Optimization – Particularly Optimization under Uncertainty.

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ANL-GE-DOE meeting

1. Motivation (our playground ☺) : Management of Energy Systems under Ambient Conditions Uncertainty

Ambient Condition Effects in Energy Systems

Operation of Energy Systems is Strongly Affected by Ambient Conditions

- **Power Grid Management:** Predict Spatio-Temporal Demands *(Douglas, et.al. 1999)*

- **Power Plants:** Generation levels affected by air humidity and temperature *(General Electric)*

- **Petrochemical:** Heating and Cooling Utilities *(ExxonMobil)*

- **Buildings:** Heating and Cooling Needs *(Braun, et.al. 2004)*

- (Focus) **Next Generation Energy Systems** assume a major renewable energy penetration: Wind + Solar + Fossil *(Beyer, et.al. 1999)*

- Increased reliance on renewables must account for variability of ambient conditions, which cannot be done deterministically …

- We must optimize operational and planning decisions accounting for the uncertainty in ambient conditions (and others, e.g. demand)

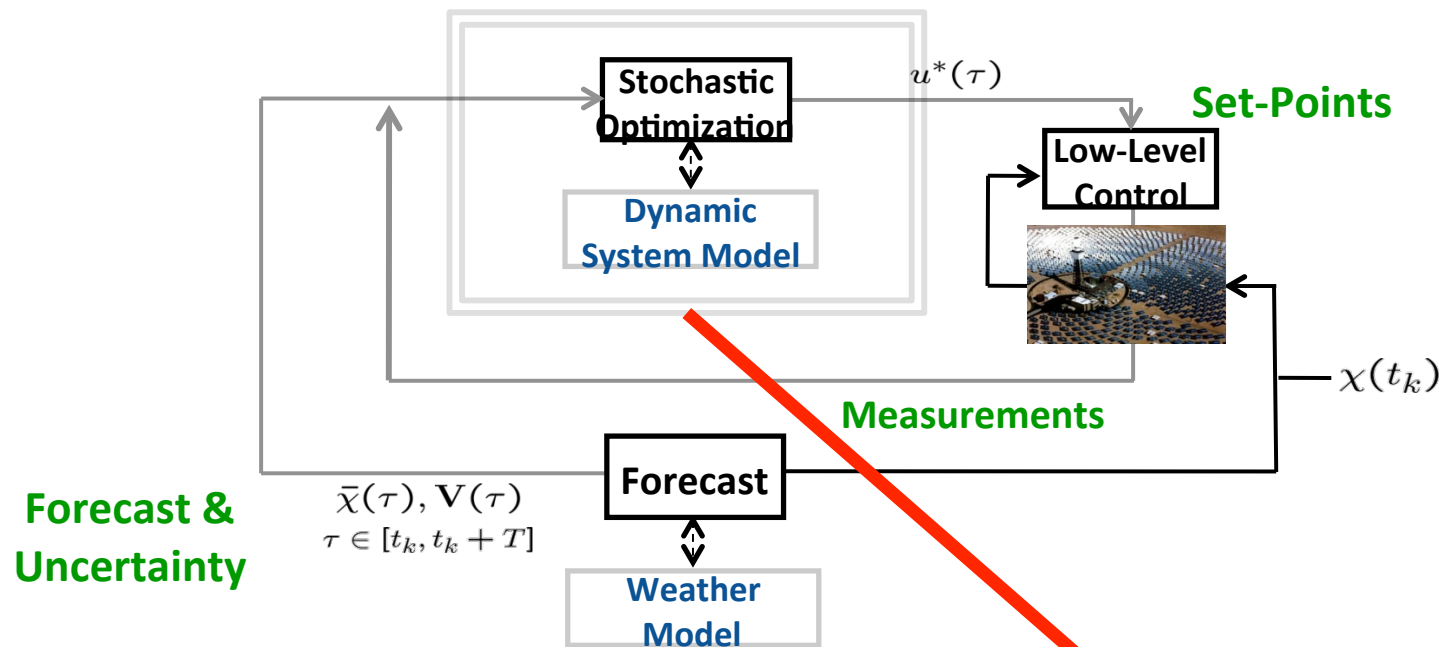- **Optimization Under Uncertainty.**
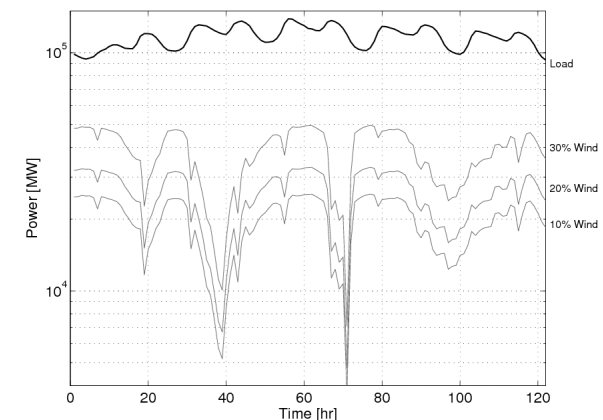
Wind Power Profiles

2. Impact: Stochastic Unit Commitment – Management of Energy Systems

Stochastic Predictive Control

$u^*(\tau)$

Stochastic Optimization

Set-Points

Low-Level Control

Dynamic System Model

$\chi(t_k)$

Measurements

Forecast & Uncertainty

$\bar{\chi}(\tau), \mathbf{V}(\tau)$
$\tau \in [t_k, t_k + T]$

Forecast

Weather Model

Two-stage Stoch Prog

$$\underset{x_0}{Min}\Big\{ f_0(x_0) + \mathbb{E}\Big[\underset{x}{Min}\, f(x,\omega) \Big]\Big\}$$

subj. to.

$$g_0(x_0) \;=\; b_0$$

$$g_i(x_0, x_i) \;=\; b_i \quad i = 1,2\ldots S$$

$$x_0 \geq 0, \quad x_i \geq 0$$

Stochastic NLMPC

$$\underset{u(t)}{\min} \quad \underset{\chi(t)\in\Omega}{\mathbf{E}} \left[\int_{t_\ell}^{t_\ell + N} \varphi(z(t), y(t), u(t), \chi(t))\, dt \right]$$

$$\frac{dz}{dt} \;=\; \mathbf{f}(z(t), y(t), u(t), \chi(t))$$

$$0 \;=\; \mathbf{g}(z(t), y(t), u(t), \chi(t))$$

$$0 \;\geq\; \mathbf{h}(z(t), y(t), u(t), \chi(t))$$

$$z(0) \;=\; x_\ell$$

Stochastic Unit Commitment with Wind Power (SAA)

$$\min \quad \text{COST} = \frac{1}{N_s} \sum_{s \in \mathcal{S}} \left(\sum_{j \in \mathcal{N}} \sum_{k \in \mathcal{T}} c^p_{sjk} + c^u_{jk} + c^d_{jk} \right)$$

$$\text{s.t.} \quad \sum_{j \in \mathcal{N}} p_{sjk} + \sum_{j \in \mathcal{N}_{wind}} p^{wind}_{sjk} = D_k, s \in \mathcal{S}, k \in \mathcal{T}$$

$$\sum_{j \in \mathcal{N}} \overline{p}_{sjk} + \sum_{j \in \mathcal{N}_{wind}} p^{wind}_{sjk} \geq D_k + R_k, s \in \mathcal{S}, k \in \mathcal{T}$$

