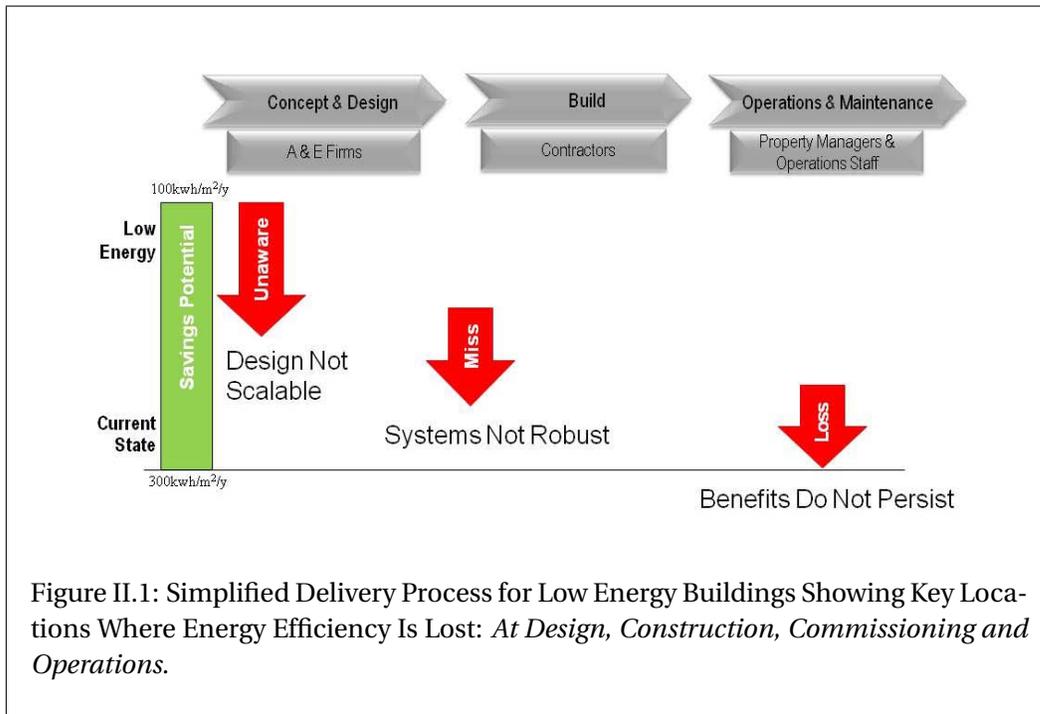


Figure II.1: Simplified Delivery Process for Low Energy Buildings Showing Key Locations Where Energy Efficiency Is Lost: *At Design, Construction, Commissioning and Operations.*

- The number of these components is large and there is considerable uncertainty that must be addressed through the design of dynamics both through passive and active control mechanisms.

- Components are connected in a variety of ways, most often nonlinearly. Furthermore, local and system wide phenomena depend on each other in complicated ways.

- The dynamic behavior of the building is extremely difficult to predict from the behavior of individual components. Moreover, the overall system behavior may evolve along qualitatively different pathways that may display great sensitivity to small perturbations at any stage.

## II.2   Role of Mathematics & Computation

Although mathematics and computational techniques that focus on general complex systems are relevant for building systems [1, 3] the design and operation of buildings offer unique computational challenges and requirements that must be addressed in order to produce tools which will have a transformative impact on the industry and how buildings are designed, constructed and operated. Key issues which must be addressed in buildings that differentiate this application domain are the usage of the buildings which must take into account uncertainty in occupancy and loads including weather and power supply. Also, it is essential to address the different stages of the building life-cycle which must be considered holistically from a usage perspective and then reflected in the types of computational methodology and tool chains that are developed and deployed to the industrial base.

