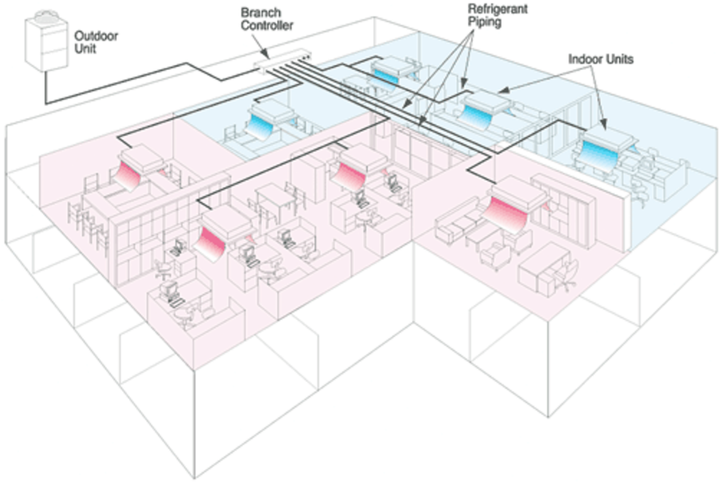
MITSUBISHI ELECTRIC RESEARCH LABORATORIES
Cambridge, Massachusetts

ANP-BBO: Attentive Neural Processes and Batch Bayesian Optimization for Scalable Calibration of Physics-Informed Digital Twins



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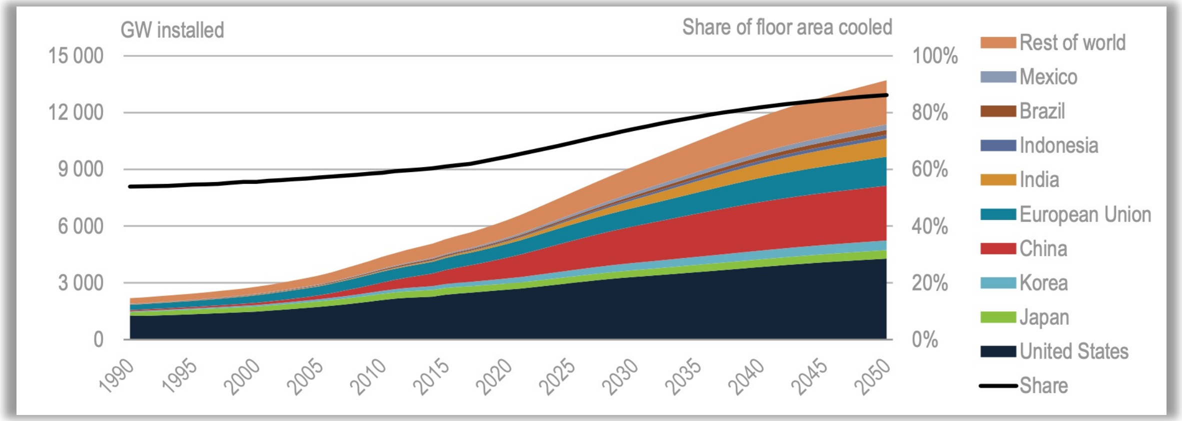
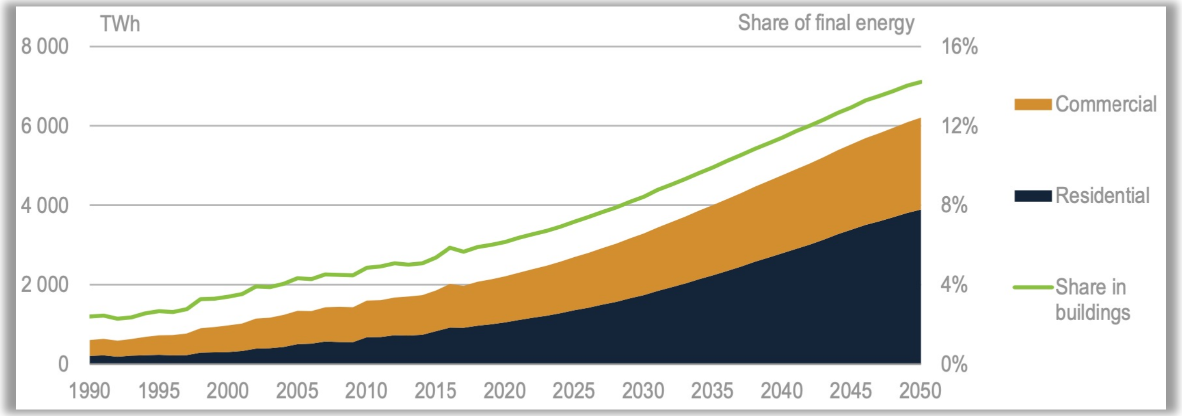
Digital Twins and Climate Change