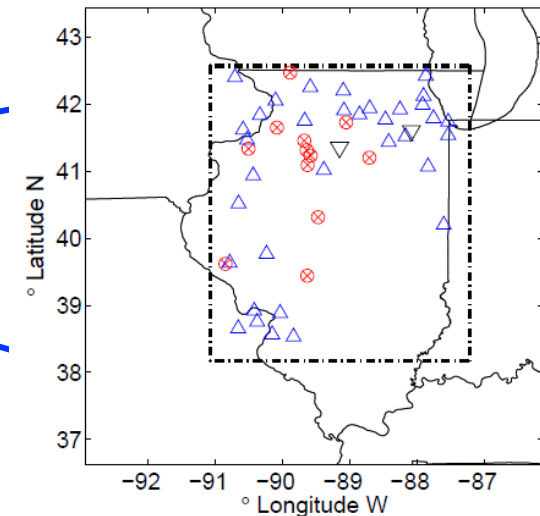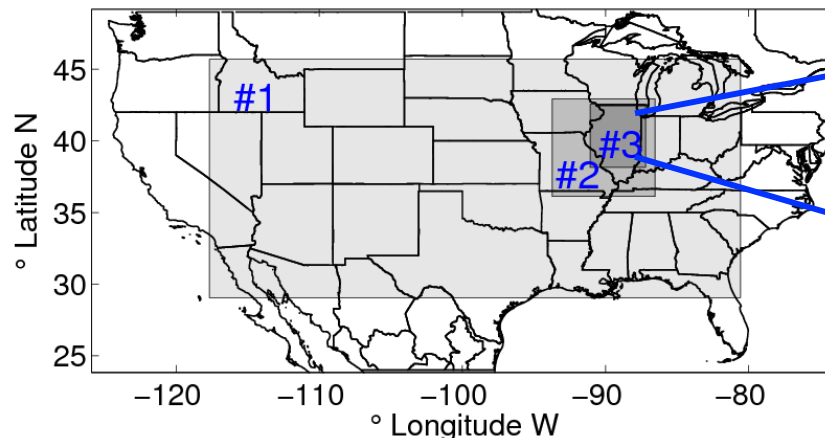ramping constr., min. up/down constr.

Thermal Units Schedule? Minimize Cost

Satisfy Demand

Have a Reserve

Dispatch through network

- Wind Forecast – WRF(Weather Research and Forecasting) Model
  - Real-time grid-nested 24h simulation
  - 30 samples require 1h on 500 CPUs (Jazz@Argonne)

Zavala & al 2010.

Wind power forecast and stochastic programming

- Unit commitment & energy dispatch with <u>uncertain wind power generation for the State of Illinois, assuming 20% wind power penetration, using the same windfarm sites as the one existing today.</u>

wind
power
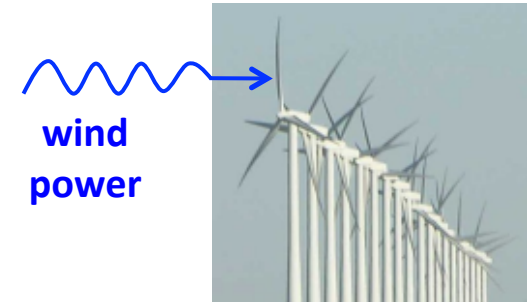
- Full integration with 10 thermal units to meet demands. Consider dynamics of start-up, shutdown, set-point changes

- The solution is only 1% more expensive then the one with exact information. Solution on average infeasible at 10%.
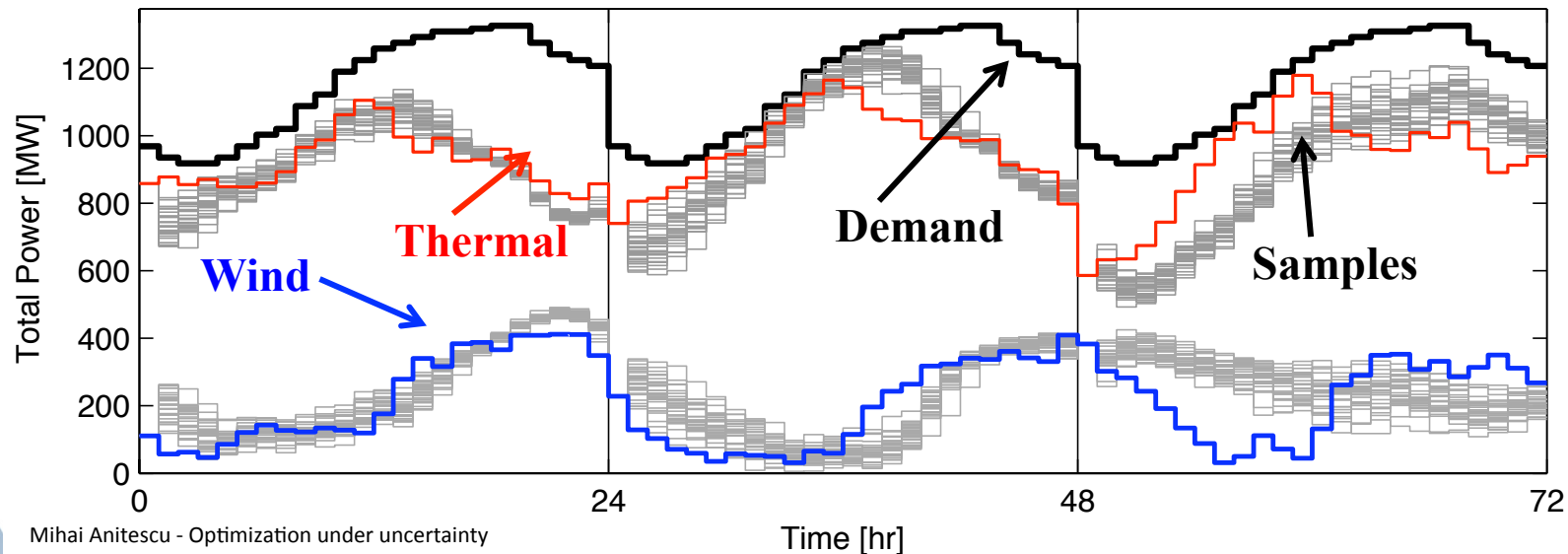
Some Considerations in Using Supercomputing for Power Grid

- Is it really worth using a supercomputer for this task? (We need the answer every 1hr with 24 hour time horizons.)