It is key is to bring to bear the new breakthroughs in computational science, high productivity computing, model reduction, optimal and distributed control, optimization and sensitivity analysis and distributed parameter control to the problems of modeling, simulation, estimation, actuation and real time optimal control of building energy systems. The metrics of development time, cost and quality of low energy consumption building designs can all be affected through the use of computational science and high performance and high productivity computing (HP2C).

However, there are challenges in the use of existing HP2C systems for the design of highly energy efficient buildings. Figure II.2 displays the computational performance required to conduct a "raw" or direct simulation for design with less than one hour turnaround time (typical of building design requirements). The determination of energy consumption in buildings requires understanding of coupled airflow and thermal properties of small room scale zones to whole building situations. However, this schematic, like the earlier one shown in Figure II.1 which shows the loss in efficiency across the life-cycle, hides a number of issues and opportunities. It is not enough in the turnaround time to only simulate a few trajectories associated with building operations, rather, the

dynamics of the coupled subsystems need to be understood. In addition the effects of uncertainty of the occupancy and the loads also need to be computed and made visible in all the stages of the lifecycle. It is to be expected that focus on the applied and computational mathematics for building energy efficiency will bring new mathematics forward that integrate HP2C resources with new analyses.
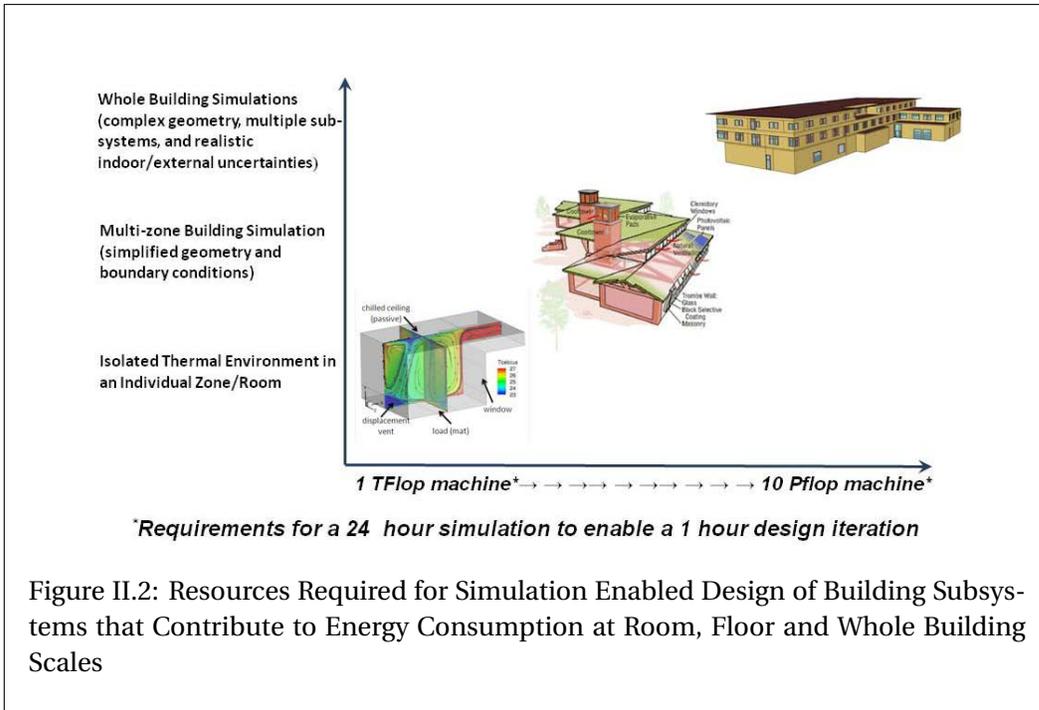


Figure II.2: Resources Required for Simulation Enabled Design of Building Subsystems that Contribute to Energy Consumption at Room, Floor and Whole Building Scales

Research investments in developing solvers for systems of nonlinear differential algebraic equations that are coupled to discrete equations and for reduced order models are needed to increase the computational robustness and to reduce the computational expense requirements, and analysis methods are needed to understand the underlying structure of multi-scale, uncertain dynamic phenomena and their control, enabling next generation design tools to deliver highly energy efficient buildings and systems.

