Preprints

B. W. Bush, E. Doris, and D. Getman, “Understanding the Complexities of Subnational Incentives in Supporting a National Market for Distributed PV.” The purpose of this work is to contribute to the discussion of the impact subnational (State, local, and utility) policies, as a group, have on the national market for solar PV technologies. Subnational policies have increased in volume in recent years and federal incentives are set to be phased out over the next few. Understanding how subnational policies intertwine within and across jurisdictions to impact market development provides information to both federal program administrators and subnational policymakers to support informed policy decision making. In order to do add value to the current discussion on subnational policies, a logic engine containing incentives for PV development was developed. The incentives used are from the US Department of Energy’s (DOE) Database of Incentives for Energy Efficiency and Renewable Energy (DSIRE), widely considered to be the most comprehensive listing of US policies and incentives. The logic engine adds value to the DSIRE database by allowing users to see the interactions of incentives along with exogenous factors such as geographic location, technology characteristics, and financial parameters. Depending on how it is queried, the database can yield insights into which combinations of incentives are available and most advantageous under particular circumstances as requested by the user. To illustrate the capabilities of the logic engine, the database was queried to identify the relative complexities of incentives at the subnational level. The goal was to identify how many incentives they qualify for, and the subset of those that result in the largest monetary benefit (the “best” combination of incentives). The outcomes inform federal program designers as to the complexity of the incentive “market” nationwide, and subnational policymakers to the complexities of incentives within their jurisdiction, as well as allow for a comparison of complexities between jurisdictions.

M. S. Melaina, Y. Sun, and B. Bush, “Retail Infrastructure Cost Comparison for Hydrogen and Electricity Light-Duty Vehicles,” presented at the SAE 2014 World Congress and Exhibition, Detroit, Michigan. Both hydrogen and plug-in electric vehicles offer significant social benefits to enhance energy security and reduce criteria and greenhouse gas emissions from the transportation sector. However, the rollout of electric vehicle supply equipment (EVSE) and hydrogen retail stations (HRS) requires substantial investments with high risks due to many uncertainties. We compare retail infrastructure costs on a common basis – cost per mile, assuming fueling service to 10% of all light-duty vehicles in a typical 1.5 million person city in 2025. Our analysis considers three HRS sizes, four distinct types of EVSE and two distinct EVSE scenarios. EVSE station costs, including equipment and installation, are assumed to be 15% less than today’s costs. We find that levelized retail capital costs per mile are essentially indistinguishable given the uncertainty and variability around input assumptions. Total fuel costs per mile for battery electric vehicle (BEV) and plug-in hybrid vehicle (PHEV) are, respectively, 21% lower and 13% lower than that for hydrogen fuel cell electric vehicle (FCEV) under the home-dominant scenario. Including fuel economies and vehicle costs makes FCEVs and BEVs comparable in terms of costs per mile, and PHEVs are about 10% less than FCEVs and BEVs. To account for geographic variability in energy prices and hydrogen delivery costs, we use the Scenario Evaluation, Regionalization and Analysis (SERA) model and confirm the aforementioned estimate of cost per mile, nationally averaged, but see a 15% variability in regional costs of FCEVs and a 5% variability in regional costs for BEVs.

L. J. Vimmerstedt, B. W. Bush, D. D. Hsu, D. Inman, and S. Peterson, “Maturation of Biomass-to-Biofuels Conversion Technology Pathways for Rapid Expansion of Biofuels Production: A System Dynamics Perspective,” Biofpr. The potential for rapid expansion of the biofuels industry is explored using a system-dynamics simulation model named the Biomass Scenario Model (BSM), emphasizing how policy incentives and technological learning-by-doing can accelerate industry growth. The BSM simulates major sectors of the biofuels industry, including feedstock production and logistics, conversion, distribution, and end use, as well as their interaction with one another. The model represents conversion of biomass to biofuels as a set of technology pathways, each having characteristics that include allowable feedstocks, capital and operating costs, and allowable products. Simulations indicate that coordination of investments—with respect to timing, pathway, and target sector within the biofuels industry—is needed to accelerate learning-by-doing and most effectively expand biofuels production to meet Renewable Fuel Standards (RFS). Metrics of effectiveness include timing and magnitude of increased production, incentive cost and cost-effectiveness, and avoidance of windfall profits. Due to risks and uncertainties, investment costs and optimal investment targets—such as relative value of investment in more-mature versus less-mature pathways—can be explored through scenarios but not predicted with precision. During rapid growth, dynamic competition intensifies, including competition for cellulosic feedstocks and ethanol market shares. Rapid growth in ethanol production occurs in simulations that allow higher blending proportions of ethanol in gasoline-fueled vehicles, even up to RFS-targeted volumes of biofuel.
Y. Alhassid and B. Bush, “Stochastic approach to giant dipole resonances in hot rotating nuclei,” Phys. Rev. Lett., vol. 63, no. 22, pp. 2452–2455. <http://link.aps.org/doi/10.1103/PhysRevLett.63.2452>A stochastic macroscopic approach to giant dipole resonances (GDR’s) in hot rotating nuclei is presented. In the adiabatic limit the theory reduces exactly to a previous adiabatic model where the unitary invariant metric is used to calculate equilibrium averages. Nonadiabatic effects cause changes in the GDR cross section and motional narrowing. Comparisons with experiments where deviations from the adiabatic limit are substantial are shown and can be used to determine the damping of the quadrupole motion at finite temperature.

Y. Alhassid and B. Bush, “Effects of thermal fluctuations on giant dipole resonances in hot rotating nuclei,” Nuclear Physics A, vol. 509, no. 3, pp. 461–498. <http://www.sciencedirect.com/science/article/pii/0375947490900873>We present a macroscopic approach to giant dipole resonance (GDR) in highly excited nuclei, using a unified description of quadrupole shape thermal fluctuations. With only two free parameters, which are fixed by the zero-temperature nuclear properties, the model reproduces well experimental GDR cross sections in the 100 A 170 mass range for both spherical and deformed nuclei. We also investigate the cross-section systematics as a function of both temperature and angular velocity and the sensitivity of the GDR peak to the nuclear shape. We conclude that at low temperatures (T < 1 MeV) the GDR cross section is sensitive to changes in the nuclear energy surface. Higher-temperature (T > 2 MeV) cross sections are dominated by large fluctuations (triaxial in particular) and are much less sensitive to the equilibrium shape.

Y. Alhassid and B. Bush, “Orientation fluctuations and the angular distribution of the giant-dipole-resonance rays in hot rotating nuclei,” Phys. Rev. Lett., vol. 65, no. 20, pp. 2527–2530. <http://link.aps.org/doi/10.1103/PhysRevLett.65.2527>A recent macroscopic approach to the giant dipole resonances in hot rotating nuclei is extended to include the angular distributions of the rays emitted in the resonance decay. It provides a uniform description of thermal fluctuations in all quadrupole shape degrees of freedom within the framework of the Landau theory. In particular, the inclusion of fluctuations in the nuclear orientation with respect to the rotation axis is crucial in reproducing the observed attenuation of the angular anisotropy. The theory is applied to recent precision measurements in 90Zr and 92Mo and is the first to reproduce well both the observed giant-dipole-resonance cross sections and the angular anisotropies.

Y. Alhassid and B. Bush, “Time-dependent shape fluctuations and the giant dipole resonance in hot nuclei: Realistic calculations,” Nuclear Physics A, vol. 514, no. 3, pp. 434–460. <http://www.sciencedirect.com/science/article/pii/037594749090101X>Effects of time-dependent shape fluctuations on the giant dipole resonance (GDR) in hot rotating nuclei are investigated. Using the framework of the Landau theory of shape transitions we develop a realistic macroscopic stochastic model to describe the quadrupole time-dependent shape fluctuations and their coupling to the dipole degrees of freedom. In the adiabatic limit the theory reduces to a previous adiabatic theory of static fluctuations in which the GDR cross section is calculated by averaging over the equilibrium distribution with the unitary invariant metric. Nonadiabatic effects are investigated in this model and found to cause structural changes in the resonance cross section and motional narrowing. Comparisons with experimental data are made and deviations from the adiabatic calculations can be explained. In these cases it is possible to determine from the data the damping of the quadrupole motion at finite temperature.

Y. Alhassid and B. Bush, “Time-dependent fluctuations and the giant dipole resonance in hot nuclei: Solvable models,” Nuclear Physics A, vol. 531, no. 1, pp. 1–26. <http://www.sciencedirect.com/science/article/pii/037594749190565N>A recent macroscopic theory of time-dependent shape fluctuations in hot nuclei and their effects on the giant dipole resonance is investigated in the context of solvable models with one quadrupole shape degree of freedom. Using the framework of the Landau theory of shape transitions, both the quadrupole shape and the giant dipole degrees of freedom are described by a coupled set of stochastic equations. Two solvable models for which the dipole correlation function is found in closed form are discussed; one for a spherical nucleus and one for a deformed nucleus. The adiabatic and sudden limits of the models are examined. The latter limit is shown to produce a phenomenon known as motional narrowing. For the more general cases we introduce Monte Carlo techniques and test them against the solvable models.

Y. Alhassid and B. Bush, “Effects of orientation fluctuations on the angular distribution of the giant dipole resonance - rays in hot rotating nuclei,” Nuclear Physics A, vol. 531, no. 1, pp. 39–62. <http://www.sciencedirect.com/science/article/pii/037594749190567P>The macroscopic approach to the GDR in hot rotating nuclei is extended to include the angular distribution of the emitted GDR rays. The effects of thermal shape fluctuation and in particular fluctuations in the nuclear orientation with respect to the rotation axis, are discussed in the framework of the Landau theory. It is found that while orientation fluctuations have negligible effects on the GDR cross section, they cause significant attenuation in the angular anisotropy parameter a2 which offsets the a2 enhancement due to intrinsic shape fluctuations. It is shown
that this fluctuation theory is successful in reproducing both the observed cross section and a2 in highly excited 90Zr and 92Mo compound nuclei. The non-adiabatic effects on a2 are studied in terms of a time-dependent model for the quadrupole shape fluctuations.

Y. Alhassid and B. Bush, “The systematics of the Landau theory of hot rotating nuclei,” Nuclear Physics A, vol. 549, no. 1, pp. 12–42. <http://www.sciencedirect.com/science/article/pii/037594749290065R> The Landau theory of hot rotating nuclei, which was recently introduced to explain the universal features of the shape transitions, is shown to describe well many nuclei at moderate temperatures (T < 1 MeV) and spin. The Landau parameters are extracted from microscopic calculations. Their systematics as a function of temperature and neutron numbers is demonstrated for the neodymium isotopes with even number of neutrons. An extended Landau theory is introduced to describe better nuclei at lower temperatures and /or higher spins.

Y. Alhassid and B. Bush, “Nuclear level densities in the static-path approximation: (I). A solvable model,” Nuclear Physics A, vol. 549, no. 1, pp. 43–58. <http://www.sciencedirect.com/science/article/pii/037594749290066S> We investigate the static-path approximation (SPA) and mean-field approximation (MFA) for the level density within a solvable SU(2) model. Comparing the SPA level density to the MFA one, we find an enhancement with a great sensitivity to the interaction strength, in agreement with exact analytic results. This enhancement compensates for a corresponding suppression which occurs at negative temperatures. The saddle-point approximation used in converting the partition function to the level density works well at all but low energies.