- Let's look at the most pressing item of Supercomputing usage: power.

  – BG/P (and exascale) needs <~ 20MW of power.

  – The Midwest US has 140GW of power installed, and the peak demands runs up to 110GW.

  – We will never reduce power consumption, but we will make it more reliable, less dependent on fossil, and cheaper by better managing the peak

- If we accept this will lead to 10% more renewable penetration (our SUC study), then this is worth on the order of 10-15GW, far above what BG/P costs in power consumption.

- In addition operational constraints makes supercomputing (if uncertainty needed to account for) necessary and not just useful or convenient.

- But, even if approximations will work, this tool will be helpful as the "gold standard" for validating other algorithms to be deployed on defined computational resources.

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3. Secondary Impacts

New Platform: Optimization under Uncertainty for Next-Generation Building Systems

Deployment of Proactive Systems at Argonne National Laboratory
- Integrates New Sensors, Statistical Models, and Real-Time Optimization
- Tests in Commercial-Sized Building : ~ 500 Occupants, ~100,000 sq. ft.
- Energy Savings of Up to 30% in HVAC Energy Demand
    - Key: Anticipation Using Occupancy & Weather Information
    - Key: Adaptive Comfort and Equipment Conditions (Set-Points)
    - Key: Maximize Ambient Air Intake to Condition Building
    - Key: Provide algorithms for limited computational resources
"in thermostat"

Predicted Energy Savings at Argonne's Building
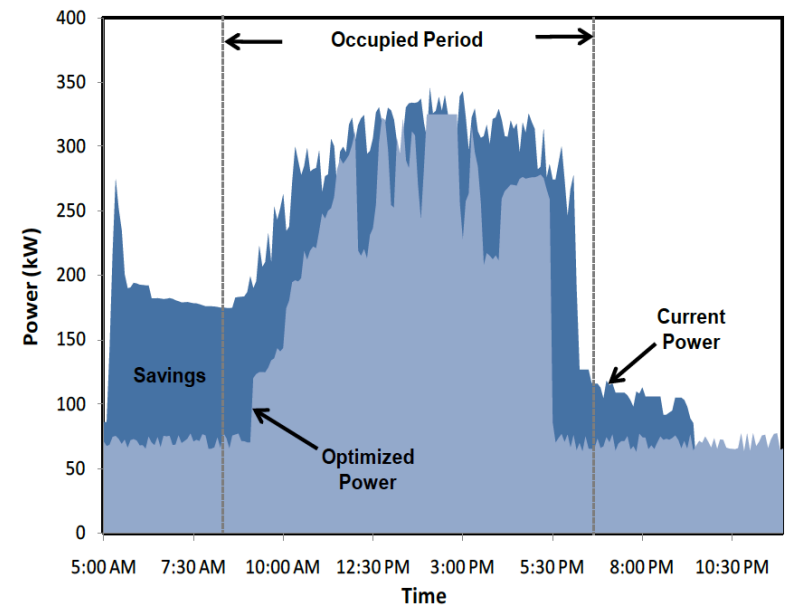
Stochastic Real-Time Optimization for Building Systems
Minimize operation cost
<u>Subject to</u>: Comfort and Hardware Constraints.
<u>Uncertainty</u>: occupancy, ambient conditions, state

Unusual Features:
•**Data Analysis and Storage**
(~1,000 Sensors per Building at High-Frequencies)
•**Statistical and Gray-Box Modeling**
(Minimize Technology Cost, Uncertainty Estimates)
•**Resiliency Requirements**
(Sustain Frequent Sensor and Equipment Faults)

SRTO-Latest Deployment (APS Building, August 23 2011)
15% Energy Savings (~ 1MWh) in First Day

Hybrid Photovoltaic-H$_2$ System
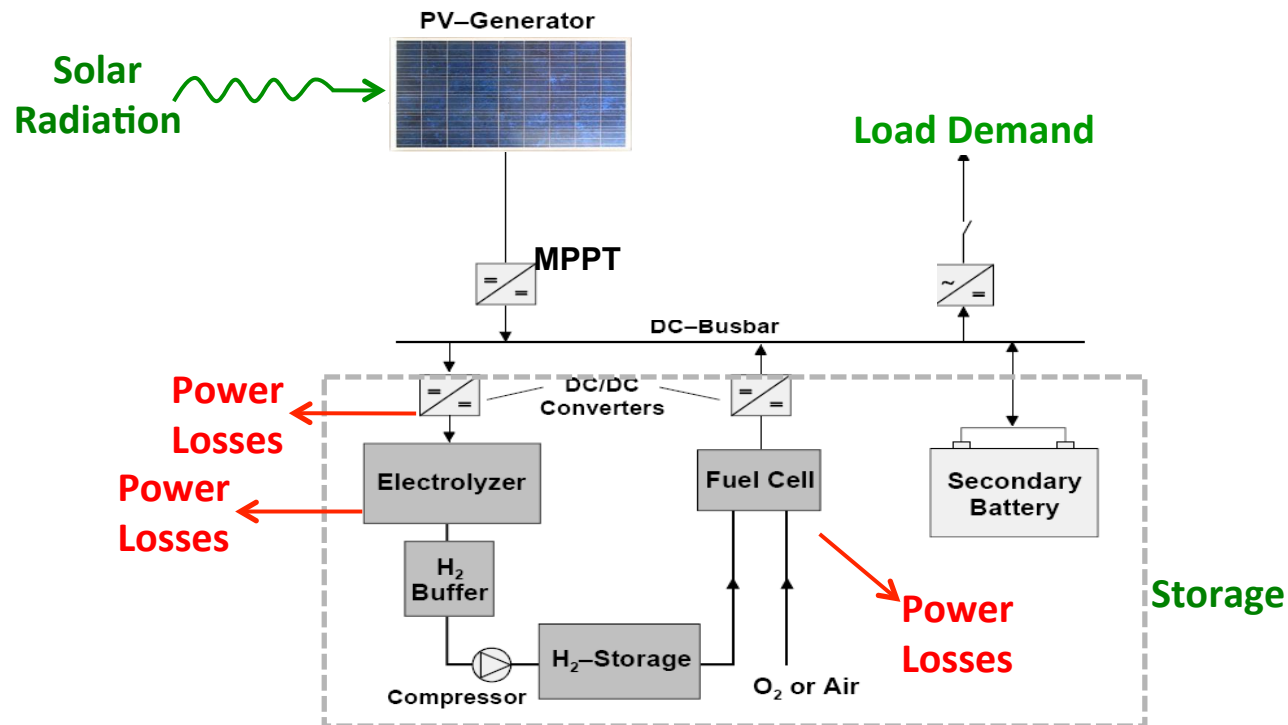
- **Operating Costs Driven by <u>Uncertain</u> Radiation** *Ulleberg, 2004*
  - **Performance Deteriorates by Multiple <u>Power Losses</u>**