Due to climate change, global trends project[1]

- space cooling demand will rise **from 60% to >85%**
- energy needs for space cooling will **>3x**

between 2016 and 2050





[1] International Energy Agency, *The Future Of Cooling*, 2018.

Digital Twins and Climate Change

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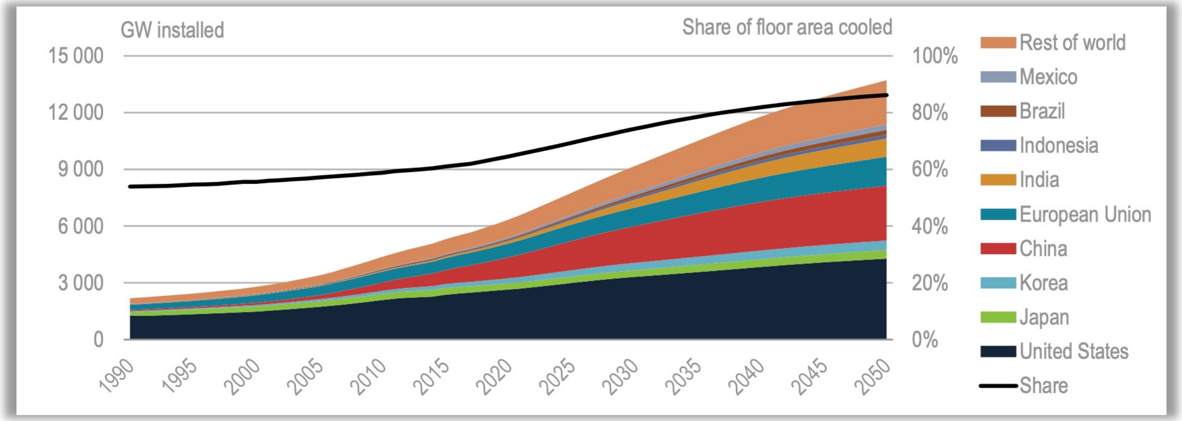
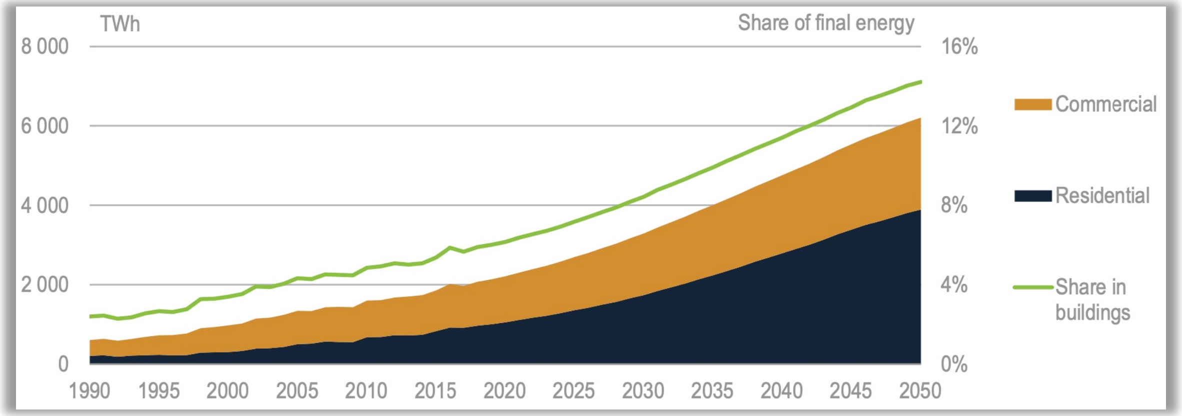
Dangerous positive feedback loop that will exacerbate climate change **unless space cooling is optimized for the same energy demand**

- ML has been identified as enabling technology for building optimization[2]
- Many field experiments for data is impractical





[1] International Energy Agency, *The Future Of Cooling*, 2018.
[2] Rolnick et al., *Tackling Climate Change with Machine Learning*, arXiv:1906.05433, 2019.