Dynamics and control is the key enabling technology for the design and operation of low energy consumption buildings. Control is often referred to as a "hidden technology" that enables performance: from [3] "The field of control provides the principles and methods used to design engineering systems that maintain desirable performance by automatically adapting to changes in the environment." As used in this document control technology covers the entire lifecycle from system design to operations. Controls — and the understanding of dynamics and how to shape either passively or actively — is a key technology to enable the design of complex energy systems such as low en-

ergy buildings. Dynamical analysis is the key to capturing and exploiting the intrinsic structure of complex systems, that is, systems that are interconnected, uncertain and have different or heterogeneous structure such as a building. Control offers the ability to shape dynamics of interconnected, multi-scale energy systems both in the stages of their design as well as in operations. Most importantly, control offers the ability to mitigate the uncertainty that dominates the operations of energy systems.

# III  Three Research Pillars: Dynamics, Controls & Design

There are three key pillars that must support the development and deployment of applied and computational mathematics to the building energy area. These are

**Dynamics:** be able to effectively characterize dynamics of large scale, heterogeneous, multiscale systems,
**Control:** be able to develop optimal control and optimization methodologies throughout the building design and operation stages,
**Model Based Design Methodology:** bring the dynamics, control and optimization elements together into tools for effective model based design and operation for the building industry.
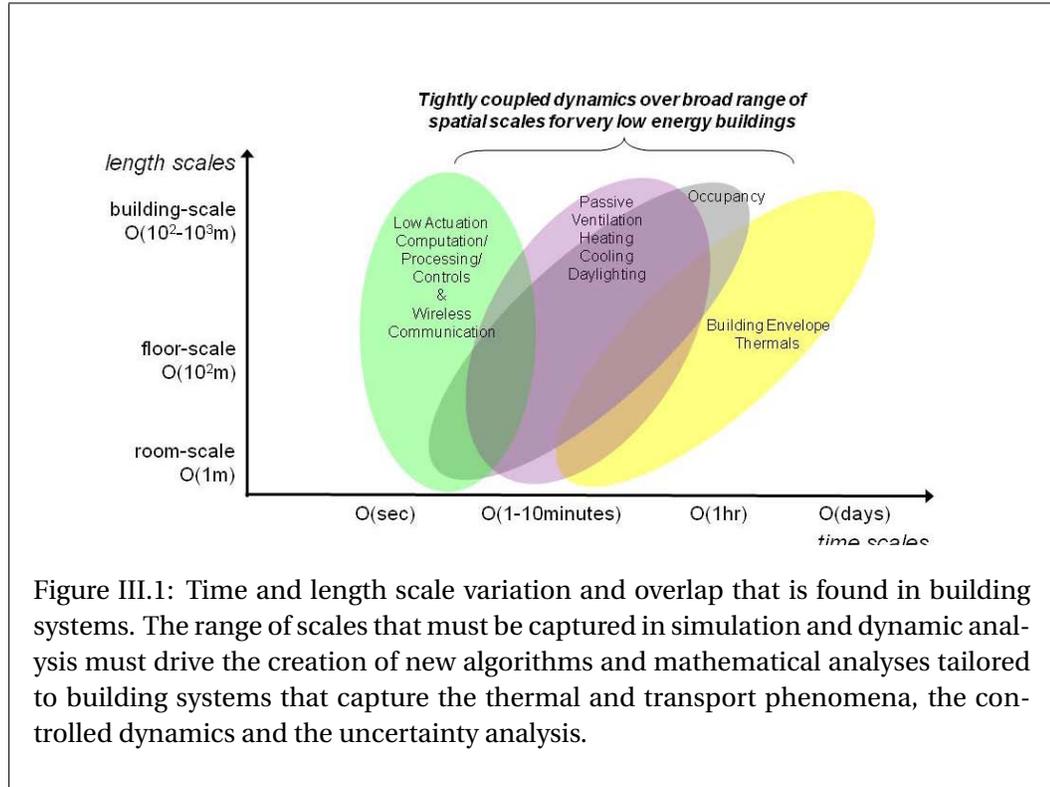
## III.1  Methodology to Characterize Dynamics of Multi-scale Energy Systems

In order to develop design specific computational methods for energy systems it is essential that one is able to sufficiently characterize the complex multi-scale dynamics by models that are amenable for use in design and control. This requirement leads to the following needs.