Model:

Problem: Operate to Minimize Operating Costs +

Maximize H$_2$ Production

<u>**Subject to:**</u> **Energy Balances; State-of-Charge, Fuel Cell**

and Electrolyzer Limits

Hybrid Photovoltaic-H$_2$ System

Load Satisfaction Deterministic ("Optimization on Mean") vs. Stochastic
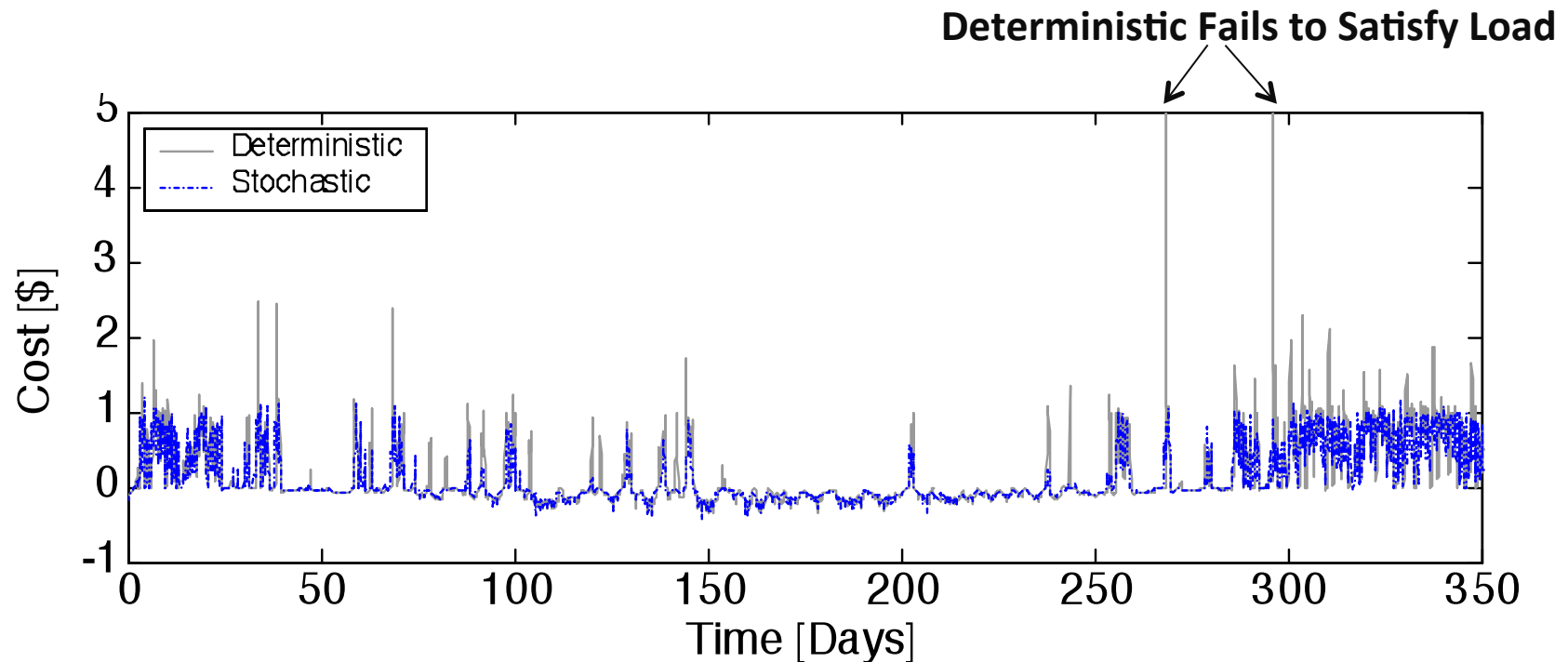
Therefore, the alternative to stochastic programming can turn out infeasible !!

Handling Stochastic Effects Particularly Critical in <u>Grid-Independent</u> Systems

3. Our Technology:

PIPS-I (Parallel Interior Point Stochastic Programming)
PIPS-S (Parallel Simplex for Stochastic Programming)

PIPS – Our Scalable Stochastic Programming Solver Using Direct Schur Complement Method

- The arrow shape of H

$$
\begin{bmatrix}
H_1 & & & & G_1^T \\
& H_2 & & & G_2^T \\
& & \ddots & & \vdots \\
& & & H_S & G_S^T \\
G_1 & G_2 & \dots & G_S & H_0
\end{bmatrix}
=
\begin{bmatrix}
L_1 & & & & \\
& L_2 & & & \\
& & \ddots & & \\
& & & L_S & \\
L_{10} & L_{20} & \dots & L_{S0} & L_c
\end{bmatrix}
\begin{bmatrix}
D_1 & & & & \\
& D_2 & & & \\
& & \ddots & & \\
& & & D_N & \\
& & & & D_c
\end{bmatrix}
\begin{bmatrix}
L_1^T & & & & L_{10}^T \\
& L_2^T & & & L_{20}^T \\
& & \ddots & & \vdots \\
& & & L_S^T & L_{S0}^T \\
& & & & L_c^T
\end{bmatrix}
$$

- Solving Hz=r

$$
L_i D_i L_i^T = H_i, \quad L_{i0} = G_i L_i^{-T} D_i^{-1}, \quad i = 1, \dots S,
$$

$$
C = H_0 - \sum_{i=1}^{S} G_i H_i^{-1} G_i^T, \quad \boxed{L_c D_c L_c^T = C.}
$$

Implicit factorization, C is **dense**, H's are sparse.

$$
w_i = L_i^{-1} r_i, \quad i = 1, \dots S,
$$

$$
\boxed{w_0 = L_c^{-1}} \left(r_0 - \sum_{i=1}^{S} L_{i0} w_i \right)
$$

$$
v_i = D_i^{-1} w_i, \quad i = 0, \dots, S
$$

$$
\boxed{z_0 = L_c^{-1} v_0}
$$

$$
z_i = L_i^{-T} \left(v_i - L_{i0}^T z_0 \right), \quad i = 1, \dots S.
$$

Back substitution   Diagonal solve   Forward substitution

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Stochastic programming – a non-trivial parallel paradigm suitable for next-generation supercomputers