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Digital twins (DTs) enable safe experiments via simulation, but they **need to be calibrated to accurately reflect truth**

[1] International Energy Agency, *The Future Of Cooling*, 2018.
[2] Rolnick et al., *Tackling Climate Change with Machine Learning*, arXiv:1906.05433, 2019.

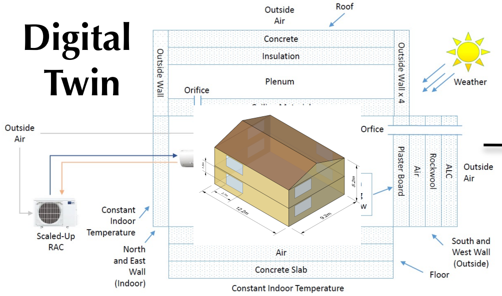
Calibration of Physics-Informed Digital Twins

Building System + HVAC

Measured data

$y^{\star}_{0:T}$

Digital Twin



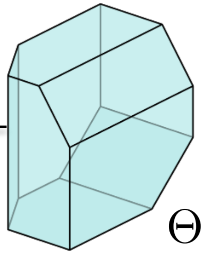
Model outputs

$y_{0:T} = \mathcal{M}_T(\theta)$

$$\boxed{J(y^{\star}_{0:T}, \mathcal{M}_T(\theta_t))}$$

Calibration Cost

Simulate model



Θ

Admissible Parameter Space

Examples of $\boldsymbol{\theta}$

Building: airflow coefficients, material properties

HVAC: heat transfer coefficients, refrigerant properties

$$\theta^{\star} = \arg\min_{\Theta} J$$

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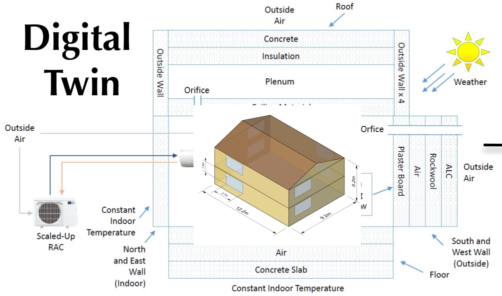
Building System + HVAC

Measured data

$y^{\star}_{0:T}$

Digital Twin



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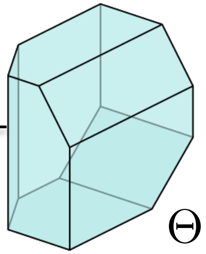


Admissible Parameter Space

Examples of $\boldsymbol{\theta}$

Building: airflow coefficients, material properties

HVAC: heat transfer coefficients, refrigerant properties

$$\theta^{\star} = \arg\min_{\Theta} J$$

Objective: Use simulations to obtain parameters $\theta^{\star}$ that minimize the calibration cost

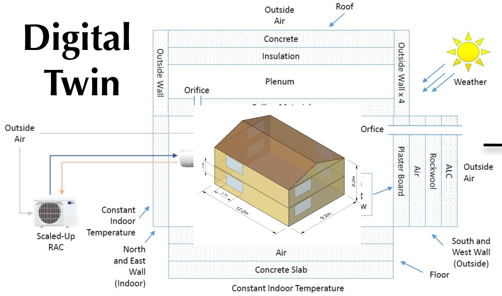
Calibration of Physics-Informed Digital Twins (via Bayesian Optimization)