Y. Alhassid and B. Bush, “Nuclear level densities in the static-path approximation: (II). Spin dependence,” Nuclear Physics A, vol. 565, no. 2, pp. 399–426. <http://www.sciencedirect.com/science/article/pii/037594749390218M> The static-path approximation (SPA) and mean-field approximation (MFA) for the partition function and level density are investigated with the inclusion of spin. The methods are studied within a solvable model, the nuclear SU(3) Elliot model. The SPA partition function is enhanced compared with the MFA partition function and is in good agreement with the exact result at all angular velocities (or spins) and at all but low temperatures. The error made in the SPA as well as in the saddle-point approximation used in the conversion from angular velocity to spin is only weakly dependent on the spin and is small at not too low temperatures (or excitation energies).

Y. Alhassid, B. Bush, and S. Levit, “Landau theory of shapes, shape fluctuations and giant dipole resonances in hot nuclei,” Nuclear Physics A, vol. 482, no. 1–2, pp. 57–64. <http://www.sciencedirect.com/science/article/pii/037594749290065R> Universal features of evolution of the equilibrium nuclear shapes with temperature and angular momentum are predicted by the Landau theory of nuclear shape transitions. The general dependence of the nuclear free energy on the deformation given by this theory also provides a unified description of thermal fluctuations of all quadrupole degrees of freedom. Using this unified theory we calculate the giant dipole absorption by hot rotating nuclei and investigate its systematics as a function of nuclear spin and temperature. Direct comparison with experimental data is presented.

Y. Alhassid, B. Bush, and S. Levit, “Thermal Shape Fluctuations, Landau Theory, and Giant Dipole Resonances in Hot Rotating Nuclei,” Phys. Rev. Lett., vol. 61, no. 17, pp. 1926–1929. <http://link.aps.org/doi/10.1103/PhysRevLett.61.1926> A macroscopic approach to giant dipole resonances (GDR’s) in hot rotating nuclei is presented. It is based on the Landau theory of nuclear shape transitions and provides a unified description of thermal fluctuations in all quadrupole shape degrees of freedom. With all parameters fixed by the zero-temperature nuclear properties the theory shows a very good agreement with existing GDR measurements in hot nuclei. The sensitivity of the GDR peak to the shape of hot nuclei is critically examined. Low-temperature experimental results in Er show clear evidence for changes in the nuclear energy surface, while higher-temperature results are dominated by the fluctuations.

M. Blue and B. W. Bush, “Information content in the Nagel-Schreckenberg cellular automaton traffic model,” Phys. Rev. E, vol. 67, no. 4, p. 047103. <http://link.aps.org/doi/10.1103/PhysRevE.67.047103> We estimate the set dimension and find bounds for the set entropy of a cellular automaton model for single lane traffic. Set dimension and set entropy, which are measures of the information content per cell, are related to the fractal nature of the automaton [S. Wolfram, Physica D 10, 1 (1989); Theory and Application of Cellular Automata, edited by S. Wolfram (World Scientific, Philadelphia, 1986)] and have practical implications for data compression. For models with maximum speed vmax, the set dimension is approximately log(vmax+2)/2.5, which is close to one bit per cell regardless of the maximum speed. For a typical maximum speed of five cells per time step, the dimension is approximately 0.47.

M. Blue, B. Bush, and J. Puckett, “Unified approach to fuzzy graph problems,” Fuzzy Sets and Systems, vol. 125, no. 3, pp. 355–368. <http://www.sciencedirect.com/science/article/pii/S0165011401000112> We present a taxonomy of fuzzy graphs that treats fuzziness in vertex existence, edge existence, edge connectivity, and edge weight. Within that framework, we formulate some standard graph-theoretic problems (shortest paths and minimum cut) for fuzzy graphs using a unified approach distinguished by its uniform application of guiding principles such as the construction
of membership grades via the ranking of fuzzy numbers, the preservation of membership grade normalization, and the “collapsing” of fuzzy sets of graphs into fuzzy graphs. Finally, we provide algorithmic solutions to these problems, with examples.

B. Bush and Y. Alhassid, “On the width of the giant dipole resonance in deformed nuclei,” Nuclear Physics A, vol. 531, no. 1, pp. 27–38. <http://www.sciencedirect.com/science/article/pii/037594749190566O> We derive and discuss the classical relativistic equations of motion for an action corresponding to extended nucleons interacting with massive, neutral scalar and vector meson fields. This theory, which we call classical hadrodynamics, is the classical analogue of the quantum hadrodynamics of Serot and Walecka but without the assumptions of the mean-field approximation and of point nucleons. The theory is manifestly covariant and allows for non-equilibrium phenomena, interactions among all nucleons, and meson production when used for applications such as relativistic heavy-ion collisions. We review the history of classical meson field theory, with special emphasis on issues related to self-interaction, pre-acceleration, runaway solutions, and finite-size effects. Sample calculations are presented for nucleon-nucleon collisions at plab = 200 GeV/c, where we find that the theory provides a physically reasonable description of gross features associated with the soft reactions that dominate nucleon-nucleon collisions. The equations of motion are practical to solve numerically for ultrarelativistic heavy-ion collisions.

B. W. Bush and J. Nix, “Classical hadrodynamics: application to soft nucleon-nucleon collisions,” Nuclear Physics A, vol. 560, no. 1, pp. 586–602. <http://www.sciencedirect.com/science/article/pii/037594749400748C> We present results for soft nucleon-nucleon collisions at Plab = 14.6, 30, 60, 100 and 200 GeV/c calculated on the basis of classical hadrodynamics for extended nucleons. This theory, which corresponds to nucleons of finite size interacting with massive neutral scalar and vector meson fields, is the classical analogue of the quantum hadrodynamics of Serot and Walecka but without the assumptions of the mean-field approximation and of point nucleons. The theory is manifestly Lorentz-covariant and automatically includes space-time nonlocality and retardation, nonequilibrium phenomena, interactions among all nucleons and particle production when used for applications such as relativistic heavy-ion collisions. We briefly review the history of classical meson-field theory and present our classical relativistic equations of motion, which are solved to yield such physically observable quantities as scattering angle, transverse momentum, radiated energy and rapidity. We find that the theory provides a physically reasonable description of gross features associated with the soft reactions that dominate nucleon-nucleon collisions. The equations of motion are practical to solve numerically for relativistic heavy-ion collisions.

B. W. Bush and J. Nix, “Classical hadrodynamics: A new approach to ultrarelativistic heavy-ion collisions,” Nuclear Physics A, vol. 583, no. 0, pp. 705–710. <http://www.sciencedirect.com/science/article/pii/037594749400748C> We discuss a new approach to ultrarelativistic heavy-ion collisions based on classical hadrodynamics for extended nucleons, corresponding to nucleons of finite size interacting with massive meson fields. This new theory provides a natural covariant microscopic approach that includes automatically spacetime nonlocality and retardation, nonequilibrium phenomena, interactions among all nucleons and particle production. In the current version of our theory, we consider N extended unexcited nucleons interacting with massive neutral scalar (σ) and neutral vector (v) meson fields. The resulting classical relativistic many-body equations of motion are solved numerically without further approximation for soft nucleon-nucleon collisions at plab = 14.6, 30, 60, 100 and 200 GeV/c to yield the transverse momentum imparted to the nucleons. For the future development of the theory, the isovector pseudoscalar (σ+, σ−, σ0), isovector scalar (σ+, σ−, σ0), isovector vector (σ+, σ−, σ0) and neutral pseudoscalar (σ) meson fields that are known to be important from nucleon-nucleon scattering experiments should be incorporated. In addition, the effects of quantum uncertainty on the equations of motion should be included by use of techniques analogous to those used by Moniz and Sharp for nonrelativistic quantum electrodynamics.

B. W. BUSH and R. D. SMALL, “A Note on the Ignition of Vegetation by Nuclear Weapons,” Combustion Science and Technology, vol. 52, no. 1-3, pp. 25–38. <http://www.tandfonline.com/doi/abs/10.1080/00102208708952566> We derive and discuss the classical relativistic equations of motion for an action corresponding to extended nucleons interacting with massive neutral scalar and neutral vector meson fields, is the classical analogue of the quantum hadrodynamics of Serot and Walecka but without the assumptions of the mean-field approximation and of point nucleons. The theory is manifestly Lorentz-covariant and allows for non-equilibrium phenomena, interactions among all nucleons, and meson production when used for applications such as relativistic heavy-ion collisions. We review the history of classical meson field theory, with special emphasis on issues related to self-interaction, pre-acceleration, runaway solutions, and finite-size effects. Sample calculations are presented for nucleon-nucleon collisions at plab = 200 GeV/c, where we find that the theory provides a physically reasonable description of gross features associated with the soft reactions that dominate nucleon-nucleon collisions. The equations of motion are practical to solve numerically for ultrarelativistic heavy-ion collisions.

B. W. Bush and J. Nix, “Classical Hadrodynamics: Foundations of the Theory,” Annals of Physics, vol. 227, no. 1, pp. 97–150. <http://www.sciencedirect.com/science/article/pii/0003491683710778> We derive and discuss the classical relativistic equations of motion for an action corresponding to extended nucleons interacting with massive, neutral scalar and vector meson fields. This theory, which we call classical hadrodynamics, is the classical analogue of the quantum hadrodynamics of Serot and Walecka but without the assumptions of the mean-field approximation and of point nucleons. The theory is manifestly Lorentz-covariant and allows for non-equilibrium phenomena, interactions among all nucleons, and meson production when used for applications such as relativistic heavy-ion collisions. We review the history of classical meson field theory, with special emphasis on issues related to self-interaction, pre-acceleration, runaway solutions, and finite-size effects. Sample calculations are presented for nucleon-nucleon collisions at plab = 200 GeV/c, where we find that the theory provides a physically reasonable description of gross features associated with the soft reactions that dominate nucleon-nucleon collisions. The equations of motion are practical to solve numerically for relativistic heavy-ion collisions.
Biofuels are expected to be a major contributor to renewable energy in the coming decades under the Renewable Fuel Standard (RFS). These fuels have many attractive properties that incorporate uncertainty in the pathogen behaviour and epidemic response to show the extreme variation in the consequences of a potential pandemic outbreak in the USA. Using sensitivity analysis we found the most important considerations, and the role of the Conservation Reserve Program,” Environ. Res. Lett., vol. 8, no. 2, p. 025016. Biofuels are expected to be a major contributor to renewable energy in the coming decades under the Renewable Fuel Standard (RFS). These fuels have many attractive properties including the promotion of energy independence, rural development, and the reduction of national carbon emissions. However, several unresolved environmental and economic concerns remain. Environmentally, much of the biomass is expected to come from agricultural expansion and/or intensification, which may greatly affect the net environmental impact, and economically, the lack of a developed infrastructure and bottlenecks along the supply chain may affect the industry’s economic vitality. The approximately 30 million acres (12 million hectares) under the Conservation Reserve Program (CRP) represent one land base for possible expansion. Here, we examine the potential role of the CRP in biofuels industry development, by (1) assessing the range of environmental effects on six end points of concern, and (2) simulating differences in potential industry growth nationally using a systems dynamics model. The model examines seven land-use scenarios (various percentages of CRP cultivation for biofuel) and five economic scenarios (subsidy schemes) to explore the benefits of using the CRP. The environmental assessment revealed wide variation in potential impacts. Lignocellulosic feedstocks had the greatest potential to improve the environmental condition relative to row crops, but the most plausible impacts were considered to be neutral or slightly negative. Model simulations revealed that industry growth was much more sensitive to economic scenarios than land-use scenarios—similar volumes of biofuels could be produced with no CRP as with 100% utilization. The range of responses to economic policy was substantial, including long-term market stagnation at current levels of first-generation biofuels under minimal policy intervention, or RFS-scale quantities of biofuels if policy or market conditions were more favorable. In total, the combination of the environmental assessment and the supply chain model suggests that large-scale conversion of the CRP to row crops would likely incur a significant environmental cost, without a concomitant benefit in terms of biofuel production.