- Computational pattern

2nd stage computations

1st stage computations

Optimization

| Deterministic model | Effects of uncertainty |

Optimization

Recourse problem outcome 1

Optimization

Recourse problem outcome 2

Optimization

Recourse problem outcome N
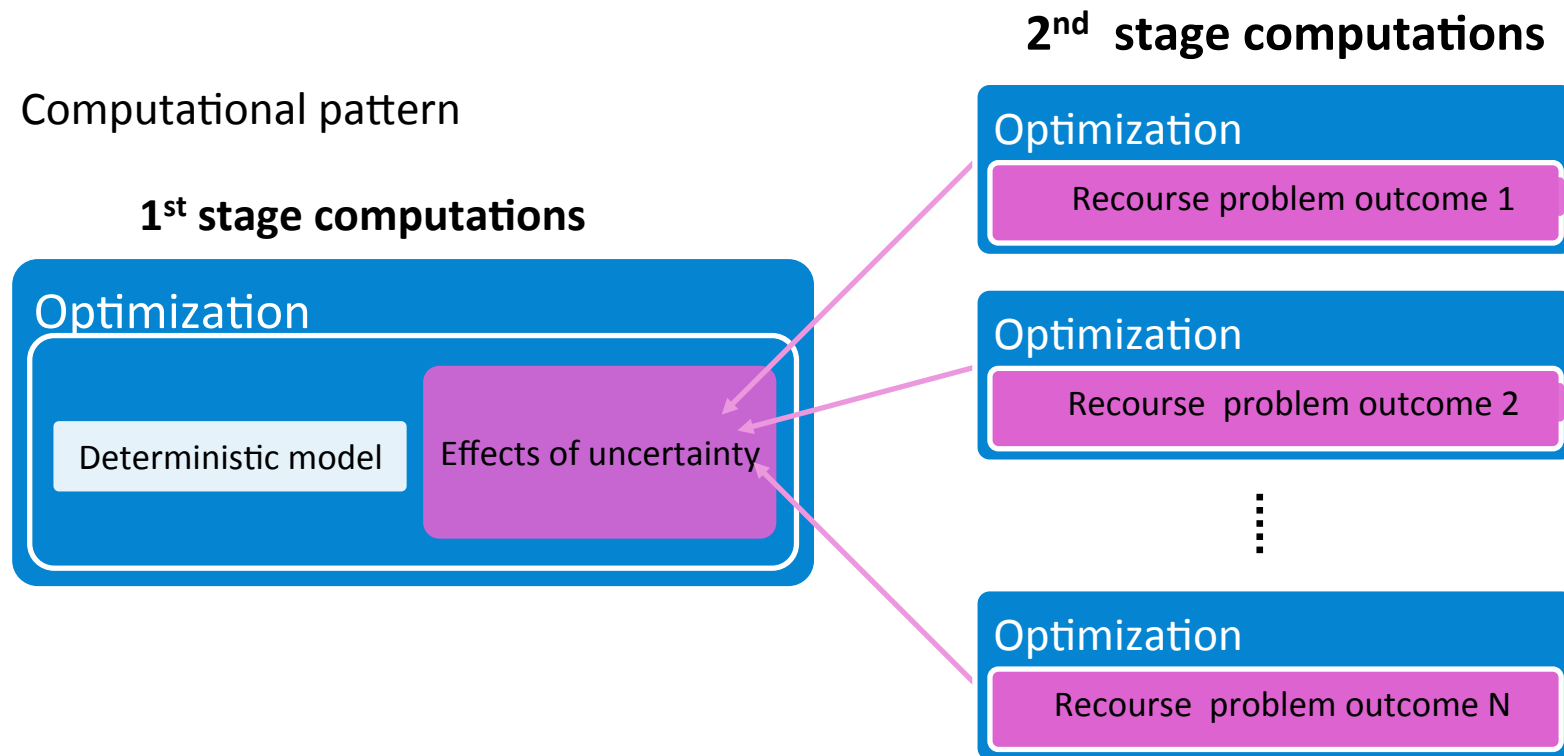
- Extra, in-node parallelization can be obtained for both 1st and 2nd stage.
- Algorithmic developments are needed to ensure efficient communication, fault resilience and good load balancing.
- Same pattern for statistical model CALIBRATION.

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Parallelizing the 1st stage linear algebra

- We distribute the 1st stage Schur complement system.

$$C = \begin{bmatrix} \tilde{Q} & A_0^T \\ A_0 & 0 \end{bmatrix}, \tilde{Q} \text{ dense symm. pos. def., } A_0 \text{ sparse full rank.}$$

- C is treated as dense.

- Alternative to PSC for problems with large number of 1st stage variables.

- Removes the memory bottleneck of PSC and DSC.

- We investigated ScaLapack, Elemental (successor of PLAPACK)
  - None have a solver for symmetric indefinite matrices (Bunch-Kaufman);
  - LU or Cholesky only.
  - So we had to think of modifying either.

Cholesky-based LDL^T-like factorization

$$\begin{bmatrix} \tilde{Q} & A^T \\ A & 0 \end{bmatrix} = \begin{bmatrix} L & 0 \\ AL^{-T} & \bar{L} \end{bmatrix} \begin{bmatrix} I & \\ & -I \end{bmatrix} \begin{bmatrix} L^T & L^{-1}A^T \\ 0 & \bar{L}^T \end{bmatrix}, \text{ where } LL^T = \tilde{Q}, \bar{L}\bar{L}^T = A\tilde{Q}^{-1}A^T$$

- Can be viewed as an "implicit" normal equations approach.

- In-place implementation inside Elemental: no extra memory needed.

- Idea: modify the Cholesky factorization, by changing the sign after processing p columns.

- It is much easier to do in Elemental, since this distributes elements, not blocks.

- Twice as fast as LU

- Works for more general saddle-point linear systems, *i.e.,* pos. semi-def. (2,2) block.

PIPS Solver Capabilities

- **Hybrid MPI/SMP running on Blue Gene/P**
  - Successfully (though incompletely due to allocation limit) run on up to **32,768** nodes (**96**% strong scaling) for Illinois problem with grid constraints. 3B variables, maybe largest ever solved?

