



# The Promise of Supercomputing for Optimal Management of Energy Systems

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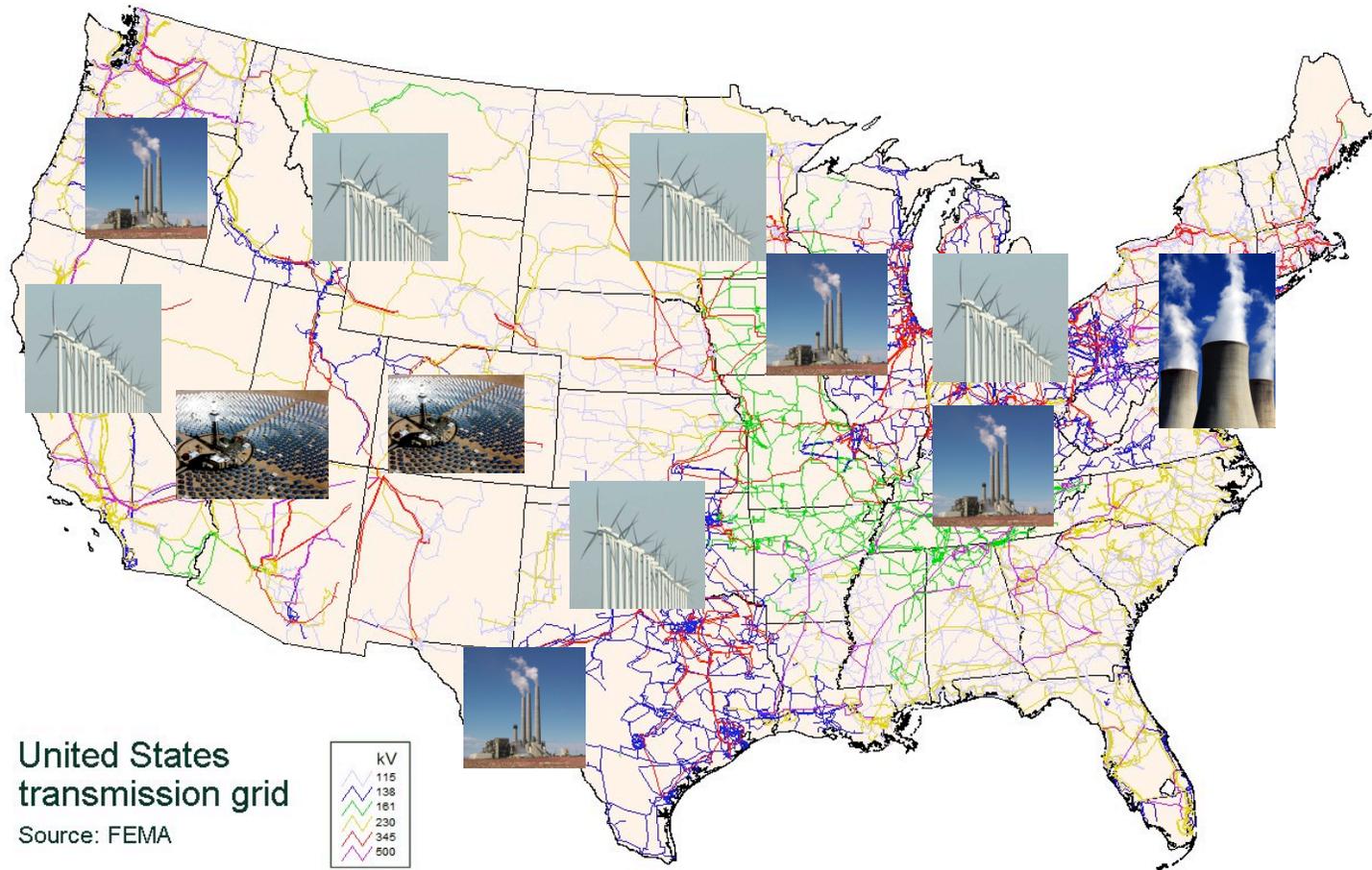
**Supercomputing 09  
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# Electricity Supply - Billions \$/Yr Market

## Challenges of the Next-Generation Power Grid

- Major Adoption of Renewable Resources (20-30%)
- Highly Decentralized Generation and Demand



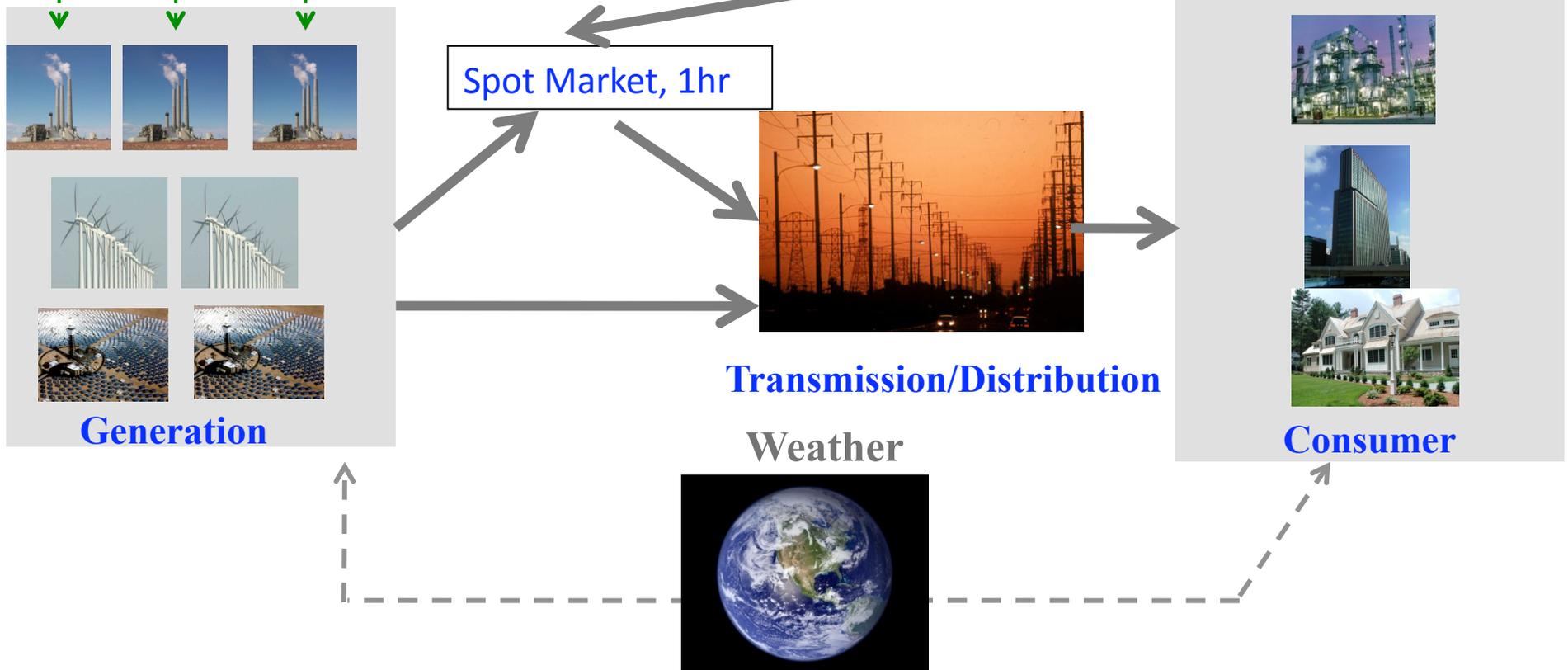
# Electricity Supply - Billions \$/Yr Market

## System Operator



ON/OFF  
Power Levels, day ahead.

Demand



**Anticipating Weather (In 1hr, 1 day, at 1km) Minimizes Reserve Cost**

# Objective 1: Uncertainty quantification in weather forecast: A test case with real data

- Importance in Energy Systems Management
  - Weather influences both energy supply (wind/solar/thermal) and demand
  - Accurate weather/climate forecast leads to an efficient proactive resource management (reduces needed reserves and cost, though not consumption directly).
- Weather forecasting at the renewable energy (RE) system scale (1km) is a grand challenge:
  - very large-system, difficult to simulate
  - Chaotic,
  - incomplete/missing physics
  - unknown initial conditions, uncertain forcings
  - Lack of information makes deterministic prediction impossible, we must quantify and compute uncertainty in weather forecast (i.e. its probability distribution).
- **Objective 1: Is there hope of predicting the probability **distribution** of weather at RE scale **operationally** ? (24 hour ahead in 1 hour at 1 km)?**



## Objective 2: What is the economic impact of using weather (and demand/pricing) forecast in energy management

- The impact strongly depends on the decision system and of the way it accounts for risk.
- We posit the decision problem under uncertainty as a stochastic programming problem.
- Note that we do not expect to reduce consumption, (that is design, not management), but we expect to be able to reduce cost, and implicitly
  - Reduce the risk of not meeting demand
  - Reduce the peak requirements on power grid and this increase resilience by optimally answering to the appropriate incentives (such as electricity pricing).
- Question 2: For realistic Independent System Operator Problems, Building Systems, and Photovoltaic Systems, what are the expected cost reductions?



# Forecast and Uncertainty

# Uncertainty in dynamical systems: 1. Data

- Assume a time-discretized process with imperfect initial state and forcing information and noisy measurements.

The dynamic model is depicted as for  $k = 0, \dots, K$

$$\mathbf{x}_k^{in} = M(\mathbf{x}_{k-1}^{in}) + W_k, \quad (1)$$

$$\mathbf{z}_k^{obs} = H(\mathbf{x}_k^{in}) + V_k, \quad (2)$$

where

$$W_k \approx N(\bar{\mathbf{x}}_k, Q_k^{-1})$$

and

$$V_k \approx N(\mathbf{0}, R_k^{-1}).$$

We want find  $D(\mathbf{x}_0^{in}, \dots, \mathbf{x}_K^{in})$ 's mean and variance.