**Needs**

Low energy buildings are "climate adaptive" and the energy consumption reductions depend on using interactions between prevailing climate conditions and passive technologies for their operation. Examples such as the Deutsche Post or Manitoba Hydro [2] buildings are low energy use buildings that utilize a range of passive technologies such as natural ventilation and daylighting. The consequence of these types of buildings and the use of passive means for daylighting, heating, cooling and ventilation is that the natural dynamics must be taken into account during design and operation and need to be characterized. Characterization is not simply more refined or faster time domain simulation, rather, analysis including detailed quantitative understanding of the dynamics of heterogeneous interconnected systems at different time and length scales must be taken into account.

Getting the dynamics wrong in a design can result in time consuming engineering efforts during operation and very expensive to fix. The low energy KfW building in Frankfurt, Germany required tuning of three years to get the performance right [4]. Industry simply cannot accept this kind of risk.

Figure III.1: Time and length scale variation and overlap that is found in building systems. The range of scales that must be captured in simulation and dynamic analysis must drive the creation of new algorithms and mathematical analyses tailored to building systems that capture the thermal and transport phenomena, the controlled dynamics and the uncertainty analysis.

## Current State and Gaps

The current state of being able to characterize dynamics in buildings is very low. While simulation capabilities for building energy models are increasingly being used in design and are being encouraged through standards like LEED, these capabilities are mainly used today to capture the dynamics of the building envelope and steady state conditions of the energy and the associated control systems. This capability is well established since the development of building simulation and is embodied in a number of tools. The steady state conditions are insufficient though to fully seize computational capabilities to design and operate high performance buildings. The range of different physics that need to be captured and the time scales (seconds to days) tax any simulator used in the available tools and the length scales create very large scale issues in gridding the building layout. New algorithms must be developed that can be used to move across the scales and to isolate and reveal couplings of subsystems that drive essential dynamics and are critical to design control algorithms and to develop diagnostic algorithms for building operations. Figure III.1 shows both the range and the interactions of length and time scales that must be addressed in building problems.

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**Proposed Approach and Research Agenda**

The methodology to close the gap on being able to describe the dynamics of buildings that have strong use of passive technologies are to extract, shape and quantify large scale dynamic systems that are composed of very different, that is heterogeneous, physical, computational and communication subsystems. Specific needs and how the state of the art will be advanced are the following:

- New dynamical system theory tools will extract invariant dynamics and reveal underlying coupled thermal, airflow and equipment dynamics, from high fidelity models for robust control of low energy system designs. The current state of the art is to obtain a large number of simulations that give limited and imprecise knowledge of the dynamics of the building operation.

- Dynamical system tools will provide optimal control design of multi-scale, fully coupled building, equipment, thermo-fluid, and control models. The current state of the art is to design supervisory control sequences for building operation based on empirical and historical knowledge of building operation.

- Uncertainty quantification methods and tools will provide predicted building performance through the simulation of energy and thermal models using probabilistic methods that describe the effects of the uncertainty of inputs (e.g. uncertainty in human behavior, physics, and network traffic) on the model outputs. The current state of the art is to recognize sensitivity of building performance during commissioning and operation phases.

- Fast parameter sampling, probabilistic analysis, uncertainty quantification and propagation methods for energy and thermal simulations will establish performance bounds during design of low energy consumption performance. The current state of the art uses Monte Carlo sampling of subsystem models to characterize sensitivity of performance during conceptual and preliminary design stages.