C. M. Clark, Y. Lin, B. G. Bierwagen, L. M. Eaton, M. H. Langholtz, P. E. Morefield, C. E. Ridley, L. Vimmerstedt, S. Peterson, and B. W. Bush, “Growing a sustainable biofuels industry: economics, environmental considerations, and the role of the Conservation Reserve Program,” Environ. Res. Lett., vol. 8, no. 2, p. 025016. Biofuels are expected to be a major contributor to renewable energy in the coming decades under the Renewable Fuel Standard (RFS). These fuels have many attractive properties including the promotion of energy independence, rural development, and the reduction of national carbon emissions. However, several unresolved environmental and economic concerns remain. Environmentally, much of the biomass is expected to come from agricultural expansion and/or intensification, which may greatly affect the net environmental impact, and economically, the lack of a developed infrastructure and bottlenecks along the supply chain may affect the industry’s economic vitality. The approximately 30 million acres (12 million hectares) under the Conservation Reserve Program (CRP) represent one land base for possible expansion. Here, we examine the potential role of the CRP in biofuels industry development, by (1) assessing the range of environmental effects on six end points of concern, and (2) simulating differences in potential industry growth nationally using a systems dynamics model. The model examines seven land-use scenarios (various percentages of CRP cultivation for biofuel) and five economic scenarios (subsidy schemes) to explore the benefits of using the CRP. The environmental assessment revealed wide variation in potential impacts. Lignocellulosic feedstocks had the greatest potential to improve the environmental condition relative to row crops, but the most plausible impacts were considered to be neutral or slightly negative. Model simulations revealed that industry growth was much more sensitive to economic scenarios than land-use scenarios—similar volumes of biofuels could be produced with no CRP as with 100% utilization. The range of responses to economic policy was substantial, including long-term market stagnation at current levels of first-generation biofuels under minimal policy intervention, or RFS-scale quantities of biofuels if policy or market conditions were more favorable. In total, the combination of the environmental assessment and the supply chain model suggests that large-scale conversion of the CRP to row crops would likely incur a significant environmental cost, without a concomitant benefit in terms of biofuel production.

J. M. Fair, D. R. Powell, R. J. LeClaire, L. M. Moore, M. L. Wilson, L. R. Danelsberg, M. E. Samsa, S. M. DeLand, G. Hirsch, and B. W. Bush, “Measuring the uncertainties of pandemic influenza,” International Journal of Risk Assessment and Management, vol. 16, no. 1, pp. 1–27. Biofuels are expected to be a major contributor to renewable energy in the coming decades under the Renewable Fuel Standard (RFS). These fuels have many attractive properties that incorporate uncertainty in the pathogen behaviour and epidemic response to show the extreme variation in the consequences of a potential pandemic outbreak in the USA. Using sensitivity analysis we found the most important
disease characteristics are the fraction of the transmission that occur prior to symptoms, the reproductive number, and the length of each disease stage. Using data from the historical pandemics and for potential viral evolution, we show that response planning may underestimate the pandemic consequences by a factor of two or more.

S.-J. Lee, B. Bush, and R. George, “Analytic science for geospatial and temporal variability in renewable energy: A case study in estimating photovoltaic output in Arizona,” Solar Energy, vol. 85, no. 9, pp. 1945–1956.<http://www.sciencedirect.com/science/article/pii/S0038092X11001745>To assess the electric power grid environment under the high penetration of photovoltaic (PV) generation, it is important to construct an accurate representation of PV power output for any location in the southwestern United States at resolutions down to 10-min time steps. Existing analyses, however, typically depend on sparsely spaced measurements and often include modeled data as a basis for extrapolation. Consequently, analysts have been confronted with inaccurate analytic outcomes due to both the quality of the modeled data and the approximations introduced when combining data with differing space/time attributes and resolutions. This study proposes an accurate methodology for 10-min PV estimation based on the self-consistent combination of data with disparate spatial and temporal characteristics. Our Type I estimation uses the nearby locations of temporally detailed PV measurements, whereas our Type II estimation goes beyond the spatial range of the measured PV incorporating alternative data set(s) for areas with no PV measurements; those alternative data sets consist of: (1) modeled PV output and secondary cloud cover information around space/time estimation points, and (2) their associated uncertainty. The Type I estimation identifies a spatial range from existing PV sites (30–40 km), which is used to estimate accurately 10-min PV output performance. Beyond that spatial range, the data-quality-control estimation (Type II) demonstrates increasing improvement over the Type I estimation that does not assimilate the uncertainty of data sources. The methodology developed herein can assist the evaluation of the impact of PV generation on the electric power grid, quantify the value of measured data, and optimize the placement of new measurement sites.

R. D. Small and B. W. Bush, “Smoke Production from Multiple Nuclear Explosions in Nonurban Areas,” Science, vol. 229, no. 4712, pp. 465–469. <http://www.sciencemag.org/content/229/4712/465>The amount of smoke that may be produced by wildland or rural fires as a consequence of a large-scale nuclear exchange is estimated. The calculation is based on a compilation of rural military facilities, identified from a wide variety of unclassified sources, together with data on their geographic positions, surrounding vegetation (fuel), and weather conditions. The ignition area (corrected for fuel moisture) and the amount of fire spread are used to calculate the smoke production. The results show a substantially lower estimated smoke production (from wildland fires) than in earlier “nuclear winter” studies. The amount varies seasonally and at its peak is less by an order of magnitude than the estimated threshold level necessary for a major attenuation of solar radiation.

R. D. Small, B. W. Bush, and M. A. Dore, “Initial Smoke Distribution for Nuclear Winter Calculations,” Aerosol Science and Technology, vol. 10, no. 1, pp. 37–50. <http://www.tandfonline.com/doi/abs/10.1080/02786828908959219>Mappings showing the initial distribution of smoke from a 3000 MT strike against over 4000 targets in the United States are presented. An attack of this magnitude would attempt to deprive the United States of all military capabilities and to destroy its industrial capacity. Most urban areas would be affected and damage to the economic base would be substantial. Smoke distributions are derived for global climate model computation grids. Such distributions represent part of the initial conditions for a simulation of climate modification. A much finer grid (2 × 1.5 degree) mapping is also given. In the latter, mountain systems are resolved, and the possible influence of topography on smoke movement is discussed. Injection profiles determined from large area fire calculations show that the initial distribution and smoke mass centroid depend on the burning rate and fuel loading. Low fuel loadings or long burn times indicate a constant mixing ratio injection with a fairly low altitude centroid. A two-level constant mass density profile with a midtroposphere centroid is more appropriate for cities that burn rapidly or have higher combustible loadings. Wind patterns at a typical injection height indicate the effect of a nonuniform source on the initial global spread of smoke.

K. L. Summers, T. P. Caudell, K. Berkbigler, B. Bush, K. Davis, and S. Smith, “Graph visualization for the analysis of the structure and dynamics of extreme-scale supercomputers,” Information Visualization, vol. 3, no. 3, p. 209–222. <http://dx.doi.org/10.1057/palgrave.ivs.9500079>We are exploring the development and application of information visualization techniques for the analysis of new massively parallel supercomputer architectures. Modern supercomputers typically comprise very large clusters of commodity SMPs interconnected by possibly dense and often non-standard networks. The scale, complexity, and inherent non-locality of the structure and dynamics of this hardware, and the operating systems and applications distributed over them, challenge traditional analysis methods. As part of the à la carte (A Los Alamos Computer Architecture Toolkit for Extreme-Scale Architecture Simulation) team at Los Alamos National Laboratory, who are simulating these new architectures, we are exploring advanced visualization techniques and creating tools to enhance analysis of these simulations with intuitive three-
Increasing demand for crop-based biofuels, in addition to other biofuel markets, include the need for infrastructure for distribution and dispensing and widespread use of sustainable ethanol fuel market (or other biofuel market) requires low end-user fuel price relative to gasoline and high ethanol blends in flexible-fuel vehicles. Some portions of this system are represented dynamically with major interactions and feedbacks, especially those related to a dispensing station owner’s decision whether to offer ethanol fuel and a consumer’s choice whether to purchase that fuel. Other portions of the system are modeled with little or no dynamics; the vehicle choices of consumers are represented as discrete scenarios. This paper explores conditions needed to sustain an ethanol fuel market and identifies implications of these findings for program and policy goals. A large, economically sustainable ethanol fuel market (or other biofuel market) requires low end-user fuel price relative to gasoline and sufficient producer payment, which are difficult to achieve simultaneously. Other requirements (different for ethanol vs. other biofuel markets) include the need for infrastructure for distribution and dispensing and widespread use of high ethanol blends in flexible-fuel vehicles.

E. Warner, D. Inman, B. Kunstman, B. Bush, L. Vimmerstedt, S. Peterson, J. Macknick, and Y. Zhang, “Modeling biofuel expansion effects on land use change dynamics,” Environmental Research Letters, vol. 8, no. 1, p. 015003. <http://iopscience.iop.org/1748-9326/8/1/015003/> Increasing demand for crop-based biofuels, in addition to other human drivers of land use, induces direct and indirect land use changes (LUC). Our system dynamics tool is intended to complement existing LUC modeling approaches and to improve the understanding of global LUC drivers and dynamics by allowing examination of global LUC under diverse scenarios and varying model assumptions. We report on a small subset of such analyses. This model provides insights into the drivers and dynamic interactions of LUC...
(e.g., dietary choices and biofuel policy) and is not intended to assert improvement in numerical results relative to other works. Demand for food commodities are mostly met in high food and high crop-based biofuel demand scenarios, but cropland must expand substantially. Meeting roughly 25% of global transportation fuel demand by 2050 with biofuels requires >2 times the land used to meet food demands under a presumed 40% increase in per capita food demand. In comparison, the high food demand scenario requires greater pastureland for meat production, leading to larger overall expansion into forest and grassland. Our results indicate that, in all scenarios, there is a potential for supply shortfalls, and associated upward pressure on prices, of food commodities requiring higher land use intensity (e.g., beef) which biofuels could exacerbate.

Proceedings

C. Barrett, B. Bush, S. Kopp, H. Mortveit, and C. Reidys, “Sequential dynamical systems and applications to simulations,” in Simulation Symposium, 2000. (SS 2000) Proceedings. 33rd Annual, Washington D.C., pp. 245–252. Computer simulations are extensively used for business and science applications. However a simulation generically generates a certain class of dynamical system whose properties are poorly understood. We address some theoretical issues of computer simulations and illustrate our concepts for the simulation of circular one-lane traffic. We propose a certain class of discrete dynamical systems (SDS) that captures key features of computer simulations and then show how SDS techniques can be applied to a case of infrastructure simulations


K. Berkbigler, G. Booker, B. Bush, K. Davis, and N. Moss, “Simulating the quadrics interconnection network,” in High Performance Computing Symposium 2003, Advance Simulation Technologies Conference 2003, Orlando, Florida. We outline à la carte, an approach for simulating computing architectures applicable to extreme-scale systems (thousands of processors) and to advanced, novel architectural configurations, and describe in detail our simulation model of the Quadrics interconnection network. Our component-based design allows for the seamless assembly of architectures from representations of workload, processor, network interface, switches, etc., with disparate resolutions and fidelities, into an integrated simulation model. This accommodates different case studies that may require different levels of fidelity in various parts of a system. Simple ping timings can be modeled to approximately 100 ns. We present results comparing the simulated versus actual execution time of a 3D neutron transport application run on a machine with a Quadrics network.