- **Handles up to 100,000 first-stage variables. Previous results dealt with O(20-50).**

- **Close to real-time solutions (6 hr horizon in 1 hr wallclock; with REAL network, 32K scenarios)**
  - Further development needed, since users aim for
    - More uncertainty, more detail (x 10)
    - Faster Dynamics → Shorter Decision Window (x 10)
    - Longer Horizons (California == 72 hours) (x 3)

Components of Execution Time and Strong Scaling
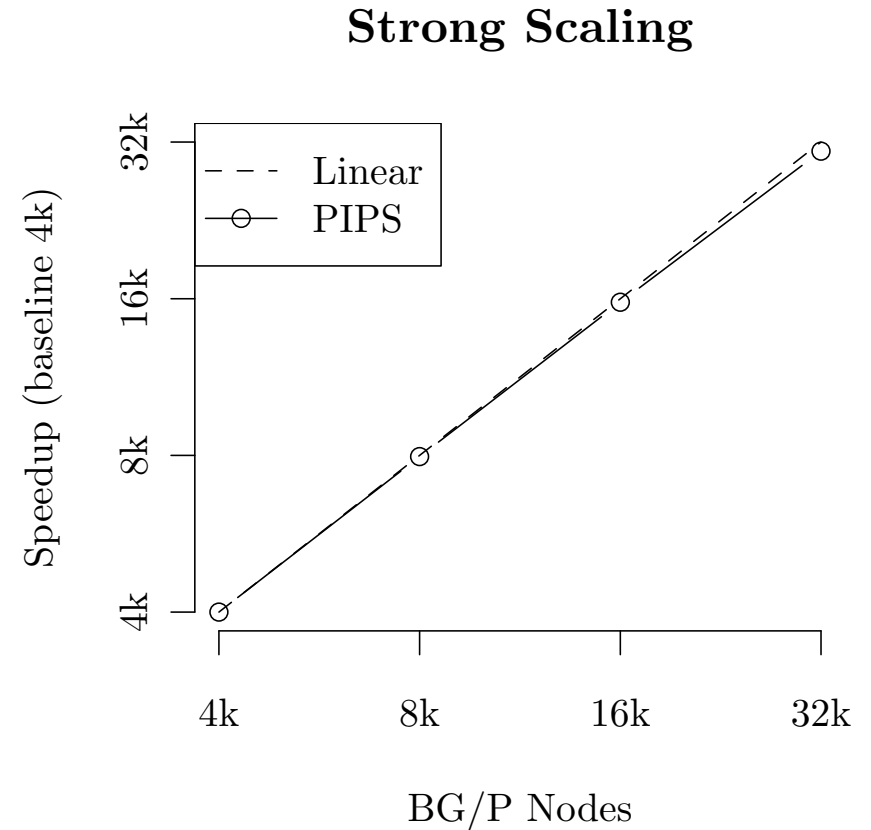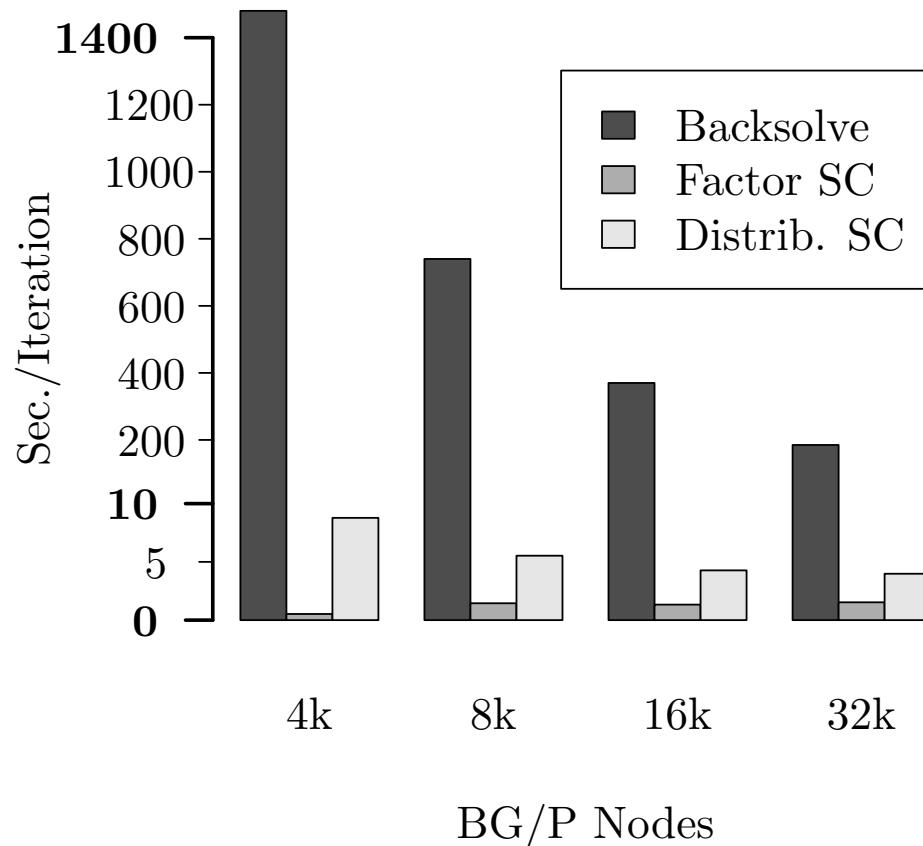
- 32K nodes=130K cores (80% BG/P)
- "Backsolve" phase embarrassingly parallel, but not Schur Complement (SC)
- Communication for "Distrib. SC" not yet a bottleneck, but we will get there.

4. Our projects

Current Sources:

- Office of Science ASCR sources: "we enable" we can get close to the problem, find scalable algorithmic patterns, demonstrate them, but the funds are for MATH and SCALABLE ALGORITHMS not to solve a problem.
  - The M2ACS center: Multifaceted mathematics
  - Stochastic Dynamic Optimization
  - Early Career -- Stochastic Programming (Zavala).
- OE sources: we actually model actual networks generators problems, etc.
- LDRD (primary) and (a bit) of EERE for solar forecasting/modeling.

- To solve REAL problems, we typically need more modeling/forecasting resources.

Anitescu: Multifaceted Mathematics for Complex Energy Systems –M2ACS

Summary:

- A 17.5M $ investment 2012-2016: ANL, PNNL, SNL, UW, UC lead by MA>

- Focuses on the **grand challenges** of analysis, design, planning, maintenance, and operation of electrical energy systems and related infrastructure in the presence of rapidly increasingly complexity of the systems.

- Four mathematical areas identified:
  – Predictive modeling that accounts for uncertainty and errors
  – Mathematics of decisions that allow hierarchical, data-driven and real-time decision making
  – Scalable solution algorithms for optimization and dynamic simulation
  – Integrative frameworks leveraging model reduction and multiscale analysis

- Mathematical aspects include: discrete and continuous optimization, dynamical systems, multi-level techniques, data-driven methods, graph-theoretical methods, and stochastic and probabilistic approaches for uncertainty and error.

- Mathematics addresses a broad class of complex energy systems subchallenges

Application Domain Subchallenges

- 1. Integrated Energy Resource Planning under Sustainability Considerations
- 2. Next-Generation Energy Delivery Architecture Design
- 3. Real-Time Interconnect-wide Monitoring and Predictive Operation
- 4. Predictive Control of Cascading Blackouts and Real-Time Contingency Analysis.