Building System + HVAC

Measured data

$y^\star_{0:T}$

Digital Twin



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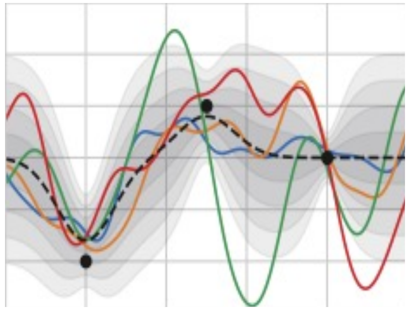
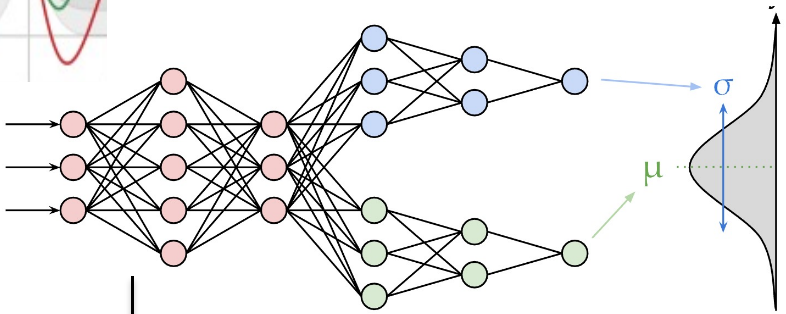


Can scale up

Approximate Calibration Cost with Probabilistic Learners



Mean, variance predictions

$\mu(\cdot), \sigma(\cdot)$

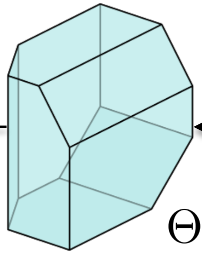
Sample efficient

Simulate model

Not gradient-based

Next parameter candidate

θ_{t+1}



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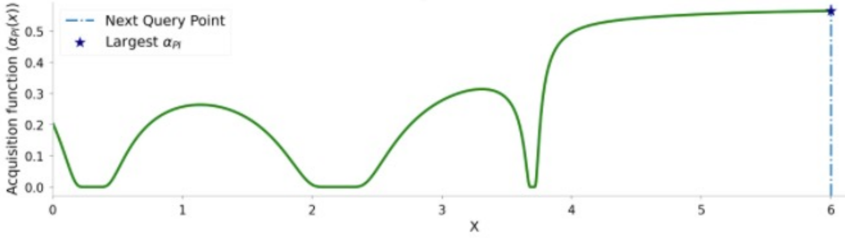

$\mathcal{A}(\cdot)$

Acquisition function

ANP-BBO: Why not GPs?

GP-BO:

✗ Inference is expensive

✗ Limited to Gaussian distributions

✗ Simulations/cost evaluation not parallelizable

Proposed ANP-BBO:

✓ Inference is cheap[1]

✓ Wide range of distributions[2]

✓ Simulations/cost evaluation can be parallelized

[1] Kim et al. *Attentive Neural Processes.* https://arxiv.org/pdf/1901.05761.pdf
[2] Garnelo et al. *Neural processes*. arXiv preprint arXiv:1807.01622.

ANP-BBO: Attentive Neural Processes-Batch Bayesian Optimization

ANP-BBO: Algorithm

GP-BO:

✗ Inference is expensive

✗ Limited to Gaussian distributions

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Proposed ANP-BBO:

✓ Inference is cheap

✓ Wide range of distributions

✓ Simulations/cost evaluation can be parallelized

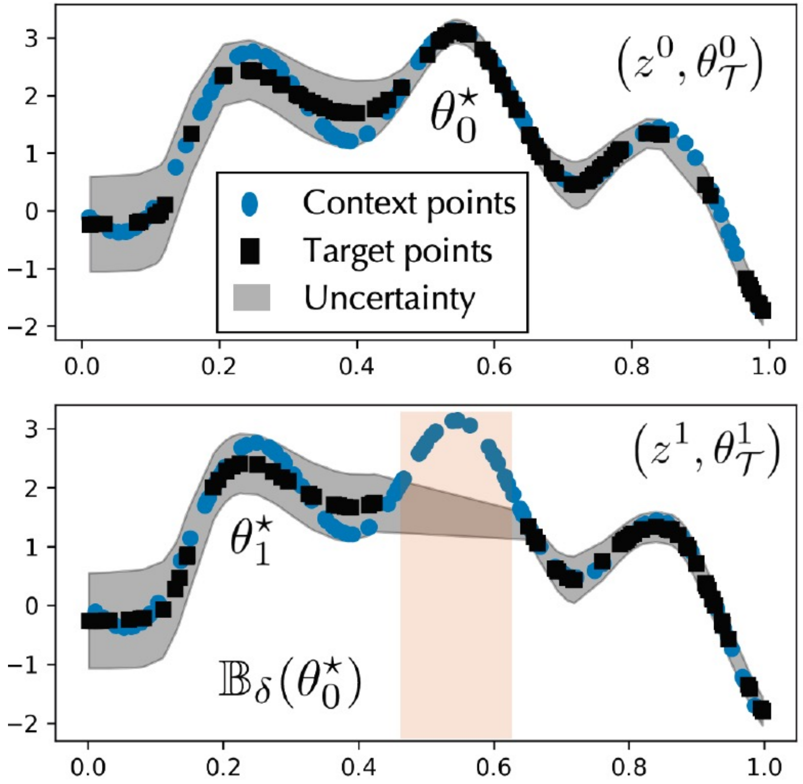
i. Current dataset after t iterations $D^t = \{(\theta, J)\}_0^{N_0+tN}$