B. W. Bush and J. R. Nix, “Classical hadrodynamics for extended nucleons,” in Proc. 8th Winter Workshop on Nuclear Dynamics, Jackson Hole, Wyoming, p. 311–316. <http://www.osti.gov/energy citations/servlets/purl/5692537-WI0CTO/> We discuss a new approach to relativistic nucleus-nucleus collisions based on classical hadrodynamics for extended nucleons, corresponding to nucleons of finite size interacting with massive meson fields. This theory provides a natural covariant microscopic approach to relativistic nucleus-nucleus collisions that includes automatically spacetime nonlocality and retardation, nonequilibrium phenomena, interactions among all nucleons, and particle production. Inclusion of the finite nucleon size cures the difficulties with preacceleration and runaway solutions that have plagued the classical theory of self-interacting point particles.

B. W. Bush and J. R. Nix, “Particle-production mechanism in relativistic heavy-ion collisions,” in Proc. 7th Int. Conf. on Nuclear Reaction Mechanism, Varenna, Italy, p. 592. <http://www.osti.gov/energy citations/servlets/purl/10162609-gv1Z8s/native/> We discuss the production of particles in relativistic heavy-ion collisions through the mechanism of massive bremsstrahlung, in which massive mesons are emitted during rapid nucleon acceleration. This mechanism is described within the framework of classical hadrodynamics for extended nucleons, corresponding to nucleons of finite size interacting with massive meson fields. This new theory provides a natural covariant microscopic approach to relativistic heavy-ion collisions that includes automatically spacetime nonlocality and retardation, nonequilibrium phenomena, interactions among all nucleons, and particle production. Inclusion of the finite nucleon size cures the difficulties with preacceleration and runaway solutions that have plagued the classical theory of self-interacting point particles. For the soft reactions that dominate nucleon-nucleon collisions, a significant fraction of the incident center-of-mass energy is radiated through massive bremsstrahlung. In the present version of the theory, this radiated energy is in the form of neutral scalar (0) and neutral vector (0) mesons, which subsequently decay primarily into pions with some photons also. Additional meson fields that are known to be important from nucleon-nucleon scattering experiments should be incorporated in the future, in which case the radiated energy would also contain isovector pseudoscalar (+,–,0), isovector scalar (+,–,0), isovector vector (+,–,0), and neutral pseudoscalar (0) mesons.
B. W. Bush, J. R. Nix, and A. J. Sierk, “Spacetime nonlocality and retardation in relativistic heavy-ion collisions,” in Presented at the 7th Winter Workshop on Nuclear Dynamics, Key West, 27 Jan. - 2 Feb. 1991, Key West, Florida, vols. -1, p. 282–287. <http://adsabs.harvard.edu/abs/1991nudy.workR....B> We discuss the exact numerical solution of the classical relativistic equations of motion for a Lagrangian corresponding to point nucleons interacting with massive scalar and vector meson fields. The equations of motion contain both external retarded Lorentz forces and radiation-reaction forces; the latter involve nonlocal terms that depend upon the past history of the nucleon in addition to terms analogous to those of classical electrodynamics. The resulting microscopic many-body approach to relativistic heavy-ion collisions is manifestly Lorentz covariant and allows for nonequilibrium phenomena, interactions with correlated clusters of nucleons, and particle production. For point nucleons, the asymptotic behavior of nucleonic motion prior to the collision is exponential, with a range in proper time of approximately 0.5 fm. However, this behavior is altered by the finite nucleon size, whose effect we are currently incorporating into our equations of motion. The spacetime nonlocality and retardation that will be present in the solutions of these equations may be responsible for significant collective effects in relativistic heavy-ion collisions.

B. W. Bush, J. R. Nix, and A. J. Sierk, “Classical hadrodynamics approach to ultrarelativistic heavy-ion collisions,” in AIP Conference Proceedings, Tucson, Arizona, vol. 243, pp. 835–837. <http://proceedings.aip.org/resource/2/apcpcs/243/1/835_1?isAuthorized=no> We discuss the exact solution of the classical relativistic equations of motion for an action corresponding to nucleons interacting with massive scalar and vector meson fields. This model—the classical analogue of the quantum hadrodynamics of Serot and Walecka—provides a manifestly Lorentz covariant approach to heavy-ion collisions, allows for nonequilibrium phenomena, interactions of correlated nucleon clusters, and particle production, and is valid when interaction times are short. We present an analysis of the nonlocality inherent in the model and discuss effects arising from the finite size of a nucleon.

B. Bush, Dauelsberg, L., LeClaire, R., Powell, D., DeLand, S., and Samwa, M., “Critical infrastructure protection decision support system (CIP/DSS) project overview,” in Proceedings of the 2005 System Dynamics Conference, Boston. <http://www.systemdynamics.org/conferences/2005/proceed/papers/LECLA332.pdf> The Critical Infrastructure Protection Decision Support System (CIP/DSS) simulates the dynamics of individual infrastructures and couples separate infrastructures to each other according to their interdependencies. For example, repairing damage to the electric power grid in a city requires transportation to failure sites and delivery of parts, fuel for repair vehicles, telecommunications for problem diagnosis and coordination of repairs, and the availability of labor. The repair itself involves diagnosis, ordering parts, dispatching crews, and performing work. The electric power grid responds to the initial damage and to the completion of repairs with changes in its operating characteristics. Dynamic processes like these are represented in the CIP/DSS infrastructure sector simulations by differential equations, discrete events, and codified rules of operation. Many of these variables are output metrics estimating the human health, economic, or environmental effects of disturbances to the infrastructures.

B. Bush, M. Duffy, D. Sandor, and S. Peterson, “Using system dynamics to model the transition to biofuels in the United States,” presented at the Third International Conference on System of Systems Engineering, Monterey, California. <http://www.nrel.gov/docs/fy08osti/43153.pdf> Transitioning to a biofuels industry that is expected to displace about 30% of current U.S. gasoline consumption requires a robust biomass-to-biofuels system-of-systems that operates in concert with the existing markets. This paper discusses employing a system dynamics approach to investigate potential market penetration scenarios for cellulosic ethanol and to help government decision makers focus on areas with greatest potential.

B. Bush, M. Duffy, D. Sandor, and S. Peterson, “Using system dynamics to model the transition to biofuels in the United States,” presented at the SoSE ’08. IEEE International Conference on System of Systems Engineering, Singapore. <http://www.nrel.gov/docs/fy08osti/43153.pdf> Today, the U.S. consumes almost 21 million barrels of crude oil per day; approximately 60% of the U.S. demand is supplied by imports. The transportation sector alone accounts for two-thirds of U.S. petroleum use. Biofuels, liquid fuels produced from domestically-grown biomass, have the potential to displace about 30% of current U.S. gasoline consumption. Transitioning to a biofuels industry on this scale will require the creation of a robust biomass-to-biofuels system-of-systems that operates in concert with the existing agriculture, forestry, energy, and transportation markets. The U.S. Department of Energy is employing a system dynamics approach to investigate potential market penetration scenarios for cellulosic ethanol, and to aid decision makers in focusing government actions on the areas with greatest potential to accelerate the deployment of biofuels and ultimately reduce the nation’s dependence on imported oil.


Bush, B. and Ivey, A., “Numerical Hurricane Model Outputs for GIS-Based Infrastructure Damage Estimation,” in
The actor-based definitions of the electric-power transmission line and natural-gas pipeline networks were developed using wind and precipitation fields forecast by numerical weather prediction (NWP) models, combined with the output of storm surge models, to provide estimates of damage to infrastructures such as the electric power grid several days before a hurricane makes landfall. Having the hourly forecasts of grid-based meteorological fields imported into a GIS enables an analyst to compute the cumulative effects over time of wind and rain, and subsequently, to overlay these with storm surge, elevation, and infrastructure data in order to categorize the forecast exposure of facilities to extreme weather. Calibrated heuristic models are then applied within the GIS to compute expected damage from the forecasted exposure. We provide examples for hurricanes from the 2005 season in the Atlantic Ocean and Gulf of Mexico using the output of several publicly available NWP model forecasts; similar methods apply to other types of extreme weather such as ice storms.


The government seeks to ensure that disruptions are infrequent, brief, manageable, and cause the least harm possible. The system dynamics (SD) approach is particularly promising as a way to understand these complex systems, interactions, and issues. Problems in critical infrastructure protection are being investigated with a collection of SD models developed expressly for these concerns, including agriculture models. This paper discusses the technical and social modeling context that makes this SD modeling effort seem uncommon. It involves a modular approach, a model-reassembling technology, a formal process for testing and evaluation, and a social process for managing the development and use of “living” models.

C. Unal, B. Bush, K. Werley, and P. Giguere, “Modeling of Interdependent Infrastructures,” in Probabilistic safety assessment and management (PSAM6) : proceedings of the 6th International Conference on Probabilistic Safety Assessment and Management, 23-28 June 2002, San Juan, Puerto Rico, USA, San Juan, Puerto Rico. An actor-based modeling methodology is used to simulate interactions among interdependent commercial infrastructures. The goal of this method is to capture the complex, nonlinear, self-organizing, emergent, and sometimes chaotic behaviors and interactions exemplified by complex systems, rather than relying on traditional aggregate mathematical and simulation techniques. A prototype model of four interdependent infrastructures was considered as an example. The actor-based definitions of the electric-power transmission line and natural-gas pipeline networks were developed to realistically simulate the dynamic interactions within each of these infrastructures and the interactions and interdependencies between these two infrastructures. A three-dimensional representation of system components and interconnectivity was developed. The visualization is an interactive, three-dimensional, geographically based, “layered” view of infrastructure interdependencies. It also links to a geographic information system for data analysis. A unique iterative natural-gas network solver algorithm was developed. Our assessment shows that a hybrid approach using an actor-based definition of infrastructure components in conjunction with iterative and commercial solvers has great promise for addressing the operation of interdependent infrastructures in a restructured and deregulated environment.


Fernandez, S.J., Bush, B., Toole, G.L., Danielsberg, L., Flaim, S., Thayer, G.R., and Ivey, A., “Predicting Hurricane Impacts on the Nation’s Infrastructure: Lessons Learned from the 2005 Hurricane Season,” in Second International Conference on Global Warming, Santa Fe, New Mexico. During the 2005 Hurricane season, many consequence predictions were available to key Federal agencies from 36 to 96 hours before each of the major hurricane US mainland landfalls. These key forecasts included the location and intensity of the hurricane at landfall, areas of significant damage to engineered infrastructure and lifeline utilities, time estimates to restore critical infrastructure services, and the conditions to be found on the ground as emergency and relief crews enter the area. Both the Department of Energy through its Visualization and Modeling Working Group and the Department of Homeland Security provided early forecasts of potential damage to the regionally critical infrastructures. These products communicated critical information that assisted in the decision-making process for emergency planning.
The analysis benefited substantially from knowledge gained from telecommunication industry models and provides the lack of means to develop modules independently and subsequently link, integrate, or merge the modules. Most development of large software systems using systems dynamics languages such as Vensim® has been hampered by modern software languages support such a capability. A software tool to facilitate group development of systems was proposed as early as 1998 (Bush, 1998), but their short-and long-term ramifications are not well known. This paper describes the Biomass Scenario Model, a system dynamics model developed under the support of the U.S. Department of Energy as the result of a multi-year project at the National Renewable Energy Laboratory. The model represents multiple pathways leading to the production of fuel ethanol as well as advanced biofuels such as biomass-based gasoline, diesel, jet fuel, and butanol). This paper details the BSM system dynamics architecture, the design of the supporting database infrastructure, the associated scenario libraries used in model runs, as well as key insights resulting from BSM simulations and analyses.

A linear theory approach is applied within each of the infrastructures, as well as the interconnections between the infrastructures. To enhance its capabilities, a generalized fluid network will be added to the infrastructure framework, which will allow for the analysis of specific fluid infrastructures (e.g., water, petroleum, oil, etc.). In this research, we describe the extension of IEISS to include water infrastructure. The resulting simulation capability (i.e., IEISS Water) will allow the simulation of transmission/distribution-level water systems in terms of infrastructure specific vulnerabilities and interdependent infrastructure vulnerabilities (e.g., power and water disruptions).