## Uncertainty in dynamical systems: 2. the posterior.

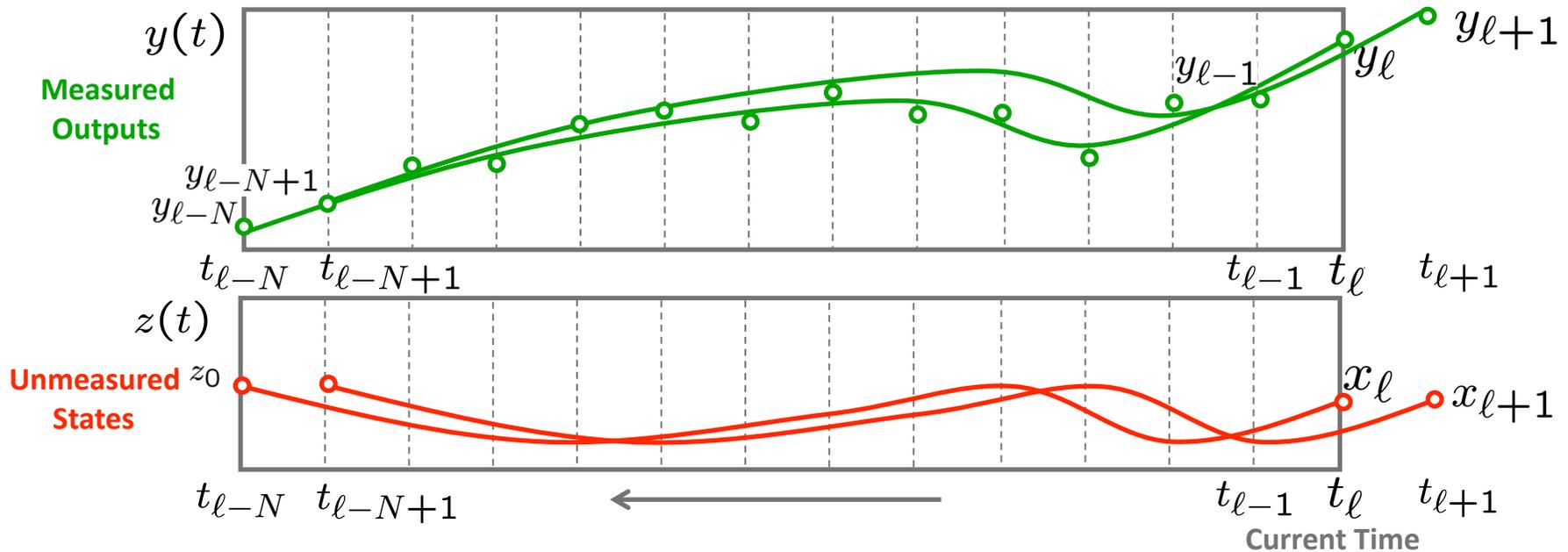
- Under the typical 4D Var assumptions (normality of noise and input and independence) we can write down the posterior ...

$$P(\mathbf{x}_k^{in}, \mathbf{x}_{k-1}^{in}, \dots, \mathbf{x}_0^{in} | z_0^{obs}, z_1^{obs}, z_2^{obs}, \dots, z_k^{obs}) = C_k \tilde{C}_k \frac{\exp\left(-\frac{1}{2}f(\mathbf{X}^{in}, \mathbf{Z}^{obs})\right)}{P(\mathbf{Z}^{obs})}.$$

$$f(\mathbf{X}^{in}, \mathbf{Z}^{obs}) = \sum_{i=0}^k (\mathbf{x}_i^{in} - \bar{\mathbf{x}}_i - \tilde{\mathbf{y}}(t_{i-1}, \mathbf{x}_{i-1}^{in}))^T Q_i^{-1} (\mathbf{x}_i^{in} - \bar{\mathbf{x}}_i - \tilde{\mathbf{y}}(t_{i-1}, \mathbf{x}_{i-1}^{in})) \\ + \sum_{i=0}^k (z_i^{obs} - h_i(\tilde{\mathbf{y}}^\perp(t_i, \mathbf{x}_i^{in})))^T R_i^{-1} (z_i^{obs} - h_i(\tilde{\mathbf{y}}^\perp(t_i, \mathbf{x}_i^{in})))$$

- A very difficult distribution to sample from.
- Solution: first, find the best estimate of the state.
- Then, approximate the prior covariance by an ergodic/Gaussian Process method.

# Step 1: Moving Horizon Best State Estimation



$$\min_{p(t), z_0} \sum (y(t_k) - \underline{y_{l-k+N}})^T V_y^{-1} (y(t_k) - \underline{y_{l-k+N}})$$

$$\min_{p(t), z_0} \sum (y(t_k) - y_{l-k+N+1})^T V_y^{-1} (y(t_k) - y_{l-k+N+1})$$

**WRF Model**

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

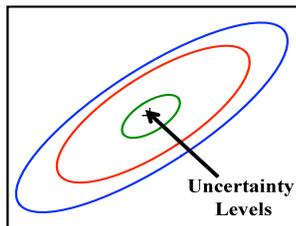
$$y(t) = \mathbf{g}(z(t), p(t), u(t))$$

$$z(0) = z_0 \text{ Uncertain}$$

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

$$y(t) = \mathbf{g}(z(t), p(t), u(t))$$

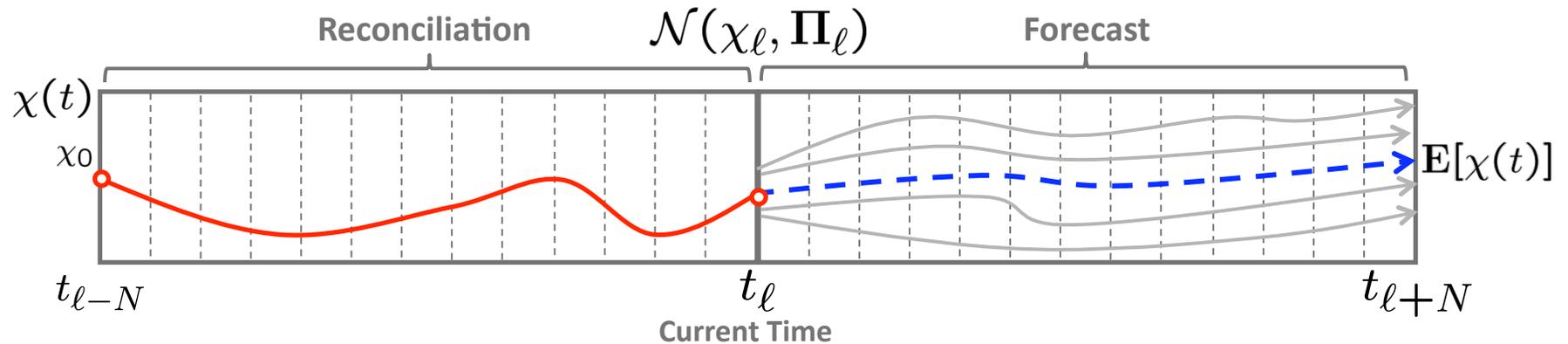
$$z(0) = z_0$$



$\Pi_\ell \rightarrow 0$

**Uncertainty in Current State  $x_\ell$**   
**Needed To Quantify Future Forecast**

## Step 2: Estimate the prior covariance matrix.



- Use some form of an ergodic hypothesis. Take  $d_{ij} \in \mathbb{R}^{N \times (2 \times 30 \text{days})}$ ,

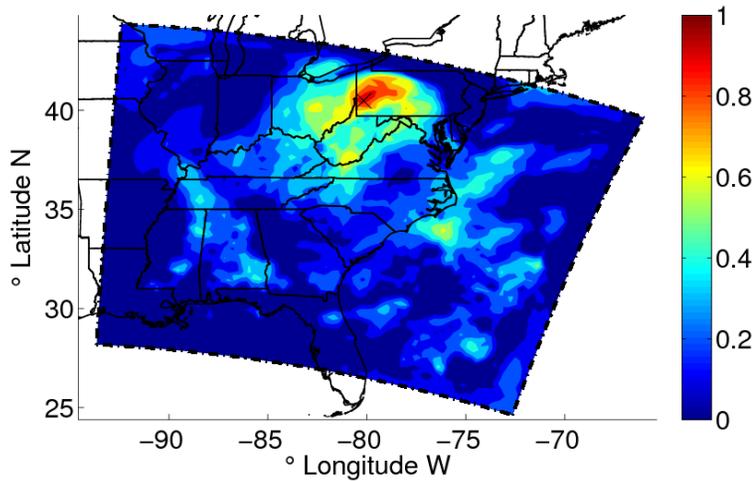
$$\mathbf{V}_{ik} \approx \mathbf{d} \mathbf{d}^T = \sum_j d_{ij} d_{kj}^T = \epsilon_i \cdot \epsilon_k = \begin{bmatrix} \epsilon_0 \cdot \epsilon_0 & \epsilon_1 \cdot \epsilon_0 & \cdots & \epsilon_n \cdot \epsilon_0 \\ \epsilon_0 \cdot \epsilon_1 & \epsilon_1 \cdot \epsilon_1 & \cdots & \epsilon_n \cdot \epsilon_1 \\ \cdots & \cdots & \cdots & \cdots \\ \epsilon_0 \cdot \epsilon_n & \epsilon_1 \cdot \epsilon_n & \cdots & \epsilon_n \cdot \epsilon_n \end{bmatrix}, \quad \mathbf{C}_{ik} = \frac{\epsilon_i \cdot \epsilon_k}{|\epsilon_i| |\epsilon_k|}.$$

- “Guess” the diagonal of the variance matrix

## Step 2 b: Fit to a Gaussian Process.

### Covariance Matrix is Huge and low rank ( $10^6 \times 10^6$ ) But ...

- Spatial Correlations Decay Exponentially *Constantinescu, et.al., 2007*
- Covariance Can be Approximated Using Gaussian Kernels *Zavala, Constantinescu & A, 2009*



$$\Pi_{:,i,j} = \exp \left( -\frac{(x_j - x_i)^2 + (y_j - y_i)^2}{L_H^2} - \frac{(z_j - z_i)^2}{L_V^2} \right)$$

# Ensemble Forecast Approach

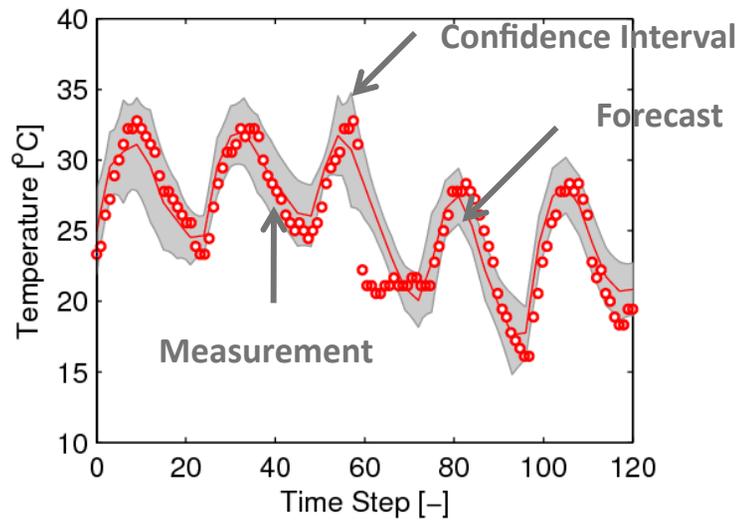
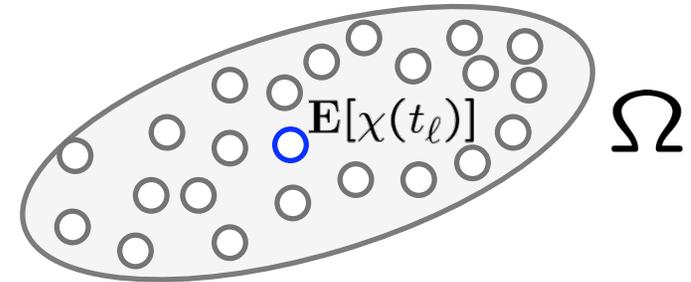
## Ensemble Forecast Approach – Use WRF as Black-Box

Sample Prior and Propagate Samples of Posterior Through Model

$$Y_{[i,j]} := \chi_i(t_{\ell+j}) = \underbrace{\mathcal{M}(\mathcal{M}(\dots\mathcal{M}(\chi_i(t_{\ell}))))}_{j \text{ times}}$$

$$E[Y] \approx \bar{Y} := \frac{1}{NS} \sum_{i=1}^{NS} Y_{[i,:]}$$

$$V \approx \frac{1}{NS - 1} \sum_{i=1}^{NS} (Y_{[i,:]} - \bar{Y})(Y_{[i,:]} - \bar{Y})^T$$