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The time scales challenge (courtesy DeMarco)

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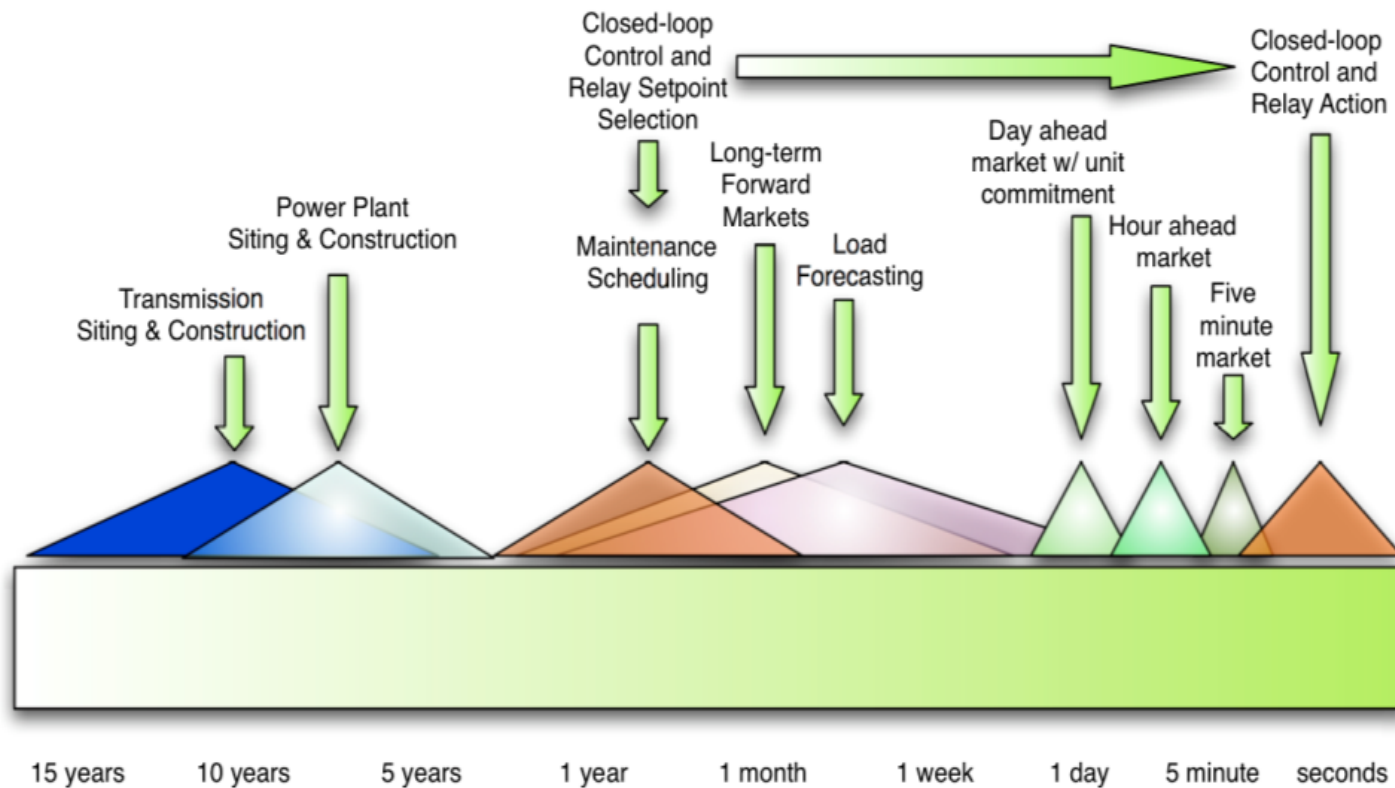
Integration Concept:

- By constant interaction of the math teams at each iteration and by gauging performance on subchallenges, integration will be achieved.

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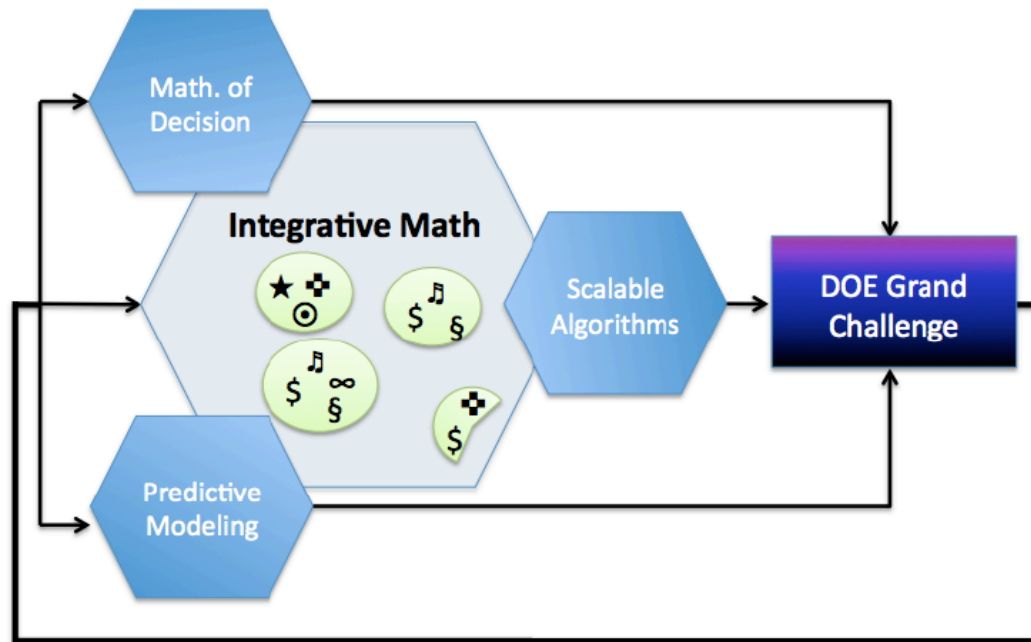
Anitescu Team: Topic Structure

Predictive modeling
Huang/Tartakovsky

- **Dynamics and stochastics** — Constantinescu, Huang, Lin, Tartakovsky
- **Stability** — DeMArco, Lee
- **Structured Lyapunov** — DeMArco
- **Graph tools** — Halappanavar, Hovland, Huang

Math. of decision
Wright/Leyffer

- **Hierarchical Decision Making** — Birge, Ferris, Munson
- **Equilibrium problems** — Birge, Ferris, Leyffer, Munson
- **Data-driven decisions** — Anitescu, Wright
- **Realtime Decisions** — Zavala

Integrative frameworks
Ferris/Watson

- **Approximation** — Leyffer
- **Multiscale reduction** — Lin, Lu
- **Rare events** — Weare
- **Relaxation** — Luedtke, Lesieutre
- **Integrative frameworks** — Ferris, Smith, Watson, Hovland