- Tools must be developed to dynamically decompose energy and building systems and provide capability for actionable, real time visualization of system level energy performance at multiple scales for energy forensics and prognostics. The current state of the art is to control subsystems such as lighting and HVAC separately to track comfort with little awareness to energy use. Today, buildings are zoned based on empirical and historical building operation.

- Computationally efficient embedded algorithms will track system dynamics and automatically detect and prevent energy waste. Thus, building control systems will be aware of energy and peak power implications of their control options, and not only regulate to maintain comfort. Tools must allow measuring and enforcing

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performance across the handoff points during design, construction and operation. The current state of the art is to have multiple manual or text based handoffs during the design and the construction phase.

- Hierarchical, optimal control laws will establish low energy consumption design principles (e.g. natural ventilation, thermally activated structures). The current state of the art is to arrange hierarchical control systems based on empirical and historical building operation.

## III.2 Control and Optimization Methodology of Multi-scale Energy Systems under Uncertainty

Uncertainty management and quantification in energy systems must be included in the development of control and optimization tools, thus robustness in both areas is essential.

### Needs

The stages, and the handoff points between the stages, of building design and operation shown in Figure II.1 have large effects on energy consumption. Moreover, even if low energy effects are designed into a building, the robustness of the design and the understanding of sensitivities of subsystems and component changes between the building delivery stages. Furthermore, the "value engineering" phase of building construction can cripple even the best of designs. It is essential that effective methodology and tools for designing and implementing control systems be effectively used in these stages. Moreover, it is necessary to bring forward ways to search the design space for optimal configurations that bring down energy consumption but also do so robustly in the face of the different uses of buildings, the loads that are seen and component variations during construction that are seen as well as degradations during operation.

### Current State and Gaps

The current state in control methodology and optimization in building design does not employ state-of-the-art methods used in other industries. Today building level control — or control sequences — are derived from history and similarity to other building designs that do not extrapolate to very low energy buildings. There is little attention to trade studies or the systematic use of optimization technologies. Moreover, in the design stage which has the greatest leverage to reduce energy consumption the pressures of cost and time preclude the examination of different systems — different configurations of heating, ventilation, cooling and daylighting solutions. At this stage the use of optimization to look quickly at different configurations and to provide information on

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multi-criteria cost functions could go a long way to assisting designers to look outside the usual offerings of equipment and controls.

During design little attention is given to diagnostics at the system level — the current offerings look mainly at components using traditional fault detection and diagnosis (FDD) techniques. Low energy buildings have much tighter coupling and dependency on subsystems (lighting, cooling, heating, etc) and diagnostics need to be developed at the system level. This is an extension of control technology that is not available today.

A number of gaps that highlight the need for control and optimization technologies are as follows:

- Achieving design performance targets for building energy usage requires whole building embedded control and fault detection, isolation and accommodation that auto-calibrate throughout the entire lifecycle of a building; achieving this requires significant advances in algorithm development over the existing industrial use of simple proportional-integral (PI) controls and component centered (or rule based) monitoring and diagnostics.

- Energy simulation models are not used for the design of controls and diagnostics. The simulation models are also not carried through the lifecycle for verification of performance during building operation. They are also not used in building management system (BMS) to ensure achievement of LEED design targets. Tool chain linkages are important as well as developing and demonstrating organizational use of models across the entire building life-cycle to effectively design, deliver and maintain building performance.

- A recurring problem in building simulation and in monitoring of building operation is how to detect anomalies and trends in a large amount of simulated or measured time trajectories. Extracting such information from data would facilitate finding operational instabilities (such as limit cycles from improperly tuned controls), equipment faults or degrading equipment. Developing data analysis methodology and model based tools is essential to maintain building design intent through operations.