Hours (August 1<sup>st</sup>-5<sup>th</sup>)

**Validation Results, Pittsburgh Area 2006**

5 Day Forecast and +/- 3s Intervals

Building applications

# Uncertainty quantification and forecast using WRF

- WRF model:  $x^{t_F} = \mathcal{M}_{t_0 \rightarrow t_F}(x^{t_0})$

- Uncertainties in the initial conditions:  $x_i^{t_0} = x_{\text{NARR}} + \mathbf{L}\xi_i$

$$\xi_i \sim \mathcal{N}(0, I), \quad i \in [1, N_S], \quad \mathbf{L}\mathbf{L}^T = \mathbf{P}, \quad \mathbf{C}_{ij} = \frac{\mathbf{P}_{ij}}{\sqrt{\mathbf{P}_{ii}\mathbf{P}_{jj}}}$$

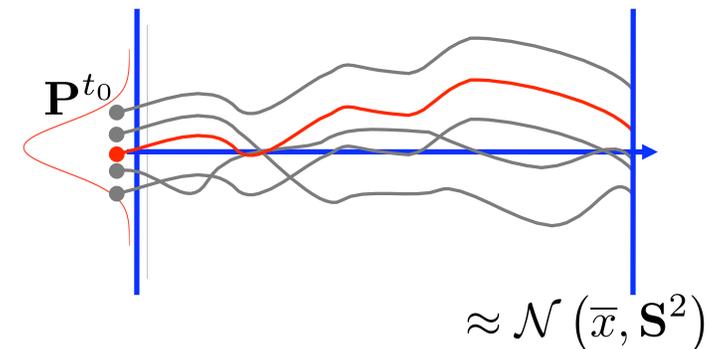
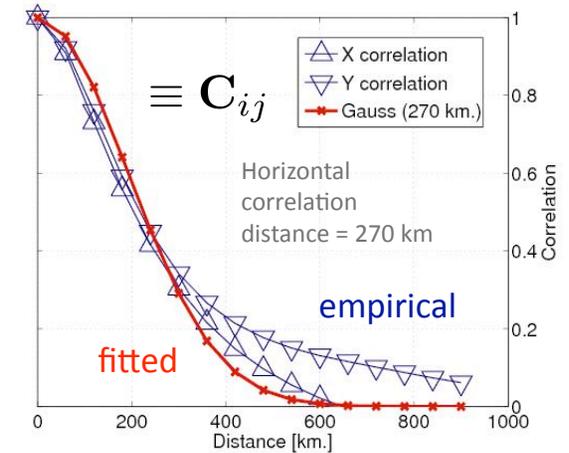
- Evolution of uncertainties through WRF:

$$x_i^{t_F} = \mathcal{M}_{t_0 \rightarrow t_F}(x_i^{t_0}) + \eta_i(t)$$

$$x_i^{t_0} \sim \mathcal{N}(x_{\text{NARR}}, \mathbf{P}^{t_0}), \quad \eta_i \sim \mathcal{N}(0, \mathbf{Q}), \quad i \in [1, N_S]$$

- Uncertainty at the final time:  $x_i^{t_F} \sim \mathcal{N}(\bar{x}, \mathbf{S}^2)$

$$\bar{x} = \frac{1}{N_S} \sum_{i=1}^{N_S} x_i \quad \mathbf{S}^2 = \frac{1}{N_S - 1} \sum_{i=1}^{N_S} (x_i - \bar{x})(x_i - \bar{x})^T$$



# Closed loop simulation using WRF

- 24-hour simulation window – restart from assimilated solution (NARR) every 12 hours

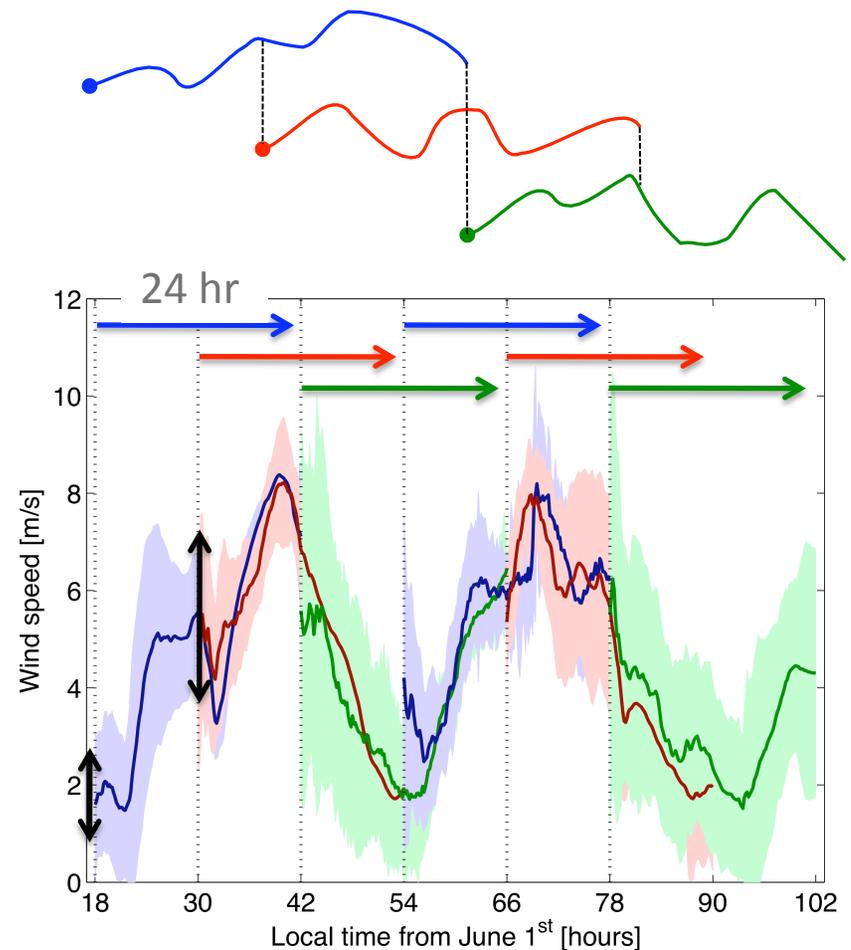
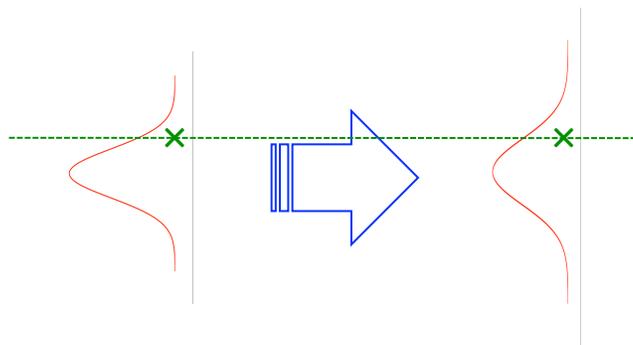
- Restart ensemble with adjusted spread based on error estimates:

$$x_i \leftarrow \bar{x} + \gamma (x_i - \bar{x}), \quad i \in [1, N_S]$$

$$\gamma = \max(1, \min(\gamma_\sigma, 4))$$

$$\gamma_\sigma = \text{mean}_{U,V,T|k=1\dots 5} \left( \frac{|x_{\text{NARR}} - \bar{x}|}{\sigma} \right)$$

- Error is underestimated: increase uncertainty

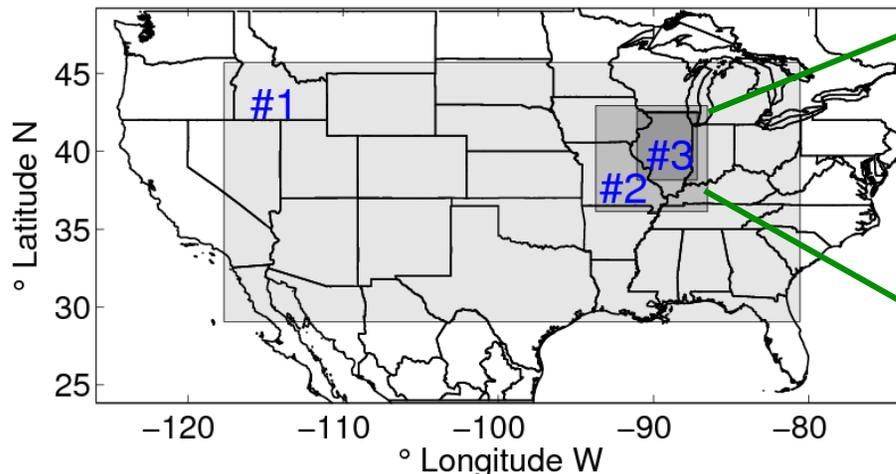




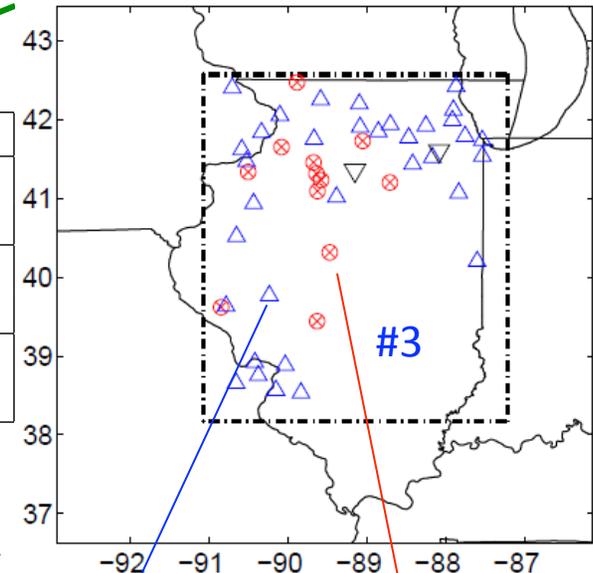
# Implementation and Estimation of Necessary Computational Resources

# Ensemble forecast and uncertainty quantification with WRF on Jazz

- Computational domain setup



Grid/Size
#1 - 32 km <sup>2</sup> 130 × 60
#2 - 6 km <sup>2</sup> 126 × 121
#3 - 2 km <sup>2</sup> 202 × 232