A linear theory approach is applied to the hydraulic simulation of a water distribution system within the Interdependent Energy Infrastructure Simulation System (IEISS). IEISS is an actor-based infrastructure modeling, simulation, and analysis tool designed to assist individuals in analyzing and understanding interdependent energy infrastructures. In particular, it has the ability to analyze and simulate the interdependent electric power and natural gas infrastructures. The ultimate goal for IEISS is a multi-infrastructure modeling framework that can be used to analyze the complex, nonlinear interactions among interdependent infrastructures including electric power, natural gas, petroleum, water, and other network based infrastructures that is scalable to multiple spatial (e.g., urban to regional) and temporal resolutions. The actor-based infrastructure components were developed in IEISS to realistically simulate the dynamic interactions within each of the infrastructures, as well as, the interconnections between the infrastructures. To enhance its capabilities, a generalized fluid network will be added to the infrastructure framework, which will allow for the analysis of specific fluid infrastructures (e.g., water, petroleum, oil, etc.). In this research, we describe the extension of IEISS to include water infrastructure. The resulting simulation capability (i.e., IEISS Water) will allow the simulation of transmission/distribution-level water systems in terms of infrastructure specific vulnerabilities and interdependent infrastructure vulnerabilities (e.g., power and water disruptions).


We are exploring the development and application of information visualization techniques for the analysis of new massively parallel supercomputer architectures. Modern supercomputers typically comprise very large clusters of commodity SMPs interconnected by possibly dense and often nonstandard networks. The scale, complexity, and inherent nonlocality of the structure and dynamics of this hardware, and the systems and applications distributed over it, challenge traditional analysis methods. As part of the 'a la carte team at Los Alamos National Laboratory, who are simulating these advanced architectures, we are exploring advanced visualization techniques and creating tools to provide intuitive exploration, discovery, and analysis of these simulations. This work complements existing and emerging algorithmic analysis tools. This paper gives background on the problem domain, a description of a prototypical computer architecture of interest (on the
order of 10,000 processors connected by a quaternary fat-tree communications network), and a presentation of two classes of visualizations that clearly display the switch structure and the flow of information in the interconnecting network.

**Posters**


B. Bush, L. Dauelsberg, A. Ivey, R. LeClaire, D. Powell, S. DeLand, and M. Sansa, “Critical Infrastructure Protection Decision Support System (CIP/DSS) Project Overview,” presented at the 3rd International Conference of the System Dynamics Society, Boston. The Critical Infrastructure Protection Decision Support System (CIP/DSS) simulates the dynamics of individual infrastructures and couples separate infrastructures to each other according to their interdependencies. For example, repairing damage to the electric power grid in a city requires transportation to failure sites and delivery of parts, fuel for repair vehicles, telecommunications for problem diagnosis and coordination of repairs, and the availability of labor. The repair itself involves diagnosis, ordering parts, dispatching crews, and performing work. The electric power grid responds to the initial damage and to the completion of repairs with changes in its operating characteristics. Dynamic processes like these are represented in the CIP/DSS infrastructure sector simulations by differential equations, discrete events, and codified rules of operation. Many of these variables are output metrics estimating the human health, economic, or environmental effects of disturbances to the infrastructures.


**Book Chapters**


Biofuels are promoted in the United States through aggressive legislation, as one part of an overall strategy to lessen dependence on imported energy as well as to reduce the emissions of greenhouse gases (Office of the Biomass Program and Energy Efficiency and Renewable
Energy, 2008). For example, the Energy Independence and Security Act of 2007 (EISA) mandates 36 billion gallons of renewable liquid transportation fuel in the U.S. marketplace by the year 2022 (U.S. Government, 2007). Meeting such large volumetric targets has prompted an unprecedented increase in funding for biofuels research. Language in the EISA legislation limits the amount of renewable fuel derived from starch-based feedstocks (which are already established and feed the commercially viable ethanol industry in the United States); therefore, much of the current research is focused on producing ethanol—but from cellulosic feedstocks. These feedstocks, such as agricultural and forestry residues, perennial grasses, woody crops, and municipal solid wastes, are advantageous because they do not necessarily compete directly with food, feed, and fiber production and are envisaged to require fewer inputs (e.g., water, nutrients, and land) as compared to corn and other commodity crops. In order to help propel the biofuels industry in general and the cellulosic ethanol industry in particular, the U.S. government has enacted subsidies, fixed capital investment grants, loan guarantees, vehicle choice credits, and aggressive corporate average fuel economy standards as incentives. However, the effect of these policies on the cellulosic ethanol industry over time is not well understood. Policies such as those enacted in the United States, that are intended to incentivize the industry and promote industrial expansion, can have profound long-term effects on growth and industry takeoff as well as interact with other policies in unforeseen ways (both negative and positive). Qualifying the relative efficacies of incentive strategies could potentially lead to faster industry growth as well as optimize the government’s investment in policies to promote renewable fuels. The purpose of this chapter is to discuss a system dynamics model called the Biomass Scenario Model (BSM), which is being developed by the U.S. Department of Energy as a tool to better understand the interaction of complex policies and their potential effects on the burgeoning cellulosic biofuels industry in the United States. The model has also recently been expanded to include advanced conversion technologies and biofuels (i.e., conversion pathways that yield biomass-based gasoline, diesel, jet fuel, and butanol), but we focus on cellulosic ethanol conversion pathways here. The BSM uses a system dynamics modeling approach (Bush et al., 2008) built on the STELLA software platform (isee systems, 2010) to model the entire biomass-to-biofuels supply chain. Key components of the BSM are shown in Figure 1. In addition to describing the underpinnings of this model, we will share insights that have been gleaned from a myriad of scenario- and policy-driven model runs. These insights will focus on how roadblocks, bottlenecks, and incentives all work in concert to have profound effects on the future of the industry.

Presentations


Biomass Scenario Model (BSM) is a unique, carefully validated, state-of-the-art third-generation model of the domestic biofuels supply chain which explicitly focuses on policy issues and their potential side effects. It integrates resource availability, behavior, policy, and physical, technological, and economic constraints. The model uses a system-dynamics simulation (not optimization) to model dynamic interactions across the supply chain; the BSM tracks the deployment of biofuels given technological development and the reaction of the investment community to those technologies in the context of land availability, the competing oil market, consumer demand for biofuels, and government policies over time. It places a strong emphasis on the behavior and decision-making of various economic agents among ten geographic regions domestically. The BSM has been used to develop insights into biofuels industry growth and market penetration, particularly with respect to policies and incentives applicable to each supply-chain element (volumetric, capital, operating subsidies; carbon caps/taxes; R&D investment; loan guarantees; tax credits); the model treats the major infrastructure-compatible fuels such as biomass-based gasoline, diesel, jet fuel, ethanol, and butanol. In general, scenario analysis based on the BSM shows that the biofuels industry tends not to rapidly thrive without significant external actions in the early years of its evolution. An initial focus for jumpstarting the industry typically has strongest results in the BSM in areas where effects of intervention have been identified to be multiplicative: due to industrial learning dynamics, support for the construction of biofuel conversion facilities in the near future encourages the industry to flourish. In general, we find that policies which are coordinated across the whole supply chain have significant impact in fostering the growth of the biofuels industry and that the production of tens of billions of gallons of biofuels may occur under sufficiently favorable conditions.

system-dynamics simulation (not optimization) to model dynamic interactions across the supply chain; the BSM tracks the deployment of biofuels given technological development and the reaction of the investment community to those technologies in the context of land availability, the competing oil market, consumer demand for biofuels, and government policies over time. It places a strong emphasis on the behavior and decision-making of various economic agents among ten geographic regions domestically. Although the BSM has historically been used to develop insights into cellulosic ethanol industry growth and market penetration, particularly with respect to policies and incentives applicable to each supply-chain element (volumetric, capital, operating subsidies; carbon caps/taxes; R&D investment; loan guarantees; tax credits), recent enhancements to the model allow it to treat the major infrastructure-compatible fuels such as biomass-based gasoline, diesel, and jet fuel. In general, scenario analysis based on the BSM shows that the cellulosic ethanol industry tends not to rapidly thrive without significant external actions in the early years of its evolution. An initial focus for jumpstarting the industry typically has strongest results in the BSM in areas where effects of intervention have been identified to be multiplicative: due to industrial learning dynamics, support for the construction of cellulosic ethanol conversion facilities in the near future encourages the industry to flourish; in addition, the alleviation of the bottlenecks of high-blend fuel distribution infrastructure and high-blend fuel pump availability allows the increased amount of ethanol produced to serve a viable market.


B. Bush, “Applications of the Biomass Scenario Model,” presented at the Workshop on Biofuels Projections in the AEO, Washington, D.C. <http://www.eia.gov/biofuels/workshop/presentations/2013/pdf/presentation-14-032013.pdf>U.S. policy targets 36 billion gallons per year of biofuels utilization by 2022, under the renewable fuels standard provisions of the Energy Independence and Security Act of 2007. Achieving such large scale biofuels adoption requires substantial development of new infrastructure, markets, and related systems. The U.S. Department of Energy is employing a system dynamics model, the Biomass Scenario Model (BSM), to represent the primary system effects and dependencies in the biomass-to-biofuels supply chain and to provide a framework for developing scenarios and conducting biofuels policy analysis. This approach is designed to help focus government action by determining which supply chain changes would have the greatest potential to accelerate the deployment of biofuels. Modeling the integration of all aspects of the supply chain from growing the feedstock through harvest, collection, transport, conversion, distribution of fuel and finally consumption of the fuel in applicable vehicles (including the availability of these vehicles) is critical to understanding where government funds might be utilized most effectively. This presentation provides an overview of the status of the BSM and a summary of recent results from system analysis based on it. We find that policies which are coordinated across the whole supply chain have significant impact in fostering the growth of the biofuels industry.


Patents

Christopher L. Barrett, Richard J. Beckman, Keith A. Baggerly, Michael D. McKay, Paul L. Speckman, Paula E. Stretz, Madhav V. Marathe, Stephen G. Eubank, Brian W. Bush, James P. Smith, Katherine Campbell, Kathy P. Berkbigler, Joerg Esser, Rudiger R. Jacob, Goran Konjevod, and Kai Nagel, “Urban Population Mobility Generation,” <https://patentimages.storage.googleapis.com/pdfs/US20040088392.pdf>A system and method provides a simulation of a complex network and movement and interdependencies between entities in the network. The system receives aggregated population data and a population synthesizer generates disaggregated population data representative of two different types of entities. The different entity types are then coupled to one another to form interdependent relationships. An activity generator generates typical activities for the entities. A route planner generates travel plans, including departure times and travel modes, for each entity to achieve daily activities. A micro-simulation module simulates movement of the individual entities in compliance with their travel plans. The system may include parallel processors to simulate thousands of roadway and transit segments, intersection signals and signs, transfer facilities between various transportation modes, traveler origins and destinations, and entities and vehicles. The system includes a framework and selector module that gathers the travel times from the simulation and
uses them to re-plan activities and trips and re-run the simulation. The methods of the present invention produce appropriate dynamic behavior of the transportation network as a whole.

**Magazine Articles**


**Theses**

B. W. Bush, “Track Reconstruction for Proton Decay,” Senior Thesis, California Institute of Technology, Pasadena, California. Events from the 417 day IMB detector data sample are scanned visually to reconstruct tracks present, and their possibility of coming from proton decay assessed by considering their invariant mass and residual momentum. Events from Monte Carlo simulations of neutrino background in the detector are also analyzed similarly and compared to the IMB sample. No significant signal above background has been found, so lifetime limits for the four proton decay modes studied are presented.