- Dynamical models for the simulation and optimization of whole building energy use lead to hybrid systems models that cannot be simulated robustly or fully analyzed for correctness. Advanced solvers, domain specific model reductions and novel computational algorithms are needed that can deal with time scale disparities and thousands of parameters that are specifically tailored to the types of models used in building systems.

- Practical market solutions for building simulation must have an expanded scope to address the full development of building control. Simulation and analysis tools

must map the building energy use and user comfort requirements through the entire development process and specifically to the implementation into networked embedded hardware and software deployment. The applied mathematics and computational research agenda must address the co-design problem for optimal sensor placement and control and diagnostics design and verification.

**Proposed Approach and Research Agenda**

The methodology to close the gaps on the use of controls and optimization technologies must address system level design methodologies. The gaps in the state of the art lie in the development of methodology and tools for large scale coupled dynamic systems. While some of these challenges are generic to control theory the application to buildings must fully use the structure of buildings both in the underlying physics of thermal and transport phenomena but also recognize the control performance required in energy consideration and the disturbances of loads and occupancy behavior. Specific needs and how the state of the art will be advanced are the following:

- Theory, methodology and tools will be used for verification of system level energy use including control implementation for large building systems. The current state of the art does not use any dynamic simulation and verification tools for the evaluation of control sequences. Verification is delayed to building operation on site.

- Theory and tools will be developed and used for the hybrid systems control verification needed for multi-scale energy system applications and methodology to incorporate uncertainty and sensitivity analysis will be deployed. The current state of the art does not address the sensitivity of controlled systems.

- Hybrid systems model reduction tools will be developed and used to create application specific control and diagnostic models from high fidelity model libraries to enable system optimization and control at multiple scales. The current state of the art is to use data driven fault models and not to utilize system level dynamic models for fault detection, diagnosis and prognostics.

## III.3   Multiscale Modeling and Simulation Enabled Design and Operation

The term "simulation enabled design methodology" is used here to highlight the difference between what is proposed here and what has been called historically "simulation based design." Model enabled design methodology for buildings must focus on modeling, numerical methods, algorithms and computational tools for the purpose of design,

optimization, deployment and operation of buildings. In this setting, the goal of modeling and simulation is to enable efficient design flows that optimize the design and carry this design intent into the operation of the building, leading to robustly performing low energy comfortable buildings. Simulation by itself is not adequate. Consequently, the computational sciences and challenges differ from standard forward simulations in levels of fidelity, computational times requirements and even in the nature of the equations to be solved through simulation.

**Needs**

Improving design methodology and tools are the biggest lever that exists to move buildings to a different state on energy savings. Bringing together the methodologies of characterizing dynamics of the building including passive mechanisms for heating and cooling such as natural ventilation and daylighting with active HVAC methods, the use of optimization methods to search the design space and the use of automated tools to verify and enforce performance at the hand-off points of the stages in Figure II.1 are all critical to achieving energy efficient designs in cost and time effective ways.

**Current State and Gaps**

Whole building energy and comfort analysis typically requires models for numerous physical situations: for heat and fluid transport in piping/duct networks (heat exchangers, pumps), for heat and moisture transport in structures, and for room air and species transport (computational fluid dynamics). The time required to assemble system-level models, the computational effort that is needed to exercise models of sufficient fidelity and the lack of tools to assemble multi-scale, multi-physics models currently makes the use of models in design prohibitive from a cost and schedule perspective of industrial users. The gap in the current state is a structured way of modeling the different fidelities and effectively bringing controls, optimization and uncertainty analysis together to focus attention on low energy designs — the critical features and the overall robustness of different configurations under consideration by the designer. Advanced solvers for these nonlinear differential algebraic equation systems that are coupled to discrete state, domain specific reduced order models and computational techniques to handle multi-scale, uncertain system dynamics will help to make simulation approaches more feasible computationally.

Today industry employs a disjointed collection of tools for various stages of design, involving energy analysis, system sizing, controls design, lacking standardized model and data interfaces. The tools offer no robust integration with Building Information Models, in particular regarding controls and nonconventional energy systems.