ii. Train ANP by maximizing ELBO with N new data points

iii. Select batch of N candidates during inference

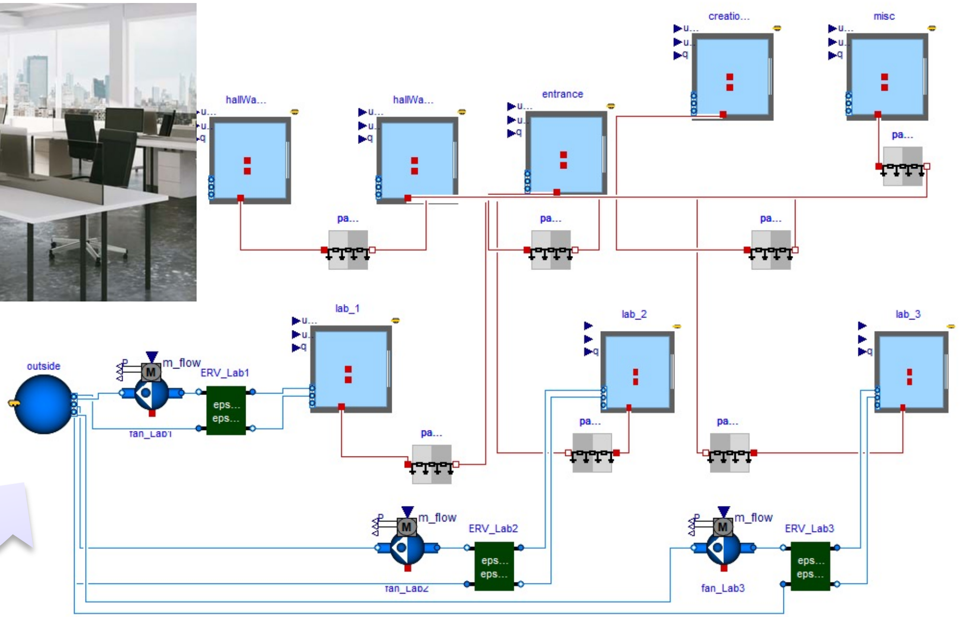
- Sample a latent, z (*Cheap inference*)
- Perform target set penalization (*Wide range*)

iv. (*Parallelizable*) Simulate to evaluate cost (via digital twin)



ANP-BBO: Calibration Results

Digital Twin of 1 Floor of Commercial Building in Tokyo, JP



Setup:

- 12 parameters to be calibrated
- 5 days of measured temp. and RH data, noisy, quantized
- 2 days for calibration, 3 days for testing

[1] ASHRAE, *Guideline 14-2014, measurement of energy, demand, and water savings*. 2014.