B. W. Bush, “Shape Fluctuations in Hot Rotating Nuclei,” Doctor of Philosophy, Yale University, New Haven, Connecticut. <http://adsabs.harvard.edu/abs/1990PhDT…….223B> We present a unified theory of quadrupole shape fluctuations in highly excited rotating nuclei using the framework of the Landau Theory of shape transitions. The theory is applied to several experimental observables. Our major application is the study of giant dipole resonances (GDRs) built on hot rotating nuclei. With only two free parameters, fixed by the ground state properties, the model reproduces well experimental GDR cross-sections and angular correlations at any temperature and spin in the 90 <= A <= 170 mass range for both spherical and deformed nuclei. A systematic study of the cross-section reveals that higher temperature cross-sections are dominated by large fluctuations (triaxial in particular) and are less sensitive to the equilibrium shape. To include non-adiabatic effects, we generalize our theory to describe time-dependent shape fluctuations using a stochastic approach based on the Langevin equation. This can produce motional narrowing of the resonance. Comparisons with experiments deviating from the adiabatic limit are used to determine the damping of quadrupole motion at finite temperature. Another application of the theory is in the study of E2 quasicontinuum spectra in warm nuclei, where it predicts enhancement of the B(E2), in accord with the experiment. Finally, we apply the fluctuation theory in improved calculations of nuclear level densities as a function of energy and spin using the static path approximation (SPA). Comparison with other calculations and experiments are made.

**Reports**

F. J. Alexander, M. Anghel, K. Berkbigler, G. Booker, B. Bush, K. Davis, A. Hoisie, N. Moss, S. Smith, T. P. Caudell, D. P. Holten, K. L. Summers, and C. Zhou, “Design, Implementation, and Validation of Network and Workload Simulations for a 30-TeraOPS Computer System,” Los Alamos National Laboratory. The magnitude of the scientific computations targeted by the US DOE ASCI project requires as-yet unavailable computational power, and unprecedented bandwidth to enable remote, realtime interaction with the compute servers. To facilitate these computations ASCI plans to deploy massive computing platforms, possibly consisting of tens of thousands of processors, capable of achieving 10-100 TeraOPS, with WAN connectivity from these to distant sites. For various reasons the current approach to building a yet-larger supercomputer—connecting commercially available SMPs with a network—may be reaching practical limits. Better hardware design and lower development costs require performance evaluation, analysis, and modeling of parallel applications and architectures, and in particular predictive capability. We outline an approach for simulating computing architectures applicable to extreme-scale systems (thousands of processors) and to advanced, novel architectural configurations, and describe our progress in its realization. The simulation environment is intended to allow (i) exploration of hardware/architecture design space; (ii) exploration of algorithm/implementation space both at the application level (e.g. data distribution and communication) and the system level (e.g. scheduling, routing, and load balancing); (iii) determining how application performance will scale with the number of processors or other components; (iv) analysis of the tradeoffs between performance and cost; and (v) testing and validating analytical models of computation and communication. Our component-based design allows for the seamless assembly of architectures from representations of workload, processor, network interface, switches, etc. with disparate resolutions, into an integrated simulation model. This accommodates different case studies that may require different levels of fidelity in various parts of a system. Our current implementation, includes low and
medium-fidelity models of the network and low-fidelity and direct execution models of the workload. It supports studies of both simulation performance and scaling, and the properties of the simulated system themselves. Ongoing work allows more realistic simulation and dynamic visualization of ASCI-like workloads on very large machines.

F. J. Alexander, K. Berkbigler, G. Booker, B. Bush, K. Davis, and A. Hoisie, “An Approach to Extreme-Scale Simulation of Novel Architectures,” Los Alamos National Laboratory, Report LA-UR-01-4087. We outline an approach for simulating computing architectures applicable to extreme-scale systems (thousands of processors) and to advanced, novel architectural configurations. We believe that simulation is the predictive tool of choice for evaluating the performance of such systems. Our component-based design allows for the seamless assembly of architectures from representations of workload, processor, network interface, switches, etc., with disparate resolutions into an integrated simulation model. This accommodates different case studies that may require different levels of fidelity in various parts of a system. Our initial prototype, comprising low-fidelity models of workload and network, aims to model at least 4096 computational nodes in a fat-tree network. It supports studies of simulation performance and scaling rather than the properties of the simulated system themselves. Future work will allow more realistic simulation and visualization of ASCI-like workloads on very large machines.

F. J. Alexander, K. Berkbigler, G. Booker, B. Bush, K. Davis, A. Hoisie, N. Moss, S. Smith, T. P. Caudell, D. P. Holten, K. L. Summers, and C. Zhou, “Design, Implementation, and Validation of Low- and Medium-Fidelity Network Simulations of a 30-TeraOPS System,” Los Alamos National Laboratory, Report LA-UR-02-6573. The magnitude of the scientific computations targeted by the US DOE ASCI project requires as-yet unavailable computational power, and unprecedented bandwidth to enable remote, realtime interaction with the compute servers. To facilitate these computations ASCI plans to deploy massive computing platforms, possibly consisting of tens of thousands of processors, capable of achieving 10-100 TeraOPS, with WAN connectivity from these to distant sites. For various reasons the current approach to building a yet-larger supercomputer–connecting commercially available SMPs with a network–may be reaching practical limits. Better hardware design and lower development costs require performance evaluation, analysis, and modeling of parallel applications and architectures, and in particular predictive capability. We outline an approach for simulating computing architectures applicable to extreme-scale systems (thousands of processors) and to advanced, novel architectural configurations, and describe our progress in its realization. The simulation environment is intended to allow (i) exploration of hardware/architecture design space; (ii) exploration of algorithm/implementation space both at the application level (e.g. data distribution and communication) and the system level (e.g. scheduling, routing, and load balancing); (iii) determining how application performance will scale with the number of processors or other components; (iv) analysis of the tradeoffs between performance and cost; and (v) testing and validating analytical models of computation and communication. Our component-based design allows for the seamless assembly of architectures from representations of workload, processor, network interface, switches, etc. with disparate resolutions, into an integrated simulation model. This accommodates different case studies that may require different levels of fidelity in various parts of a system. Our current implementation, includes low and medium-fidelity models of the network and low-fidelity and direct execution models of the workload. It supports studies of both simulation performance and scaling, and the properties of the simulated system themselves. Ongoing work allows more realistic simulation and dynamic visualization of ASCI-like workloads on very large machines.

F. J. Alexander, K. Berkbigler, G. Booker, B. Bush, K. Davis, A. Hoisie, S. Smith, T. P. Caudell, D. P. Holten, K. L. Summers, and C. Zhou, “Design and Implementation of Low- and Medium-Fidelity Network Simulations of a 30-TeraOPS System,” Los Alamos National Laboratory, Report LA-UR-02-1930. The magnitude of the scientific computations targeted by the ASCI project requires as-yet unavailable computational power. To facilitate these computations ASCI plans to deploy massive computing platforms, possibly consisting of tens of thousands of processors, capable of achieving 10-100 TeraOPS. For various reasons the current approach to building a yet-larger supercomputer–connecting commercially available SMPs with a network–may be reaching practical limits. The path to better hardware design and lower development costs involves performance evaluation, analysis, and modeling of parallel applications and architectures, and in particular predictive capability. We outline an approach for simulating computing architectures applicable to extreme-scale systems (thousands of processors) and to advanced, novel architectural configurations. The proposed simulation environment can be used for: (i) exploration of hardware/architecture design space; (ii) exploration of algorithm/implementation space both at the application level (e.g. data distribution and communication) and the system level (e.g. scheduling, routing, and load balancing); (iii) determining how application performance will scale with the number of processors or other components; (iv) analysis of the tradeoffs between performance and cost; and, (v) testing and validating analytical models of computation and communication. Our component-based design allows for the seamless assembly of architectures from representations of workload, processor, network interface, switches, etc., with disparate resolutions, into an integrated simulation model. This accommodates different case studies that may require different levels of fidelity in various parts of a system. Our initial implementation, comprising low- and medium-fidelity models for the network and a low-fidelity
model for the workload, can simulate at least 4096 computational nodes in a fat-tree network using Quadrics hardware. It supports studies of both simulation performance and scaling, and the properties of the simulated system themselves. Ongoing work allows more realistic simulation and visualization of ASCI-like workloads on very large machines.

C. L. Barrett, R. J. Beckman, K. P. Berkbigler, B. W. Bush, L. M. Moore, and D. Visarraga, “Actuated Signals in TRANSIMS,” Los Alamos National Laboratory, Report LA-UR-01-4609. This report outlines recent work implementing and calibrating actuated traffic controls and vehicle detectors in TRANSIMS. We have developed a generic control that provides a flexible approach to representing such devices. Although not modeled upon specific existing hardware or algorithms, our implementation provides a responsive control over a wide variety of demand conditions.


R. J. Beckman, B. W. Bush, K. M. Henson, and P. E. Stretz, “Portland Study Synthetic Population,” Los Alamos National Laboratory, Report LA-UR-01-4610. TRANSIMS (Transportation Analysis and Simulation System) is an integrated system of travel forecasting models designed to give transportation planners accurate, complete information on traffic impacts, congestion, and pollution. The Population Synthesizer Module constructs a regional population imitation with demographics closely matching the real population. Households are distributed spatially to approximate regional population distribution. The synthetic population’s demographics form basis for individual and household activities requiring travel and their household locations determine some of the travel origins and destinations. This report outlines how we have constructed the synthetic population for our Portland, Oregon, case study. It also briefly summarizes the characteristics of the data, and how we verified that the data was correctly generated.


K. P. Berkbiger and B. W. Bush, “TRANSIMS Network Subsystem for IOC-1,” Los Alamos National Laboratory, Report LA-UR-97-1580. The TRANSIMS network representation provides access to detailed information about streets, intersections, and signals in a road network. It forms a layer separating the other subsystems from the actual network data tables so that the other subsystems do not need to access the data tables directly or deal with the format and organization of the tables. This subsystem allows the user to construct multiple subnetworks from the network database tables. It includes road network objects such as nodes (intersections), links (road/street segments), lanes, and traffic controls (signs and signals).

K. P. Berkbiger and B. W. Bush, “TRANSIMS simulation output subsystem for IOC-1,” Los Alamos National Laboratory, Los Alamos, New Mexico, Technical Report LA-UR-97-1226. <http://www.osti.gov/energycitations/servlets/purl/501501-8MeLN/webviewable/> The output subsystem collects data from a running microsimulation, stores the data for future use, and manages the subsequent retrieval of the data. It forms a layer separating the other subsystems from the actual data files so that the other subsystems do not need to access the data files at the physical level or deal with the physical location and organization of the files. This subsystem also allows the user to specify what data is collected and retrieved, and to filter it by space and time. The collection occurs in a distributed manner such that
the subsystem’s impact on the microsimulation performance is minimized; the retrieval provides a unified view of
the distributed data.

Laboratory, Report LA-UR-97-1242. This document describes the TRAnsportation ANa lysis SIMulation System
(TRANSIMS) software architecture and high-level design for the first Interim Operational Capability (IOC-1). Our
primary goal in establishing the TRANSIMS software architecture is to lay down a framework for IOC-1. We want
to make sure that the various components of TRANSIMS are effectively integrated, both for IOC-1 and beyond, so
that TRANSIMS remains flexible, expandable, portable, and maintainable throughout its lifetime. In addition to
outlining the high-level design of the TRANSIMS software, we also set forth the software development environment
and software engineering practices used for TRANSIMS.