**Proposed Approach and Research Agenda**

The methodology to close the gaps at the design must address system level design methodologies. The gaps in the state of the art lie in the development of methodology and tools for assembling and simulating models of buildings, HVAC and controls based on BIM, for conducting simulation of energy systems with realistic feedback loop control, for assembling reduced order models from high fidelity simulations where the models are constructed with the specific goals of being usable for control design, for assessing uncertainty and robustness and for diagnostics. Specific needs and how the state of the art will be advanced are the following:

- Multi-scale grid generation, solvers for systems of nonlinear differential algebraic equations that are coupled to discrete equations, and frameworks for cosimulation will be developed for specific building applications that address the thermal and transport phenomena as well as load variations. The numerical techniques will be developed in a methodology and associated tool chain to use high fidelity models to obtain robust reduced order models suitable for control design, optimization of building subsystems and uncertainty analysis to ensure robustness of the building through construction and operation. Predictive capability must be developed with (1) high performance CFD solvers that can model three dimensional flow and energy transport through internal open spaces and ventilation of buildings made up of intricate configurations; (2) the ability to rapidly change the configuration for design optimization and (3) local resolution around energy sources and sinks. The current state of the art is to use crude steady state models of the HVAC system to support design decisions hence not addressing energy performance in suitable fidelity to drive effective decision making.

- Techniques for model-based design flows. Based on operational requirements, these flows allow the design and optimization of control sequences, the automatic implementation of these sequences in control hardware, and the verification of the control logic during operation against executable specifications that were created in the design phase. Realizing these flows requires computational science and tools that are beyond what is used today by the buildings industry.

- Techniques will be developed to obtain reduced-order models from high fidelity coupled structural and building thermal simulations suitable for use in control design and optimization. The models must be capable of accurate real time system behavior prediction under uncertain weather, user behavior and power network conditions and must be useable in software environments that utilize BIM environments for data transfer and use by designers from A&E firms to control implementation by building consultants. The current state of the art is to use crude steady state or simplistic behavioral models for control evaluation and to tune the controls on site in the actual building.

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- Techniques involving use of parallel methods for multi-criteria and stochastic optimization to speed up high fidelity coupled structural and building thermal simulation enabled system optimization studies will be developed. The use of parallel methods can be taken advantage of, but research is needed to combine stochastic effects with the other requirements: multi-criteria optimization and optimization problems with a combination of discrete and continuous parameters. The current state of the art is to use desktop simulation with at most a cursory Monte Carlo simulation of key parameters identified as critical through empirical or historical knowledge.

- Large scale data assimilation tools will be developed to visualize actionable information in real-time, preventing energy performance degradation. The current state of the art is to gather data from building operation through limited control points and little aggregation or analysis of the building operation data is used to drive either improved performance or design studies.

# IV Conclusions

A new research program in computational and applied mathematics with a broad dynamics and control research agenda that focuses on dynamics, control, optimization and simulation of multi-scale energy systems will enable computational solutions to impact building energy efficiency needs. These challenges cannot be overcome by raw computational power alone and require the development of new algorithms, a better understanding of the dynamics and new mathematical approaches to modeling, simulation, analysis and optimization of large multi-scale, multi-physics energy and control systems. It also requires bringing these elements to bear on industry in the forms of tools and processes at large scale to significantly reduce the energy use of the building stock in the US and globally.

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# VI  July 2010 Computational Science Needs in the Design, Optimization and Operation of Energy Efficient Buildings Meeting Information

A meeting was held July 8–9, 2010 in Arlington, VA. Background briefing material including the terms of reference as well as position papers prepared for the meeting can be found at the Wiki site at Computational Science July 2010 Meeting Wiki[1]. The following attended the Arlington meeting and contributed to the content of this white paper.

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[1]http://www.engineering.ucsb.edu/ mgroup/wiki/index.php

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