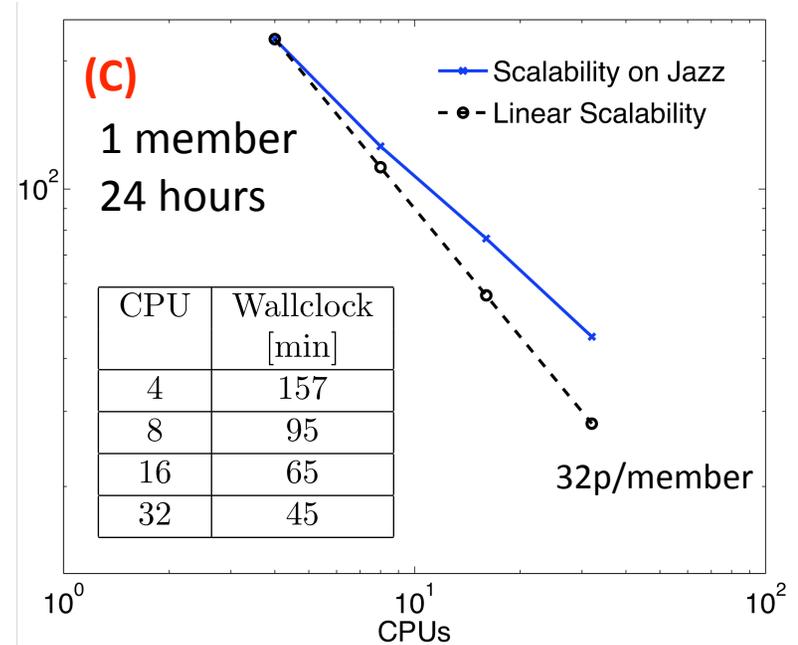
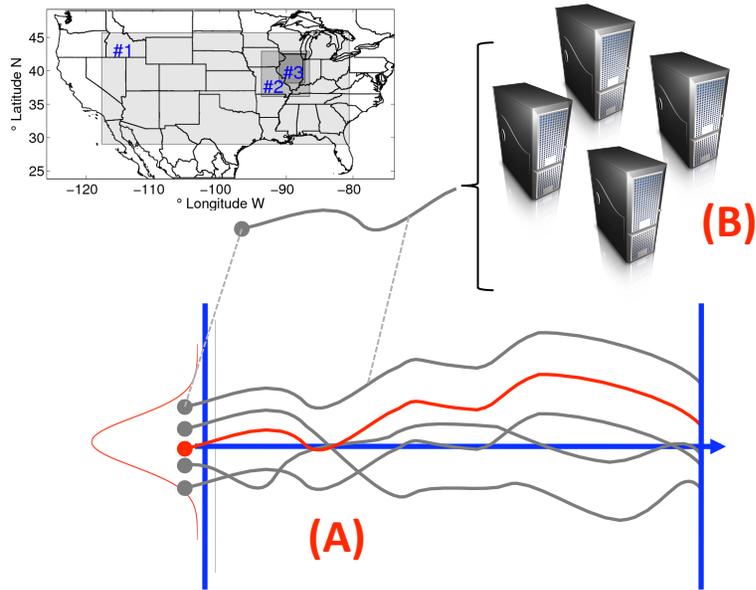
- Jazz:** 350 nodes; Intel Pentium IV Xeon@ 2.4GHz; 1 or 2 Gb RAM per node; Myrinet 2000 @ 0.25 GB/s, 6-8 μsec latency

- 24 hours** [simulation time] in **one hour** [real time] on Jazz with 30 members on **500 processors**;



# WRF scalability on Jazz

- Two-level parallelization scheme – very scalable: **(A)** realizations are independent, **(B)** each is parallelized, and **(C)** explicit



- 24 hours [simulation time] -> one hour [real time] on Jazz with 30 members; [2 km]; (almost) linear scalability with area **(C)**

- ✓ Illinois [2km]: 500 processors
- US [2 km]: ~50,000 processors
- US [1 km]: ~400,000 processors

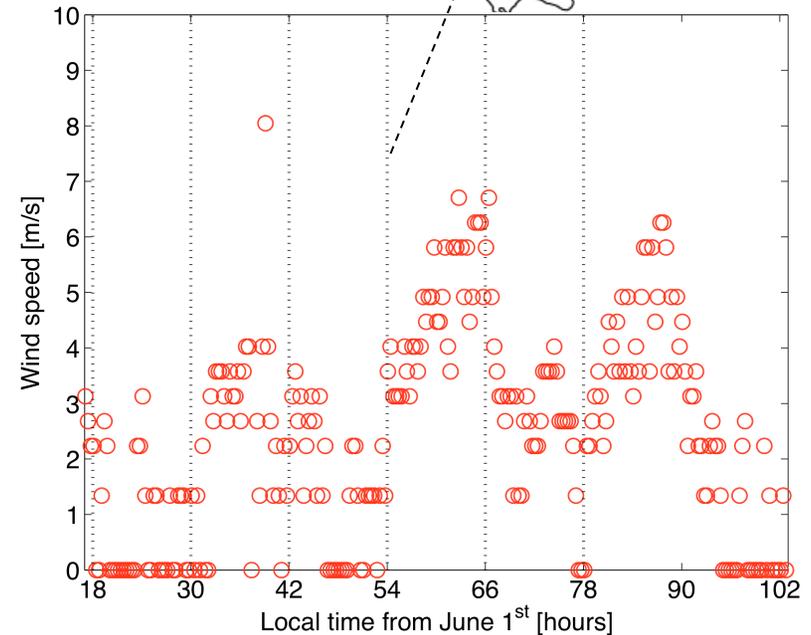
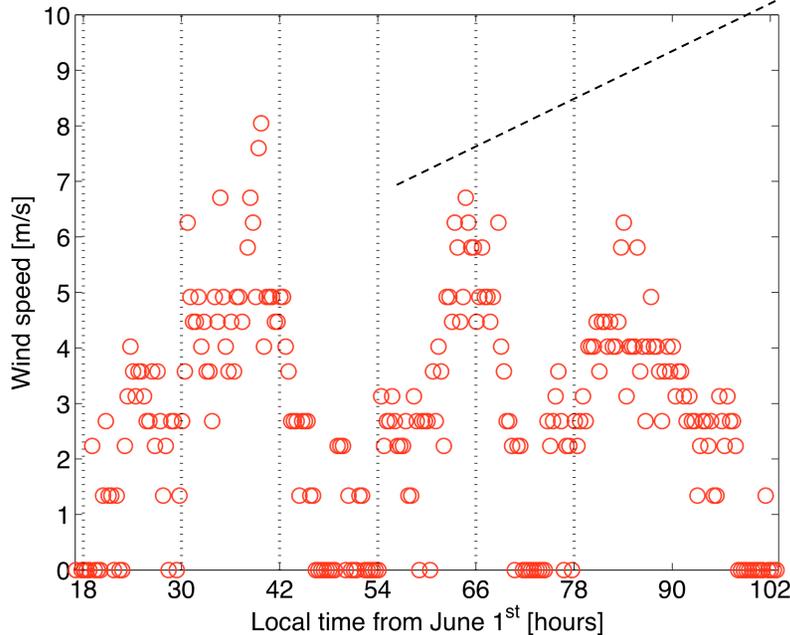
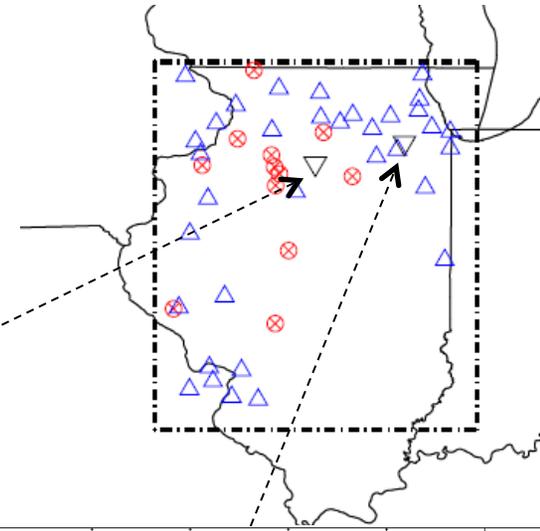




# Validation of the results

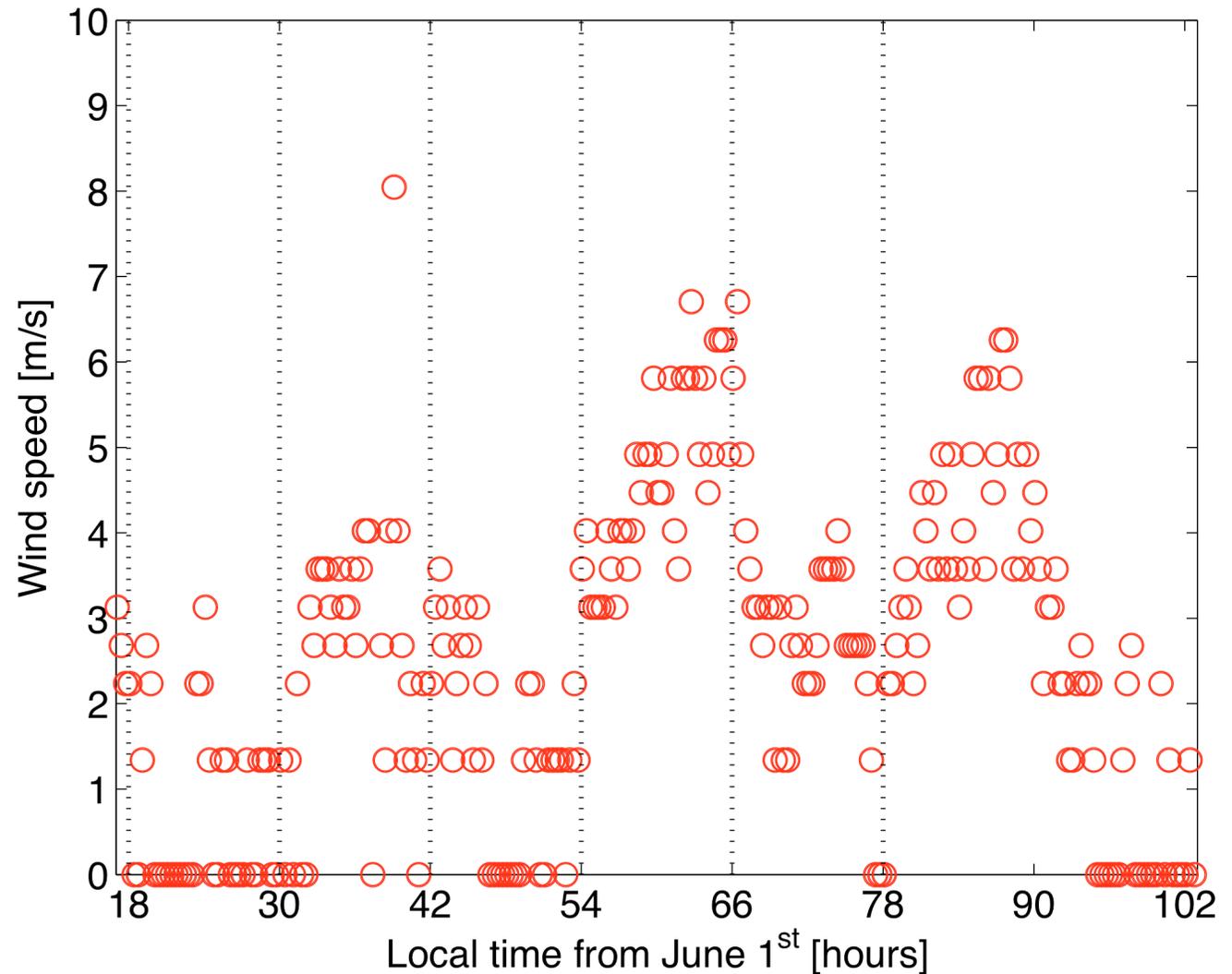
# Wind power measurements and windmill locations

- Wind turbine locations and weather stations locations in Illinois:
- Real wind and temperature measurements for hindcast (June 2006) ~every 20 min.
- Real wind power measurements for Chicago and Peru, IL:



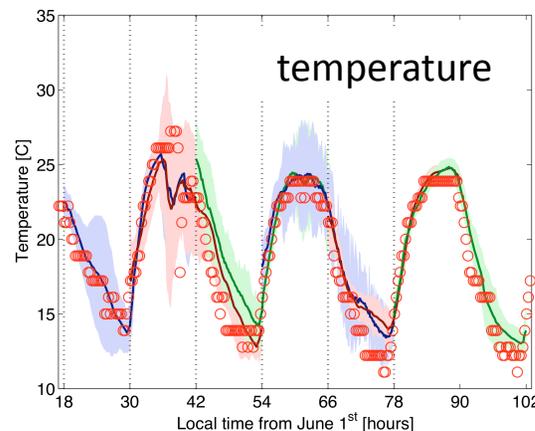
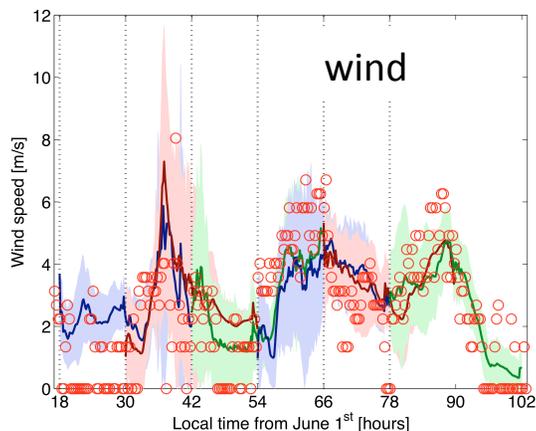
# Wind power is difficult to predict

- Wind power measurements for Chicago
- Deterministic prediction; a new one started every 12 hours
- Forecast with uncertainty

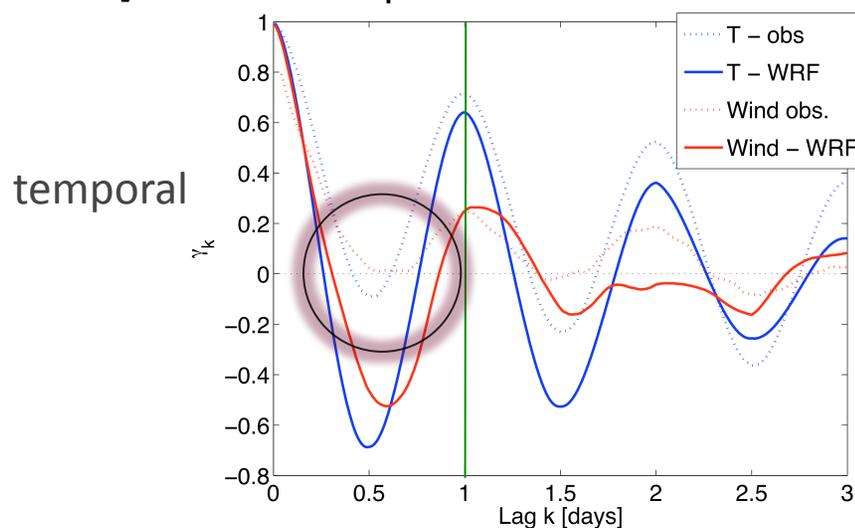
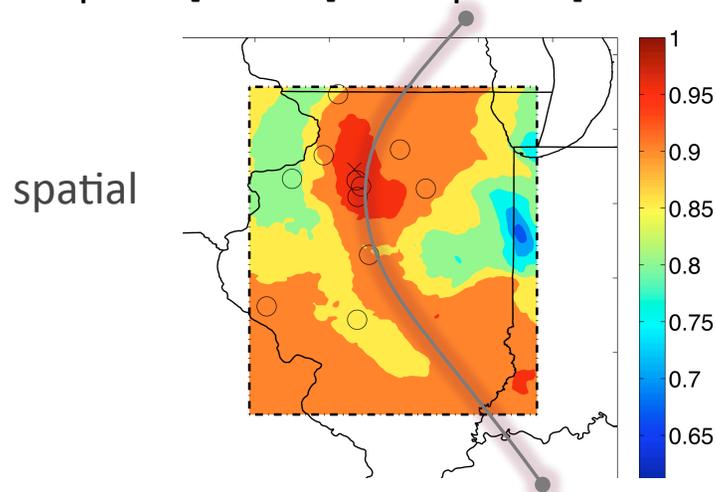


# Validation of the wind/temperature forecast and uncertainty

- Wind/temperature validation of uncertainty estimates with real measurements



- Temporal [trends] and spatial [similar outcomes] correlations provide additional info





# Optimization under Uncertainty by Stochastic Programming

# Rolling Horizon Optimization

**Benefits:** Accommodate Forecasts, Constraint Handling, Financial Objectives, Complex Models

**Deterministic**

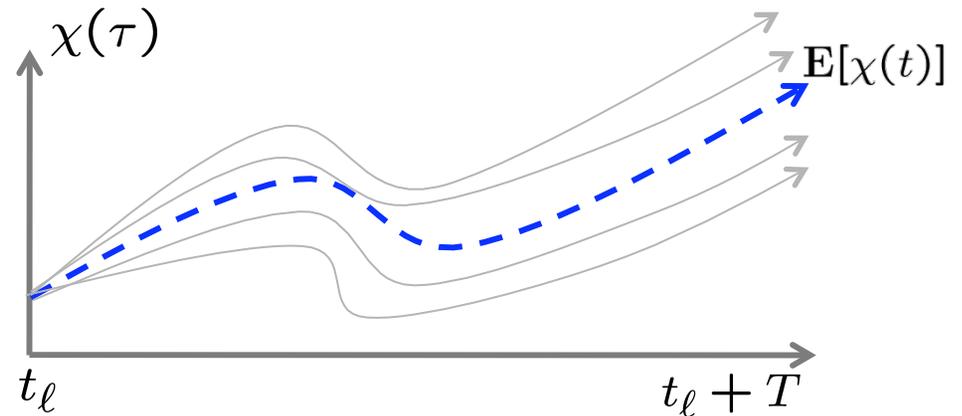
$$\min_{u(t)} \int_{t_\ell}^{t_\ell+N} \varphi(z(t), y(t), u(t), \mathbf{E}[\chi(t)]) dt$$

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

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

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

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

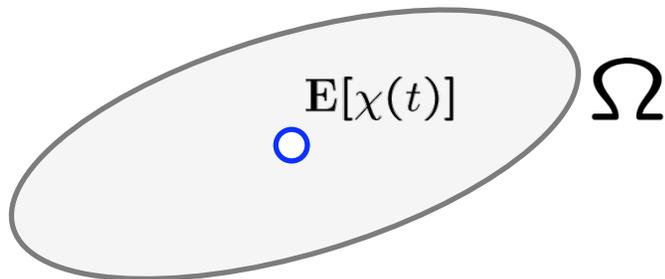


**Stochastic**

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

$$\left. \begin{aligned} \frac{dz}{dt} &= \mathbf{f}(z(t), y(t), u(t), \chi(t)) \\ 0 &= \mathbf{g}(z(t), y(t), u(t), \chi(t)) \\ 0 &\geq \mathbf{h}(z(t), y(t), u(t), \chi(t)) \end{aligned} \right\} \forall \chi(t) \in \Omega$$

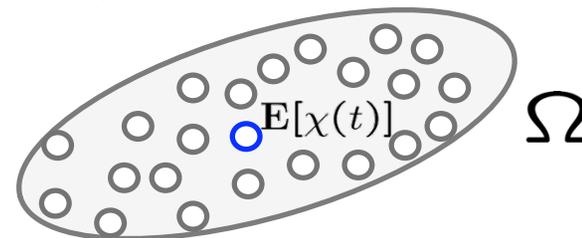
$$z(0) = x_\ell$$



Complexity (Solution Time)

1,000 – 10,000 Differential-Algebraic Equations

100-1000 Scenarios

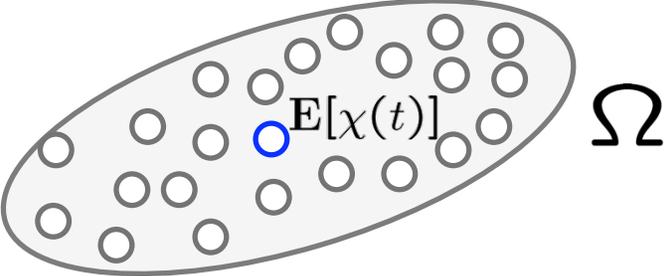


# Stochastic Rolling Horizon Optimization

## Solution Strategies

- **Dynamic Programming, Taylor Series:** Handling Constraints and Nonlinearity Cumbersome
- **Polynomial Chaos:** Dense Optimization, Multivariable Quadrature
- **Sample Average Approximation (SAA):** Sparse Optimization, Constraints, General Framework

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

$$\left. \begin{aligned} \frac{dz}{dt} &= \mathbf{f}(z(t), y(t), u(t), \chi(t)) \\ 0 &= \mathbf{g}(z(t), y(t), u(t), \chi(t)) \\ 0 &\geq \mathbf{h}(z(t), y(t), u(t), \chi(t)) \\ z(0) &= x_\ell \end{aligned} \right\} \forall \chi(t) \in \Omega$$


The diagram shows an oval representing the domain  $\Omega$ . Inside the oval, there are several small circles representing random variables  $\chi(t)$ . One circle is highlighted in blue and labeled  $\mathbf{E}[\chi(t)]$ , representing the expected value of the random variable.