01-243.

for the Analysis of the Structure and Dynamics of Extreme-Scale Supercomputers,” Los Alamos National Laboratory,
Report LA-UR-02-1929. We are exploring the development and application of information visualization techniques
for the analysis of new extreme-scale supercomputer architectures. Modern super-computers typically comprise
very large clusters of commodity SMPs interconnected by possibly dense and often nonstandard networks. The scale,
complexity, and inherent nonlocality of the structure and dynamics of this hardware, and the systems and applications
distributed over it, challenge traditional analysis methods. As part of the a la carte team at Los Alamos National
Laboratory, who are simulating these advanced architectures, we are exploring advanced visualization techniques and
creating tools to provide intuitive exploration, discovery, and analysis of these simulations. This work complements
existing and emerging algorithmic analysis tools. Here we gives background on the problem domain, a description of
a prototypical computer architecture of interest (on the order of 10,000 processors connected by a quaternary fat-tree
network), and presentations of several visualizations of the simulation data that make clear the flow of data in the
interconnection network.

A. Berscheid and B. Bush, “Critical Infrastructure Protection Decision Support System Metropolitan Models:

A. Berscheid and B. Bush, “Critical Infrastructure Protection Decision Support System Models and Simulations:
Bioterrorism,” Los Alamos National Laboratory.

A. Berscheid, W. Beyeler, B. Bush, L. Dauelsberg, S. DeLand, A. Fishman, A. Ivey, M. Jusko, L. Moore, D. Powell,
L. Olson, R. Richardson, J. St. Aubin, M. Samsa, and D. Thompson, “CIP/DSS Phase IV Architecture and Analysis


M. P. Blue and B. W. Bush, “Set Entropy of Block Configurations That Appear in the TRANSIMS Simulation,” Los
Alamos National Laboratory, Report LA-UR-01-4277.

Alamos National Laboratory, Report LA-UR-04-7649.

M. Blue, B. Bush, and J. Puckett, “Applications of Fuzzy Logic to Graph Theory,” Los Alamos National Labora-
tory, Report LA-UR-96-4792. Graph theory has numerous applications to problems in systems analysis, operations
research, transportation, and economics. In many cases, however, some aspects of the graph-theoretic problem are
uncertain. In these cases, it can be useful to deal with this uncertainty using the methods of fuzzy logic. This
paper discusses the taxonomy of fuzzy graphs, formulates some standard graph-theoretic problems (shortest paths,
maximum flow, minimum cut, and articulation points) in terms of fuzzy graphs, and provides algorithmic solutions
to these problems, with examples.

tory, LA-UR-04-6147.

B. Bush, “Energy Infrastructure Modeling at Los Alamos National Laboratory,” Los Alamos National Laboratory,
Report LALP-03-027/LA-UR-03-0658.

The problem of laying out, or drawing, a graph arises in a wide variety of contexts. Automatically drawing computer network (e.g., LAN or WAN) configurations, object-oriented class diagrams, or database entity-relationship diagrams are examples of graph drawing. Estimating the layout of street networks containing some intersections with unknown locations is an example of the problem of drawing a graph. This paper discusses an algorithm for drawing general undirected graphs that relies on constructing a dynamical system analogous to the graph and evolving the state of the system to an equilibrium configuration. This configuration provides an aesthetically pleasing layout of the graph. We present an implementation of the algorithm as a C++ class. We also demonstrate the use of the class in a command-line executable program compilable on a variety of computer platforms as well as in an interactive 32-bit Windows program that animates the layout process.

The TRANSIMS database subsystem provides low-level services for accessing and modifying TRANSIMS data. It forms a layer separating the other subsystems from the actual data files so that the other subsystems do not need to access the data files at the physical level or deal with the physical location and organization of the files. This subsystem also organizes the data and supports a variety of metadata. It uses a relational model for the storage of data.

The TRANSIMS input editor provides a means for managing the TRANSIMS database, editing road network data, and setting up scenarios for simulation via its graphical user interface (GUI). It separates the user from the lower-level layers of TRANSIMS software involved with data management. It has functions for manipulating data in the TRANSIMS database; for creating, importing, altering, validating, and viewing road network data; and for setting up simulation output tables. The input editor is integrated into the ArcView geographic information system (GIS) and the Oracle relational database. One can also customize or extend the input editor using the Avenue programming language.

The Hierarchical Data Format (HDF) is a general-purposed scientific data format developed at the National Center for Supercomputing Applications. It supports metadata, compression, and a variety of data structures (multidimensional arrays, raster images, tables). FORTRAN 77 and ANSI C programming interfaces are available for it and a wide variety of visualization tools read HDF files. The author discusses the features of this file format and its possible uses in TRANSIMS.

This report discusses the uses of programming by object-orientation. Included in this report are the following: overview of concepts; software development; user interfaces; and databases.

B. W. Bush and J. R. Nix, “New Approach to the Interaction of Cosmic Rays with Nuclei in Spacecraft Shielding and the Human Body,” Los Alamos National Laboratory, Report LA-12452-MS. The interaction of high-energy cosmic rays with nuclei in spacecraft shielding and the human body is important for manned interplanetary missions and is not well understood either experimentally or theoretically. We present a new theoretical approach to this problem based on classical hadrodynamics for extended nucleons, which treats nucleons of finite size interacting with massive meson fields. This theory represents the classical analogue of the quantum hadrodynamics of Serot and Walecka without the assumptions of the mean-field approximation and point nucleons. It provides a natural...
covanvar microscopic approach to collisions between cosmic rays and nuclei that automatically includes space-time non-locality and retardation, nonequilibrium phenomena, interactions among all nucleons, and particle production. Unlike previous models, this approach is manifestly Lorentz covariant and satisfies a priori the basic conditions that are present when cosmic rays collide with nuclei, namely an interaction time that is extremely short and a nucleon mean-free path, force range, and internucleon separation that are all comparable in size. We review the history of classical meson-field theory and derive the classical relativistic equations of motion for nucleons of finite size interacting with massive scalar and vector meson fields.

B. W. Bush and R. D. Small, “Smoke Produced by Nonurban Target-Area Fires Following a Nuclear Exchange,” Pacific-Sierra Research Corporation, Report 1515. The amount of smoke that may be produced by wildland or rural fires as a consequence of a large-scale nuclear exchange is estimated. The calculation is based on a compilation of rural military facilities, identified from a wide variety of unclassified sources, together with data on their geographic positions, surrounding vegetation (fuel), and weather conditions. The ignition area (corrected for fuel moisture) and the amount of fire spread are used to calculate the smoke production. The results show a substantially lower estimated smoke production (from wildland fires) than in earlier nuclear winter studies. The amount varies seasonally and at its peak is less by an order of magnitude that the estimated threshold level necessary for a major attenuation of solar radiation.


B. W. Bush and R. D. Small, “Nuclear Winter Source-Term Studies: The Classification of U. S. Cities,” Pacific-Sierra Research Corporation, Report 1628. A theory for classifying U.S. cities according to their burnable densities is developed. Urban land use, which is closely related to combustible loadings, is shown to be a classification correlate superior to the conventional measures of city rank such as population, urban area, or population density. Six classes of cities are defined. The basic division is regional and the classification is shown to account for the demographic and economic characteristics that distinguish U.S. urban areas. Estimates of smoke production based on analysis of sample cities from each group would systematically account for differences in urban geographies.

B. W. Bush and R. D. Small, “Nuclear Winter Source-Term Studies: Ignition of Silo-Field Vegetation by Nuclear Weapons,” Pacific-Sierra Research Corporation, Report 1628. Smoke produced by the ignition and burning of live vegetation by nuclear explosions has been suggested as a major contributor to a possible nuclear winter. This report considers the mechanics of live vegetation ignition by a finite-radius nuclear fireball. For specified plant properties, the amount of fireball radiation absorbed by a plant community is calculated as a function of depth into the stand and range from the fireball. The spectral regions of plant energy absorption and the overlap with the emitted fireball thermal spectra are discussed. A simple model for the plant response to the imposed thermal load is developed. First, the temperature is raised; the change depends on the plant structure, moisture content, and plant canopy. Subsequent energy deposition desiccates the plant and finally raises its temperature to the threshold ignition limit. Results show the development of a variable depth ignition zone. Close to the fireball, ignition of the entire plant occurs. At greater distances (several fireball radii) portions of the plant are only partially desiccated, and sustained burning is less probable. Far from the burst, the top of the stand is weakly heated, and only a small transient temperature change results. An estimate of the smoke produced by an exchange involving the U.S. missile fields shows that the burning of live vegetation only slightly increases the total nonurban smoke production.

B. W. Bush and R. D. Small, “Smoke produced by nonurban target-area fires following a nuclear exchange. Technical report, 5 June 1984-5 January 1985,” Pacific-Sierra Research Corporation, Los Angeles, California, Technical Report PSR–1515. <http://www.osti.gov/energycitations/product.biblio.jsp?osti_id=5054780> The amount of smoke that may be produced by wildland or rural fires as a consequence of a large-scale nuclear exchange is estimated. The calculation is based on a compilation of rural military facilities, identified from a wide variety of unclassified sources, together with data on their geographic positions, surrounding vegetation (fuel), and weather conditions. The ignition area (corrected for fuel moisture) and the amount of fire spread are used to calculate the smoke production. The results show a substantially lower estimated smoke production (from wildland fires) than in earlier nuclear winter studies. The amount varies seasonally and at its peak is less by an order of magnitude that the estimated threshold level necessary for a major attenuation of solar radiation.


B. W. Bush, C. R. Files, and D. R. Thompson, “Empirical Characterization of Infrastructure Networks,” Los Alamos National Laboratory, Report LA-UR-01-5784. Critical infrastructure protection is a recognized problem of national importance. Infrastructure networks such as electric power, natural gas, communications, and transportation systems have an inherent graph-theoretic structure. Quantitatively characterizing the essential properties of infrastructure networks for various domains lays a valuable foundation for studying the universal features (especially criticality, robustness, etc.) and specific characteristics of such networks. We construct an extensive reference data set of infrastructure network graphs: 44 graphs of 13 types with nearly one million vertices and over one million edges. After regularizing these graphs, we compute more than fifty metrics related to connectivity, distance scale, cyclicity, cliquishness, and redundancy. We contrast these metrics for different types of infrastructures, study their interrelationships, and use them to cluster and classify systems. We consider both intact networks and networks that have been degraded by the removal of some vertices or edges either at random or systematically—this provides insight as to the robustness of the network if it were subject to a natural disaster or an attack.


B. Bush, T. Jenkin, D. Lipowicz, D. Arent, and R. Cooke, “Variance Analysis of Wind and Natural Gas Generation under Different Market Structures: Some Observations,” National Renewable Energy Laboratory, Golden, Colorado, Research Report TP-6A20-52790. <http://www.nrel.gov/docs/fy12osti/52790.pdf> Does large scale penetration of renewable generation such as wind and solar power pose economic and operational burdens on the electricity system? A number of studies have pointed to the potential benefits of renewable generation as a hedge against the volatility and potential escalation of fossil fuel prices. Research also suggests that the lack of correlation of renewable energy costs with fossil fuel prices means that adding large amounts of wind or solar generation may also reduce the volatility of system-wide electricity costs. Such variance reduction of system costs may be of significant value to consumers due to risk aversion. The analysis in this report recognizes that the potential value of risk mitigation associated with wind generation and natural gas generation may depend on whether one considers the consumer’s perspective or the investor’s perspective and whether the market is regulated or deregulated. We analyze the risk and return trade-offs for wind and natural gas generation for deregulated markets based on hourly prices and load over a 10-year period using historical data in the PJM Interconnection (PJM) from 1999 to 2008. Similar analysis is then simulated and evaluated for regulated markets under certain assumptions.