R-x: Room number x, x ∈ {1,2,3}

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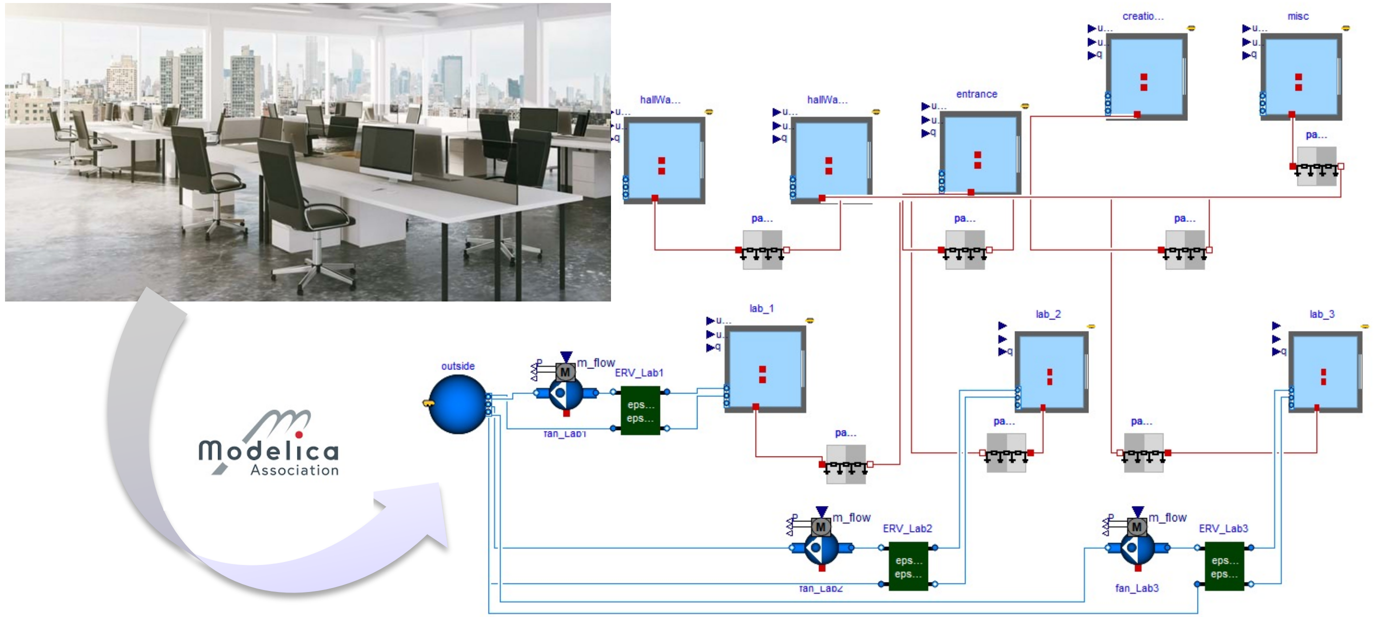
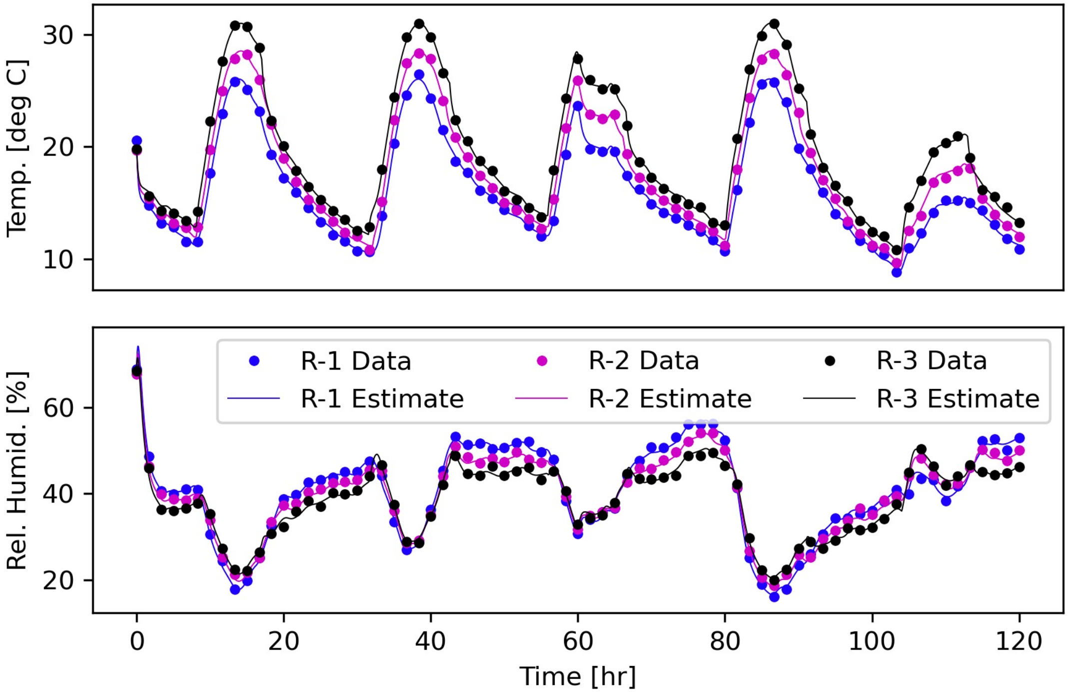