## Nonlinear Programming: Exploit Fine and Coarse Structures at Linear Algebra Level

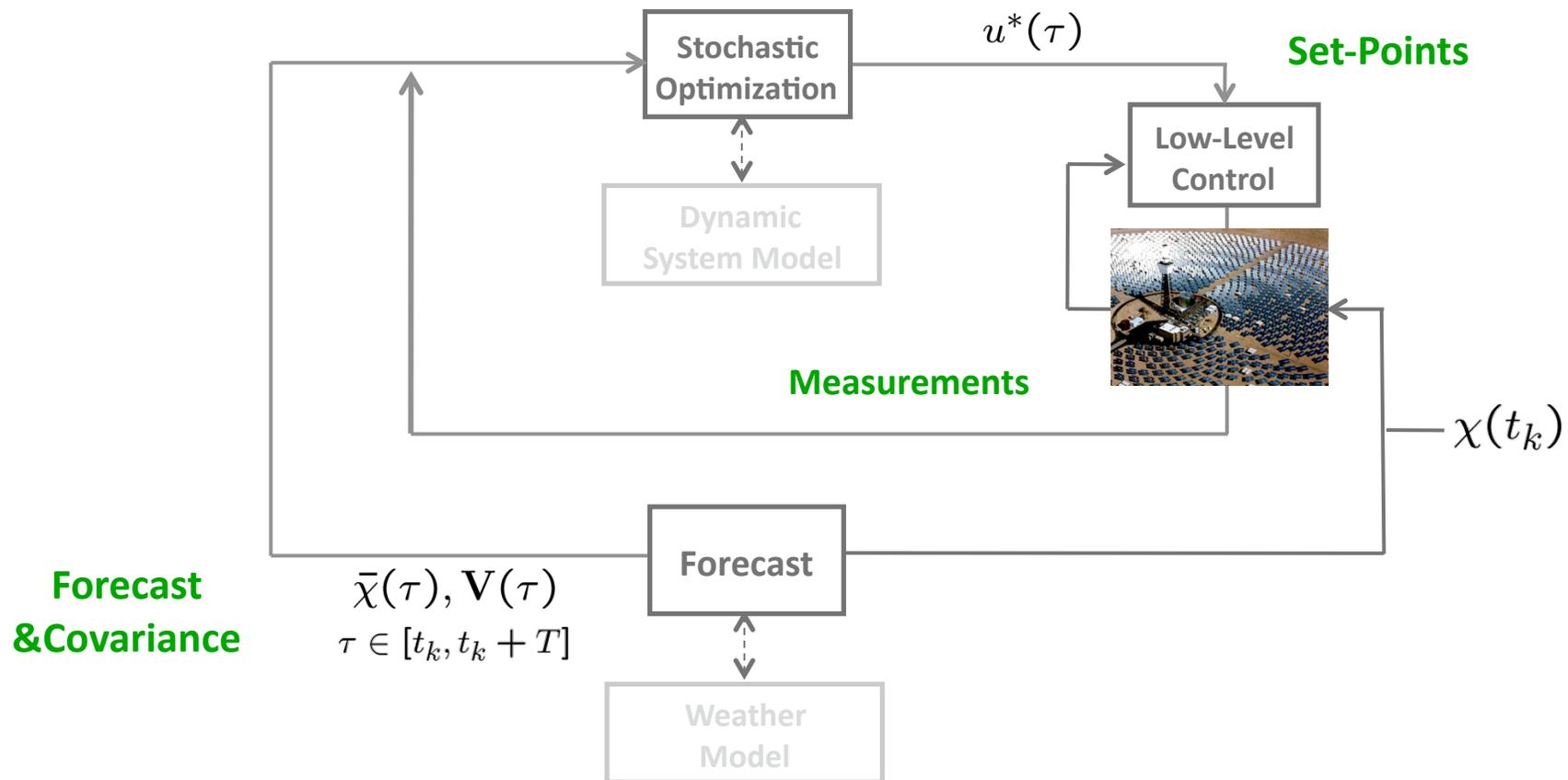
$$\min_{\mathbf{u}} \frac{1}{S} \sum_{k=1}^S \varphi(z_k, y_k, \mathbf{u}, \chi_k)$$

$$\text{s.t. } \begin{aligned} \mathbf{c}(z_k, y_k, \mathbf{u}, \chi_k) &= 0 \\ \mathbf{h}(z_k, y_k, \mathbf{u}, \chi_k) &\leq 0 \\ k &= 1, \dots, S \end{aligned}$$

$$\begin{bmatrix} \mathbf{K}_1 & & & Q_1 \\ & \mathbf{K}_2 & & Q_2 \\ & & \dots & \vdots \\ & & & \mathbf{K}_S & Q_S \\ Q_1^T & Q_2^T & \dots & Q_S^T & D_{\mathbf{u}} \end{bmatrix} \begin{bmatrix} \Delta s_1 \\ \Delta s_2 \\ \vdots \\ \Delta s_S \\ \Delta \mathbf{u} \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_S \\ r_{\mathbf{u}} \end{bmatrix}$$



# Basic Operational Setting



**Quantifying Uncertainty Key Enabler**



# Digression about the Suitability of Stochastic Programming for Energy Systems w Renewables

## SAA Stochastic Programming Approximation.

$$\begin{aligned} \min_{\mathbf{u}} \quad & \frac{1}{S} \sum_{k=1}^S \varphi(z_k, y_k, \mathbf{u}, \chi_k) \\ \text{s.t.} \quad & \mathbf{c}(z_k, y_k, \mathbf{u}, \chi_k) = 0 \\ & \mathbf{h}(z_k, y_k, \mathbf{u}, \chi_k) \leq 0 \\ & k = 1, \dots, S \end{aligned}$$

- One weakness of stochastic programming is that it assumes a distribution is given. In most applications of interest, the distribution has to be modeled from data using some knowledge of the application.
- If the uncertainty originates in weather forecast, there is a strong empirical and theoretical basis to create the distribution, or, at least to sample from it.
- To our knowledge this is the first time even a moderately complex energy system was managed using stochastic programming with real and **operational** weather uncertainty.



# Sequential Decision Making Under Uncertainty: Stochastic Dynamic Programming

- Stoc DP is the most distinguished framework, though rarely (ever ?) approached from HPC.
- Example: In Production and Inventory Planning:

– Recursive Cost at the beginning of stage  $t$  :

$$f_t(I, \omega_{1:(t-1)}) = \min_{\substack{\max(0, d_t - I) \leq x \\ \min(C, d_t + B - I)}} E_t \left[ c_t(x, \omega_t) + f_{t+1}(I + x - d_t, \omega_{1:t}) \right]$$

- **Functional approximation in an  $T \times D$  ( $D \sim 1000s$ ) dimensional space !!!** It suffers from the curse of dimensionality ... but so does sampling.
- Could HPC make inroads? We believe so but development cost restricts us to rolling horizon.





# Applications

# App 1: The operator's (ISO-IL) problem Unit commitment with wind power generation

[E.M. Constantinescu V. Zavala, M. Anitescu, M. Rocklin, S. Lee]

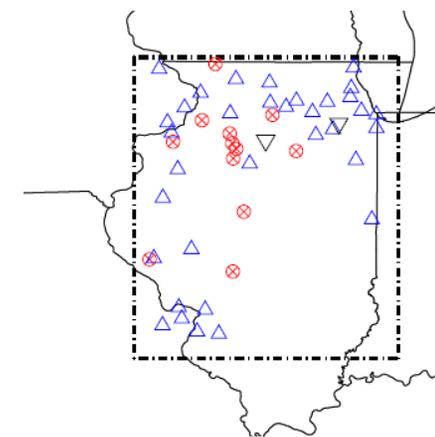
- Deterministic problem:

$$\begin{aligned}
 & \min_{p_{j,k}, \bar{p}_{j,k}, \dots} \sum_{j \in \mathcal{N}} \sum_{k \in \mathcal{T}} c_{j,k}^p + c_{j,k}^u + c_{j,k}^d \\
 & \text{s.t.} \quad \sum_{j \in \mathcal{N}} p_{j,k} + \sum_{j \in \mathcal{N}_{wind}} \mathbb{E} \{ p_{j,k}^{wind} \} = D_k \\
 & \quad \sum_{j \in \mathcal{N}} \bar{p}_{j,k} + \sum_{j \in \mathcal{N}_{wind}} \mathbb{E} \{ p_{j,k}^{wind} \} \geq D_k + R_k \\
 & \quad \dots
 \end{aligned}$$



- Stochastic program formulation:

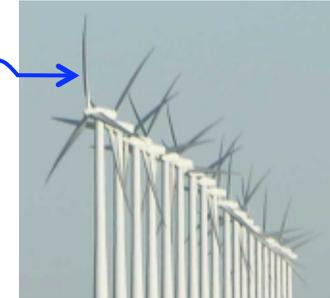
$$\begin{aligned}
 & \min_{p_{s,j,k}, \bar{p}_{s,j,k}, \dots} \frac{1}{N_S} \sum_{s \in \mathcal{S}} \left( \sum_{j \in \mathcal{N}} \sum_{k \in \mathcal{T}} c_{s,j,k}^p + c_{j,k}^u + c_{j,k}^d \right) \\
 & \text{s.t.} \quad \sum_{j \in \mathcal{N}} p_{s,j,k} + \sum_{j \in \mathcal{N}_{wind}} p_{s,j,k}^{wind} = D_k \\
 & \quad \sum_{j \in \mathcal{N}} \bar{p}_{s,j,k} + \sum_{j \in \mathcal{N}_{wind}} p_{s,j,k}^{wind} \geq D_k + R_k \\
 & \quad \dots
 \end{aligned}$$



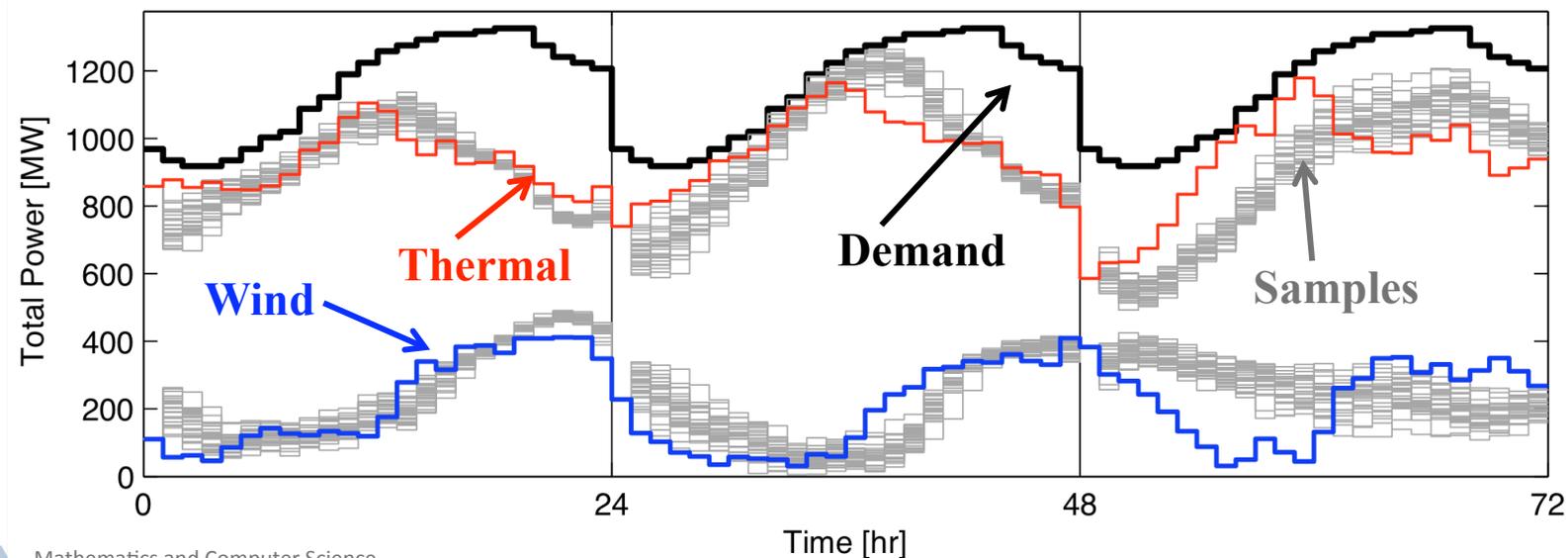
# Wind power forecast and stochastic programming