B. Bush, M. Melaina, P. Penev, and W. Daniel, “SERA Scenarios of Early Market Fuel Cell Electric Vehicle Introductions: Modeling Framework, Regional Markets, and Station Clustering,” National Renewable Energy Laboratory, Golden, Colorado, Technical Report NREL/TP-5400-56588. <http://www.nrel.gov/docs/fy13osti/56588.pdf> The availability of fueling infrastructure has become a major barrier to the early market success of hydrogen fuel cell electric vehicles (FCEVs). Various models have addressed infrastructure development during the early transition phase, but few long-term models have captured development dynamics in a manner that is consistent with real-world planning activities. This report describes the development and analysis of detailed temporal and spatial scenarios for early market infrastructure clustering and vehicle rollout using the Scenario Evaluation, Regionalization and Analysis (SERA) model. The scenarios reconcile nationwide scenario dynamics from a National Academy of Sciences study (NAS 2008) with observations and lessons learned from California’s early market strategy and planning activities (CaFCP 2012). The report provides an overview of the SERA scenario development framework and discusses the
The approach used to develop the nationwide scenario. The capability to focus on detailed infrastructure rollout dynamics within particular regions and states is then discussed with reference to Northeast Corridor states. The report also provides a description of the enhanced station placement algorithms developed to simulate both urban area network coverage and station clustering in neighborhoods with high densities of early adopters. Results from the national scenario analysis suggest that long-term levelized delivered costs for hydrogen tend toward $6.00/kg nationally, and zero cumulative cash flow is achieved in about 2018 or 2025 if hydrogen is priced at $11.00/kg and $6.75/kg, respectively. The capability to focus on dynamics within particular regions and to articulate detailed station placement strategies within urban areas adds realism and a planning perspective to these national scenario results.


R. H. Byrne, B. W. Bush, and T. Jenkin, “Long-term Modelling of Natural Gas Prices,” Sandia National Laboratories, SAND2013-2898. There are many factors that influence the price of natural gas. These include weather forecasts, economic activity, storage inventory, market expectations, and in the longer term supply and demand fundamentals. These factors can also influence the price volatility on a variety of timescales. While accurately predicting natural gas prices over long periods is probably futile, there are several reasons for modeling future long-term prices. First, business decisions for long-term investments, e.g. whether or not to invest in a power plant that burns natural gas, require estimates of future prices over a multi-decade time horizon. Second, price paths, probability density functions, and volatility estimates are necessary to price different types of derivative products. A third example, which was the motivation for this effort, is that estimating the future uncertainty of electricity prices over a multi-decade horizon under different generation mix scenarios requires some sort of estimate of input prices for natural gas and other fossil fuels. There are several options for modeling long-term price movements of natural gas. One is to develop a multi-factor model, develop longterm estimates of the factors, and then use these to construct the expected price path. Another option is to fit a mean-reverting stochastic model to historical data. Both approaches have pitfalls. Developing accurate long-term estimates of factors that contribute to natural gas prices is virtually impossible because of the inability to predict unforseen events. By fitting a stochastic model to historical data, one is assuming that the distribution of prices in the future will match the past. This is often a false assumption. Distributions (and correlations) of price dynamics often change over time, and the past is not necessarily a good predictor of the future. The approach taken for this effort was a stochastic fit to historical data. To incorporate some uncertainty into the price paths, the model accurately replicates historical distributions about 58% of the time. If there is a strong belief that the future distributions will match historical distributions, an acceptance-testing method is outlined for generating price paths that perfectly match the distribution of historical data.


D. Inman, L. Vimmerstedt, E. Newes, B. Bush, and S. Peterson, “Biomass scenario model scenario library: definitions, construction, and description,” National Renewable Energy Laboratory, Golden, Colorado, Technical Report. <http://dx.doi.org/10.2172/1129277>Understanding the development of the biofuels industry in the United States is important to policymakers and industry. The Biomass Scenario Model (BSM) is a system dynamics model of the biomass-to-biofuels system that can be used to explore many aspects of the industry. Because of the complexity of the model, as well as the wide range of possible future conditions that affect biofuels industry development, we have not developed a single reference case but instead have designed a set of six incentive-focused scenarios. The purpose of this report is to describe the scenarios that comprise the BSM scenario library. At present, we have the following six incentive-focused scenarios in our library: minimal incentives scenario; ethanol-focused incentives scenario; equal access to incentives scenario; output-focused incentives scenario; pathway-diversity-focused incentives scenario; and the point-of-production-focused incentives scenario. This report describes the model settings and rationale for each scenario.


T. Jenkin, V. Diakov, E. Drury, B. Bush, P. Denholm, J. Milford, D. Arent, R. Margolis, and R. Byrne, “The Use of Solar and Wind as a Physical Hedge against Price Variability within a Generation Portfolio,” National Renewable Energy Laboratory, Golden, Colorado, Technical Report NREL/TP-6A20-59065. <http://www.nrel.gov/docs/fy13osti/59065.pdf> This study provides a framework to explore the potential use and incremental value of small- to large-scale penetration of solar and wind technologies as a physical hedge against the risk and uncertainty of electricity cost on multi-year to multi-decade timescales. Earlier studies characterizing the impacts of adding renewable energy (RE) to portfolios of electricity generators often used a levelized cost of energy or simplified net cash flow approach. In this study, we expand on previous work by demonstrating the use of an 8760 hourly production cost model (PLEXOS) to analyze the incremental impact of solar and wind penetration under a wide range of penetration scenarios for a region in the Western U.S. We do not attempt to “optimize” the portfolio in any of these cases. Rather we consider different RE penetration scenarios, that might for example result from the implementation of a Renewable Portfolio Standard (RPS) to explore the dynamics, risk mitigation characteristics and incremental value that RE might add to the system. We also compare the use of RE to alternative mechanisms, such as the use of financial or physical supply contracts to mitigate risk and uncertainty, including consideration of their effectiveness and availability over a variety of timeframes.


Y. Lin, E. Newes, B. Bush, S. Peterson, and D. Stright, “Biomass Scenario Model Documentation: Data and References,” National Renewable Energy Laboratory, Golden, Colorado, Technical Report NREL/TP-6A20-57831. <http://www.osti.gov/bridge/servlets/purl/1082565/> The Biomass Scenario Model (BSM) is a system dynamics model that represents the entire biomass-to-biofuels supply chain, from feedstock to fuel use. The BSM is a complex model that has been used for extensive analyses; the model and its results can be better understood if input data used for initialization and calibration are well-characterized. It has been carefully validated and calibrated against the available data, with data gaps filled in using expert opinion and internally consistent assumed values. Most of the main data sources that feed into the model are recognized as baseline values by the industry. This report documents data sources and references in Version 2 of the BSM (BSM2), which only contains the ethanol pathway, although subsequent versions of the BSM contain multiple conversion pathways. The BSM2 contains over 12,000 total input values, with 506 distinct variables. Many of the variables are opportunities for the user to define scenarios, while others are simply used to initialize a stock, such as the initial number of biorefineries. However, around 35% of the distinct variables are defined by external sources, such as models or reports. The focus of this report is to provide insight into which sources are most influential in each area of the supply chain. We find that data based on POLYSYS datasets and U.S. Department of Agriculture baseline projections are the most utilized sources in the feedstock sector, whereas the conversion module relies heavily on data found in National Renewable Energy Laboratory technical reports dealing with the techno-economic characteristics of different technologies. The distribution, dispensing, and fuel use modules utilize data on gasoline stations from the National Association of Convenience Stores.


In support of the national goals for biofuel use in the United States, numerous technologies have been developed that convert biomass to biofuels. Some of these biomass-to-biofuel conversion technology pathways are fully commercial, while others are in earlier stages of development. The advancement of a new pathway towards commercialization involves various types of improvements, including yield improvements through chemical and biochemical refinements, process engineering, and financial performance. Actions of private investors and public programs can accelerate the demonstration and deployment of new conversion technology pathways. These investors (both private and public) will pursue a range of pilot-, demonstration-, and pioneer-commercial-scale biorefinery investments, because the most cost-effective set of investments for advancing the maturity of the pathway is unknown. In some cases whether or not the pathway itself will ultimately be technically and financially successful is unknown. This report presents results from the Biomass Scenario Model—a system dynamics model of the biomass-to-biofuels system—that estimate effects of investment in one particular demonstration and deployment plan. This plan is a multi-stage combination of pilot, demonstration, and pioneer-commercial-scale biorefineries. The report discusses challenges in estimating effects of such investments. The report concludes that investment in demonstration and deployment appears to have a substantive positive effect on the development of the biofuels industry, and that other conditions, such as supportive policies, are likely to have major impacts on the effectiveness of such investments.


Software


G. B. Booker, B. W. Bush, P. T. Giguere, J. V. Holland, S. P. Linger, M. L. Salazar, C. Unal, and K. A. Werley, Interdependent Energy Infrastructure Simulation System. Los Alamos National Laboratory. The IEISS software models energy transmission network systems (such as electric power systems and natural gas pipelines) and simulates their physical behavior, including the interdependencies between systems (such as when the energy supplied by one system is used to operate components of another system). Each physical, logical, or functional entity in the model has a variety of attributes and behaviors that mimic its real-world counterpart. The software supports the analysis of the complex, non-linear, and emergent interactions between energy infrastructures at the state, regional, or national scale. (Databases are not supplied with the software, however.) Specifically, the simulation can be used to visualize the interconnectivity between different energy systems, predict the outcome of incidents affecting the networks, measure the economic effects of disruptions in service, assess system robustness under varied future plans and forecasts, and identify components critical for the operation of the systems.


B. W. Bush, T. Cleland, L. Lauer, and D. R. Thompson, CIP/DSS “Conductor” Tool. Los Alamos National Laboratory. The “Conductor” is a Java-based tool to merge source code from Vensim (a system dynamics application code available from Ventana Systems, http://www.vensim.com) into a single file. Its main use is to merge separate modules of a larger system into a single version which can be executed by Vensim. It also has functionality to perform simple checks for software coding conventions, and model browsing. The software also contains extensive support for database connectivity.

B. W. Bush, L. R. Dauelsberg, M. H. Ebinger, R. J. LeClaire, D. R. Powell, S. Rasmussen, D. R. Thompson, C. J. Wilson, M. S. Witkowski, A. Ford, and D. Newsom, Metropolitan Critical Infrastructure Model. Los Alamos National Laboratory. The Metropolitan Critical Infrastructure Model simulates the dynamics of fourteen critical infrastructures (agriculture, banking/finance, chemical industry, defense industrial base, emergency services, food, government, information/telecommunications, key resources, postal, public health transportation, water, energy) in urban areas at a highly aggregate level (i.e., total capacities/capabilities are represented instead of individual facilities). The purpose of the models is to simulate disruption scenarios, evaluate the consequences of such disruptions, and estimate the effectiveness of mitigation actions. The models include high-level infrastructure interdependencies, damage and recovery simulations, potential lost productivity and recovery cost, and aggregate market models. Dynamic processes like these are represented in the CIP/DSS infrastructure sector simulations by differential equations,
discrete events, and codified rules of operation. The consequences are computed in terms of human health and safety, economic, public confidence, national security, and environmental impacts. Realistic databases are supplied separately from the software. The system is designed to help answer the following questions: (i) What are the consequences of attacks on infrastructure in terms of national security, economic impact, public health, and conduct of government—including the consequences that propagate to other infrastructures? (ii) Are there choke points in our Nation’s infrastructures (i.e., areas where one or two attacks could have the largest impact)? What and where are the choke points? (iii) Incorporating consequence, vulnerability, and threat information into an overall risk assessment, what are the highest risk areas? (iv) What investment strategies can the U.S. make that will have the most impact in reducing overall risk?

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