Measured and simulated outputs



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Outputs coefficient of variation of RMSE is **<1%**, well within the ASHRAE guidelines <15% [1]

[1] ASHRAE, *Guideline 14-2014, measurement of energy, demand, and water savings*. 2014.

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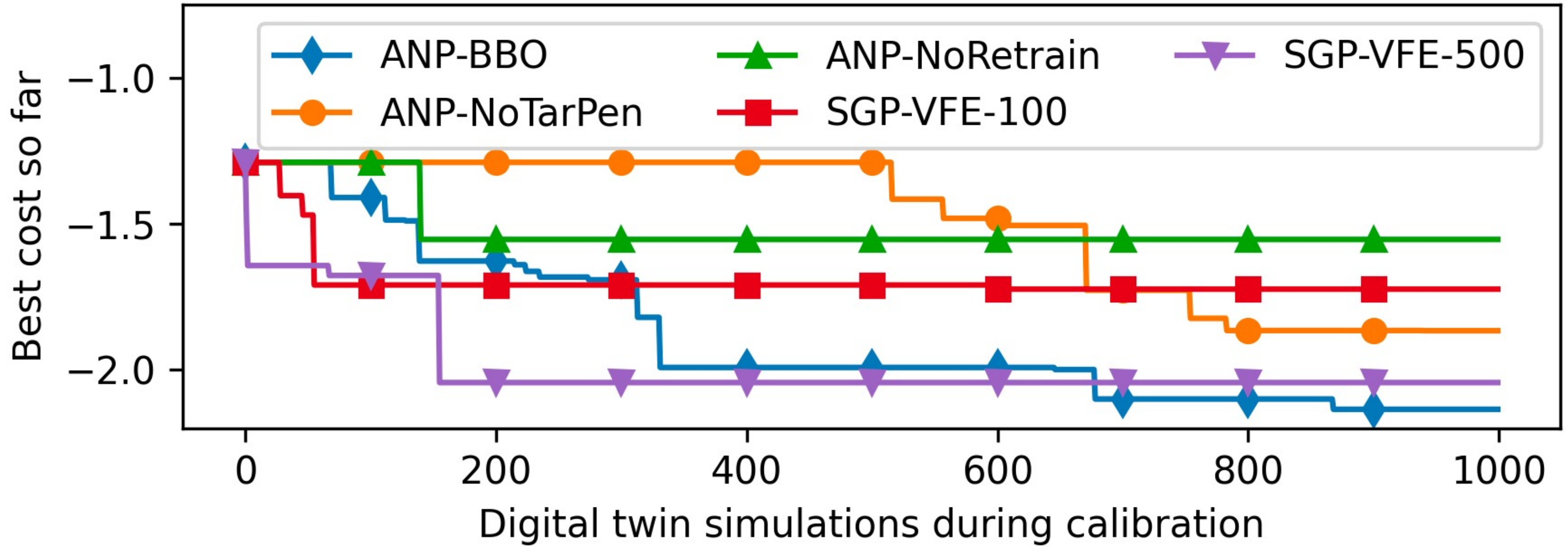
ANP-BBO: Ablation Studies

1. *ANP-BBO*: Proposed algorithm
2. *ANP-NoTarPen*: Switch off target set penalization
3. *ANP-NoRetrain*: Train ANP once with initial data, no further retraining
4. *SGP-VFE-100/500*: Use sparse Gaussian processes[1] as learner, with 100 or 500 inducing points



ANP-NoTarPen: Shows target penalization helps more than only latent sampling

ANP-NoRetrain: Lack of retraining with limited initial data does poorly

SGP-VFE: Good early, but gets stuck due to worsening approximations at scale

ANP-BBO: outperforms the others after 700 iters due to diverse and good candidates

[1] Titsias. *Variational learning of inducing variables in sparse Gaussian processes*. AISTATS, 2009.

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Changes for the Better