Scalable algorithms
Smith/Linderoth

- **Scalable dynamic simulation** — Constantinescu
- **Multilevel algorithms** — Lee, Smith
- **Decomposition algorithms** — Linderoth, Watson, Munson, Anitescu
- **Infrastructure for scalable alg.** — Anitescu, Munson

Systems Challenges
DeMarco / Huang

- **Planning under sustainability** — DeMarco
- **Delivery architecture** — Lesieutre
- **Monitoring and prediction** — Huang
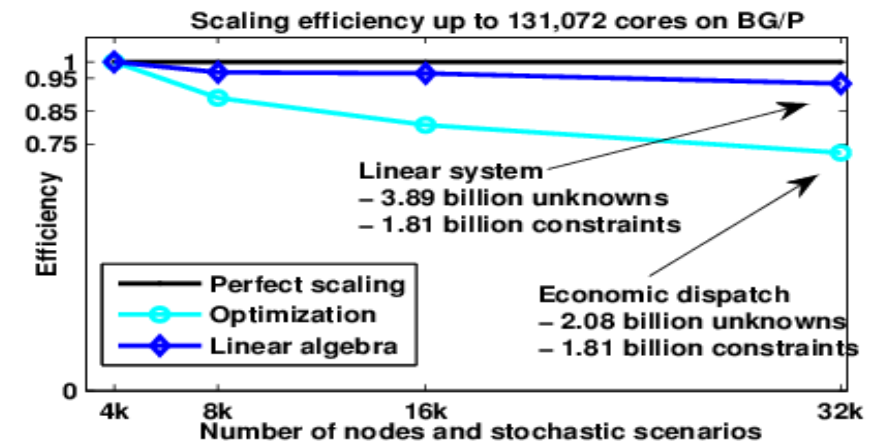- **Contingency analysis** — Lu

5 . Some Accomplishments

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27

"Real-time Optimization of Energy Systems under Uncertainty"
Mihai Anitescu, Cosmin Petra (MCS/ANL)

Scientific Objectives

- Develop *scalable algorithms* on HPC architectures for real-time electricity resource optimization under uncertainty.

- Such advances are required to solve *the stochastic energy dispatch problem*: determining optimal output of a number of electricity generation facilities, to meet the system load, while accounting for renewable energy uncertainty (variability)
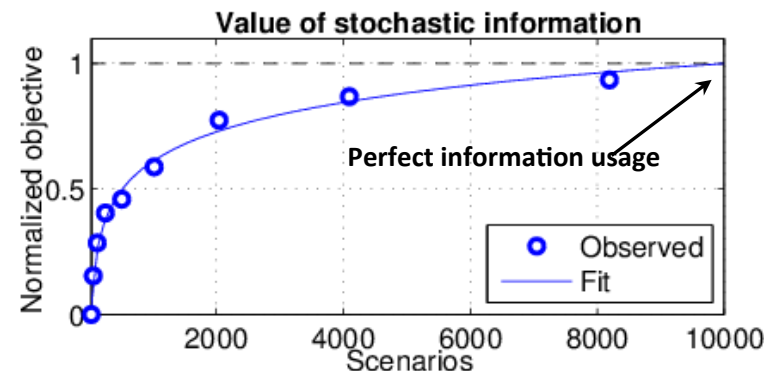

Scaling efficiency up to 131,072 cores on BG/P

Linear system
– 3.89 billion unknowns
– 1.81 billion constraints

Economic dispatch
– 2.08 billion unknowns
– 1.81 billion constraints

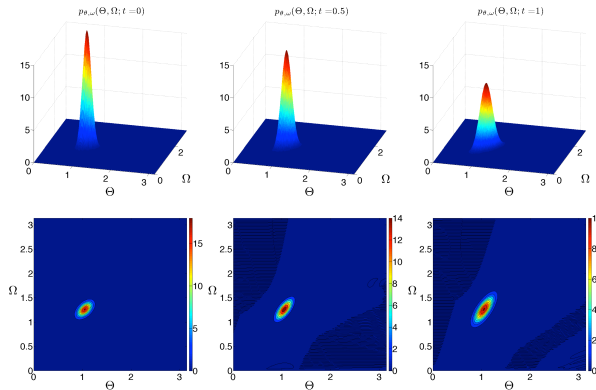Unprecedented Scalability for This Problem Class and Size

Accomplishments

- Novel *incomplete augmented sparse factorization* approach uses the cores very efficiently and fully exploits the sparsity.

- A strong scaling solution resulting in one order of magnitude reduction in time-to-solution on "Intrepid" BG/P for *Illinois energy dispatch problem with transmission and 32K wind scenario*s (4B unknowns) in operator's realtime (<1h)

- DOE INCITE Award 2012-2013 (24M core hours)

Impact

- The ability to accommodate more scenarios in **real time** gets us much closer to the ideal solution of the stochastic dispatch problem.

Value of stochastic information

Perfect information usage

Stochastic Power Grid Model

Pacific Northwest NATIONAL LABORATORY

Joint PDF of angular velocity and phase angle at three different times

Novel Ideas

PDF method with Large-Eddy-Diffusivity (LED) closure yields closed form equations for:

- **Full statistics of system states**
- **Random input parameters with arbitrary correlation (standard Fokker-Plank equation is only applicable for uncorrelated inputs)**

Power grid:

- **Probabilistic stability analysis**
- **Optimization under uncertainty**

Impact and Champions

1. **New stochastic Probability Density Function (PDF) method for generalized *Langevin* equations.**

2. **PDF method provides closed-form equation for joint PDF of *Langevin* eq. colored noise.**

3. **One of the first stochastic power-grid models.**

4. **Probabilistic stability analysis for power grid.**

Principal Investigator: Z. Huang, A.M. Tartakovsky, PNNL

Milestones/Dates/Status

	Scheduled	Actual
• Stochastic model of one generator and one load	SEP 2012	SEP 2012
• Submission to SIAM J. UQ	MAR 2013	
• Extension to multi-generators and loads	FEB 2014	FEB 2014

January 9th, 2013

Conclusions

- Complex energy systems pose an enormous number of modeling and simulation challenges.

- Computational Power will help, but it will not alone address many of the challenges.

- To demonstrate our tools on real systems, we need more system/environment modeling efforts and resources.

- This research requires sustained, multi-area, integrative thinking in mathematics.

- Increases focus on area of mathematics that were not explored up to this point and creates opportunities for FUNDAMENTAL math advances:

- Examples: resampling in stoch prog for expensive scenarios; stochastic preconditioning, fast nonlinear programming.

- We expect many more such challenges, as embodied in our MACS center.