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

wind power

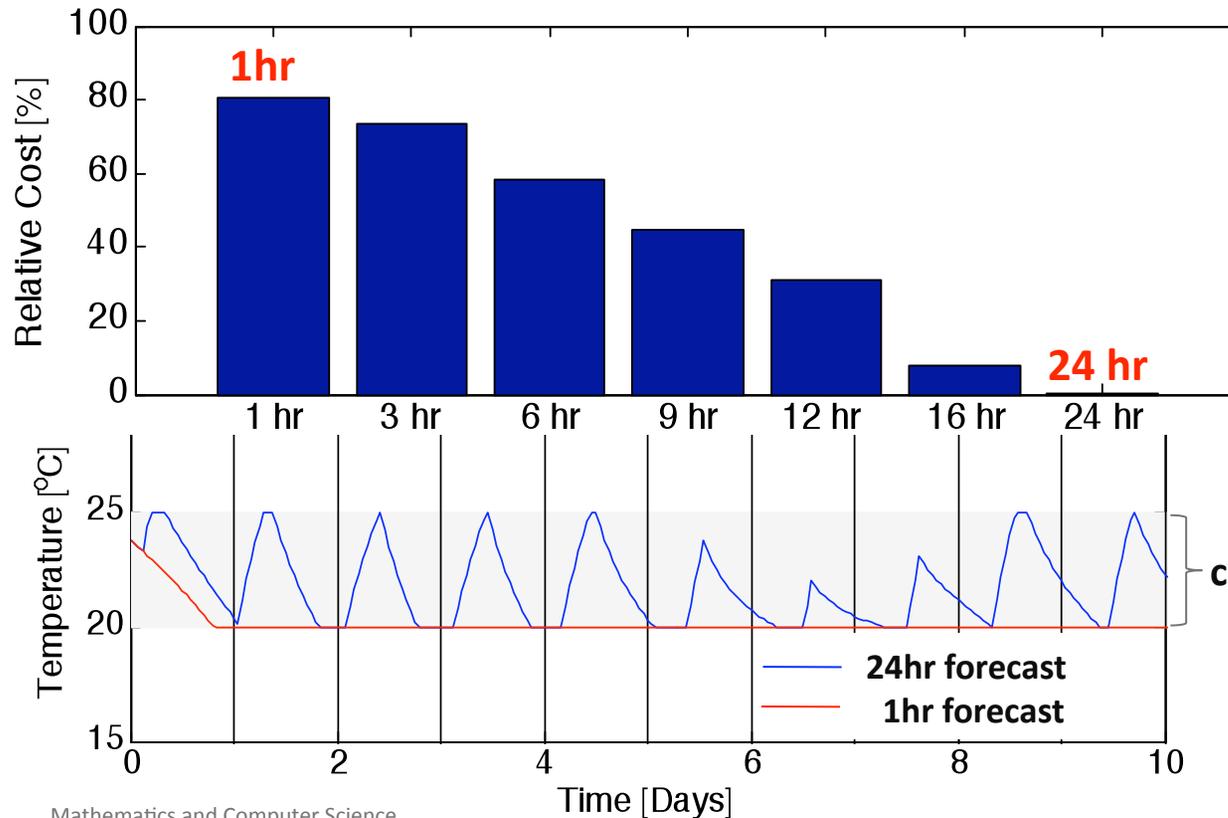


- Full integration with 10 thermal units to meet demands. Consider dynamics of start-up, shutdown, set-point changes
- The solution is only 1% more expensive than the one with exact information.

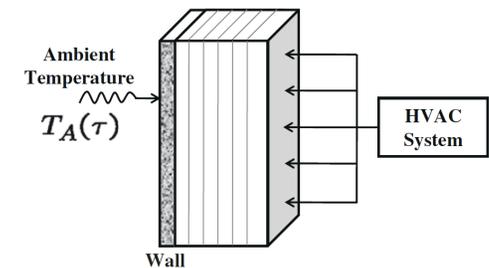
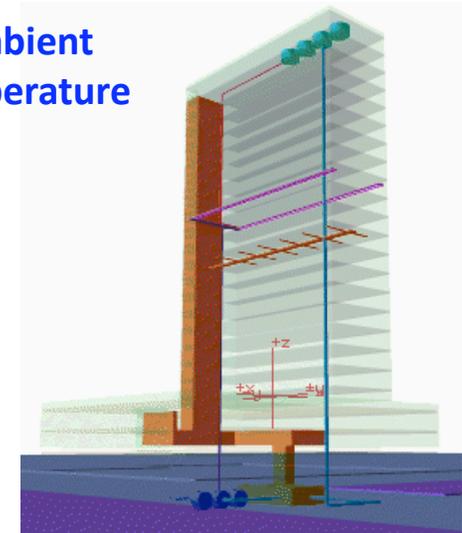


# Ap2: Thermal management of building in Pittsburgh

- Minimize annual heating and cooling costs
- Time-varying electricity prices (peak/off-peak)
- Forecast with uncertainty leads to 20-80% cost reduction (insulation quality)



ambient temperature

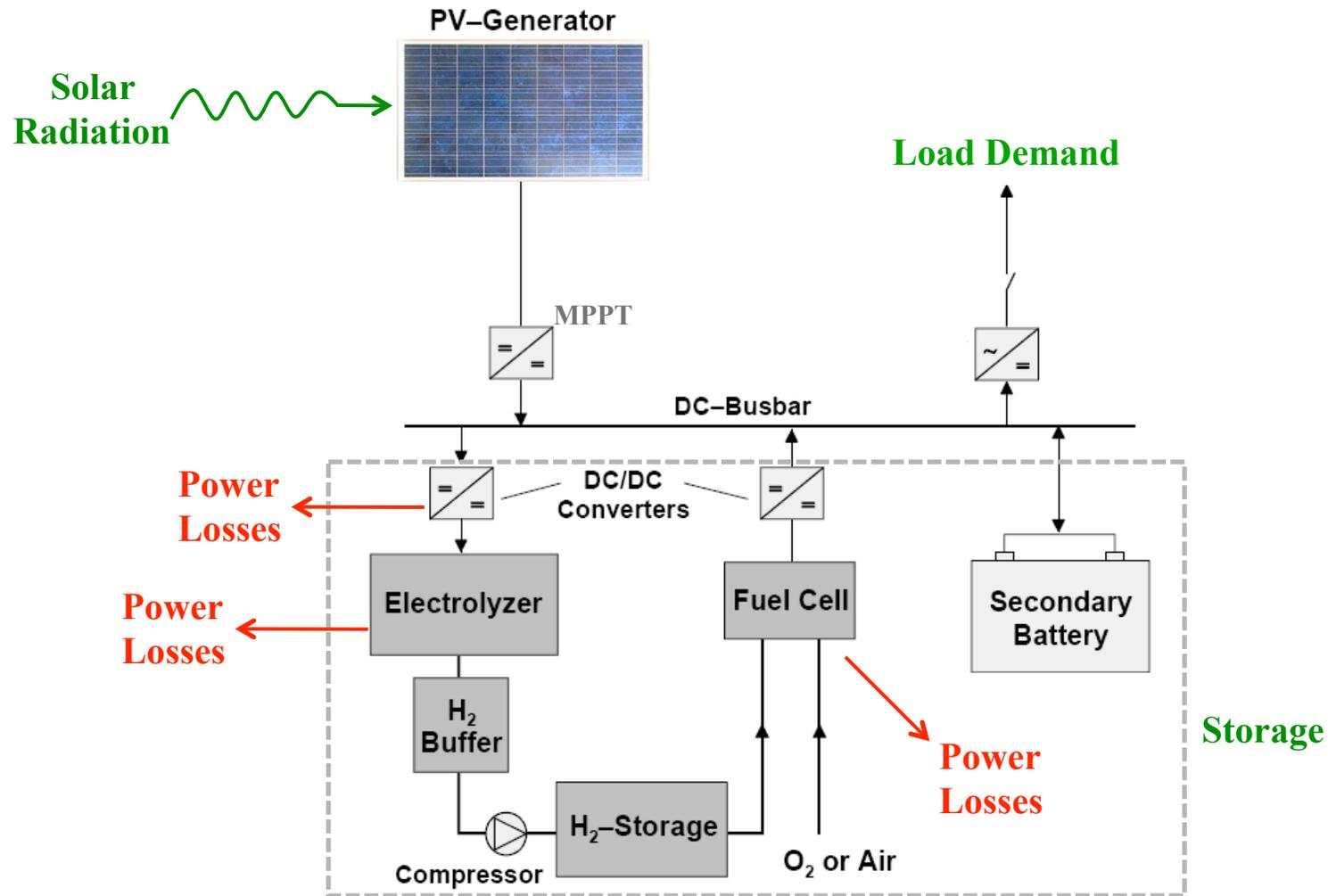


comfort zone

[Zavala, Constantinescu, Krause, and Anitescu, 2009]



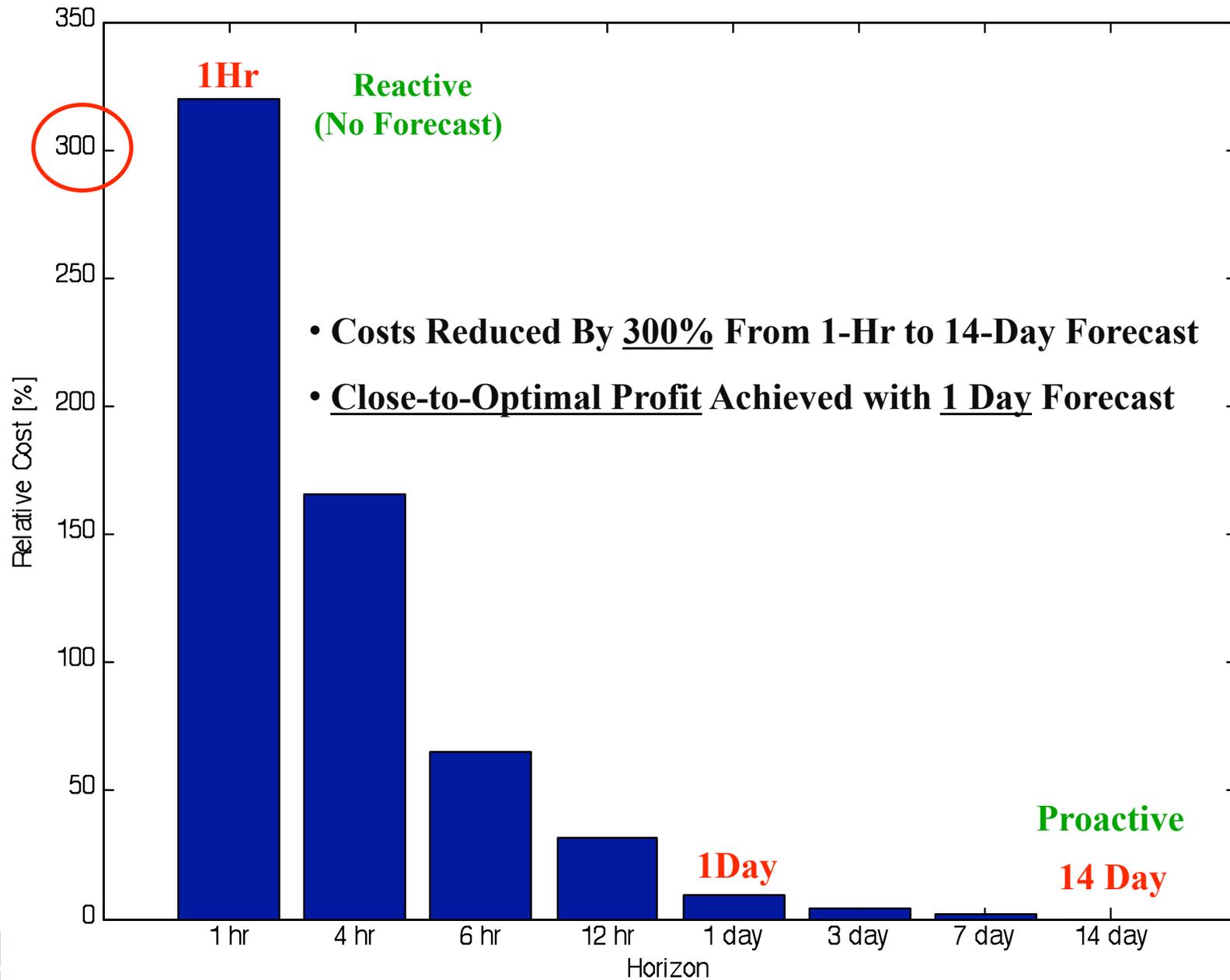
# AP3: Hybrid Photovoltaic-H<sub>2</sub> System in Chicago, IL



• **Operating Costs Driven by Solar Radiation** *Ulleberg, 2004*

• **Performance Deteriorated by Power Losses**







## Is it worth using Stochastic Programming and WRF? Or there are simple bypasses?

- The case for forecast seems clear. But how about
  - (Q1) Do I need Stochastic Programming and uncertainty? Maybe if I do deterministic programming on average it is sufficient.
  - (Q2) Do I need WRF to do it? Or can I get by with massaging historical data.
- We Present evidence of Yes on both counts.





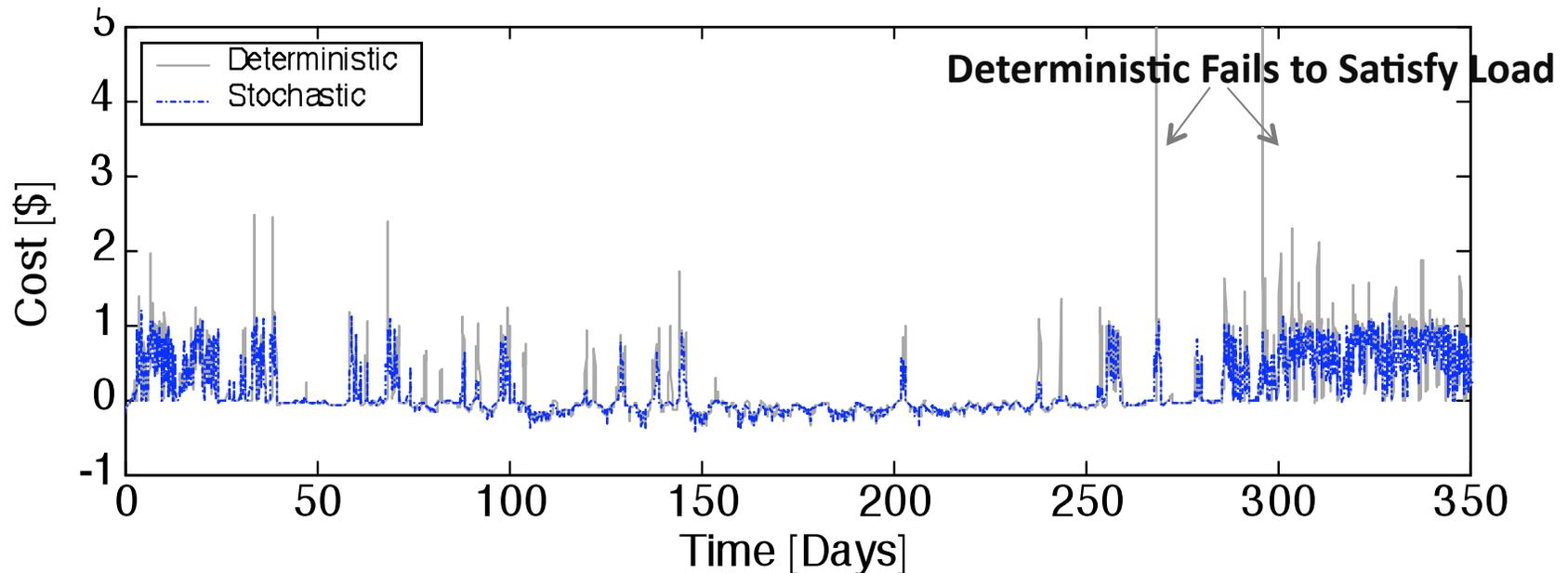
## App 1: Regional SO commitment

- Deterministic strategy (Programming on average) cannot satisfy demand beyond 10% wind penetration (The reserves help some).
- Evidence for Q1=Yes.



# App 3: Hybrid Photovoltaic-H<sub>2</sub> System

## Load Satisfaction Deterministic (“Optimization on Mean”) vs. Stochastic



Therefore, the alternative to stochastic programming can turn out **infeasible !!**

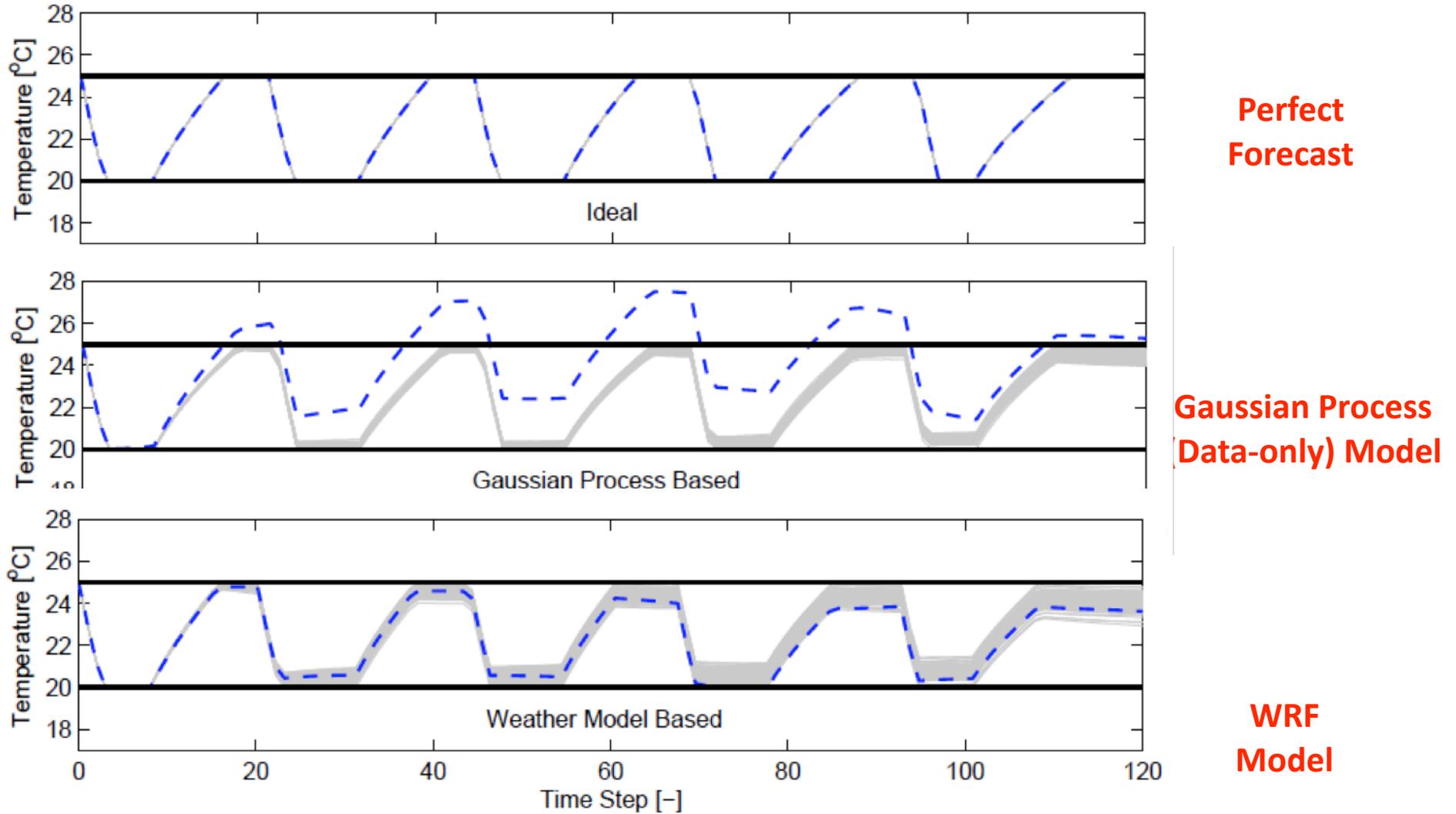
Handling Stochastic Effects Particularly Critical in Grid-Independent Systems where no recourse.

Evidence for Q1=Yes.



# App2: Thermal Management of Building Systems

Performance Optimizer using WRF and GP Model Forecasts. Evidence for Q2=Yes.



# Conclusions and Future Work

## **Integrative Study of Weather Forecast-Based Optimization**

- Far as we know this is the first integrative study using validated WRF Model for an operational setting (1km, 1 day ahead, in 1hr).
- We showed that stochastic formulation matters hugely for satisfying constraints.
- Weather uncertainty is a hard, important, problem that data-only methods (such as GP) are unlikely to crack.
- We showed that weather forecast inclusions results in 20-80% cost reduction for rolling horizon.

## **Future and On-Going Work**

- Better posterior sampling for weather forecast uncertainty.
- Dynamic Programming Formulations and comparisons with rolling horizon.
- High-resolution physics in WRF (feedback from wind farms?).
- Solving larger Stochastic MINLP problems.
- Modeling pricing and demand uncertainty.
- Real time cost-efficient techniques (buildings and PV).



# Promise of HPC for Integrated Energy Systems Management

## 1. Predicting Weather Forecast with Uncertainty **Operationally.**

**400K Processors would provide in one hour wall clock time 30 WRF Ensemble Members for the next 24 hours at 1 km resolution for the entire US. (Source: Extrapolation of Profiling)**

## 2. Stochastic Dynamic Programming as a resource management strategy for Regional System Operators. ~ 10s of billions of dollars worth of activity per year. (Source: Our educated guess).



## References. (from the Speaker's Web Site)

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•Victor M. Zavala, Mihai Anitescu and Theodore Krause. "On the Optimal On-Line Management of Photovoltaic-Hydrogen Hybrid Energy System". Preprint ANL/MCS P1569-0109 *Proceedings of the 10th International Symposium on Process Systems Engineering - PSE2009*, Rita Maria de Brito Alves, Claudio Augusto Oller do Nascimento, Evaristo Chalbaud Biscaia Jr. (Editors.) *Computer Aided Chemical Engineering*, Volume 27, Pages 1953-1958, 2009 Elsevier, Amsterdam.

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■ Emil Constantinescu, Victor Zavala, Matthew Rocklin, Sangmin Lee, and Mihai Anitescu. A Computational Framework for Uncertainty Quantification and Stochastic Optimization in Unit Commitment with Wind Power Generation. Submitted to IEEE Transactions on Power Systems.

•Victor M. Zavala, Emil M. Constantinescu, and Mihai Anitescu. Economic Impacts of Advanced Weather Forecasting in Energy System Operations. Submitted to the IEEE-PES conference

[.PDF Version.](#)

