Advanced Reduced Order Model (ROM) Prediction and Error Quantification Framework for SOFC Stacks

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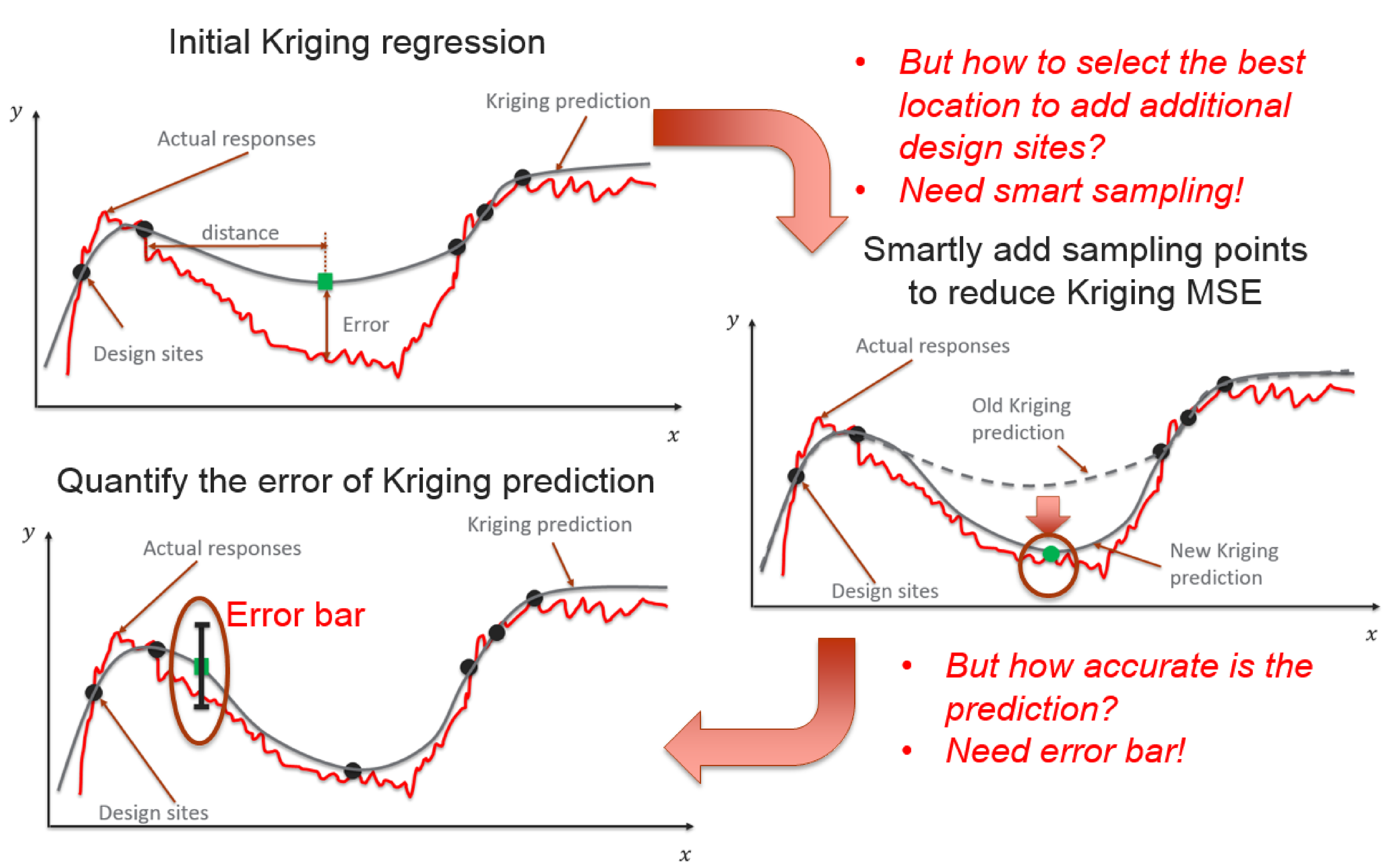
ROM OVERVIEW

Numerical modeling of solid oxide fuel cells (SOFCs) plays an important role in the development of the SOFC core technology program. PNNL developed the SOFC-MP (Solid Oxide Fuel Cell Multi-Physics) model to evaluate the flow, electrochemical, thermal, and structural performance of planar cells. Although SOFC-MP is designed for fast solution times to quickly evaluate different operating conditions for multi-cell stacks, it is often not efficient enough for integration into power system modeling. To provide quick and accurate predictions to replace the computationally expensive SOFC-MP simulations, an advanced reduced order model (ROM) is created to estimate the SOFC stack performance.

ROM TECHNICAL APPROACH

The fundamentals of the ROM are based on Kriging regression. The essence of Kriging regression is to evaluate the SOFC-MP model results at the given sampling points and then perform predictions for the selected result variables of interest. The entire framework of the advanced ROM approach consists of two main parts: smart sampling and error quantification. An adaptive sampling method needs to be integrated into the ROM tool to progressively reduce Kriging regression mean square error (MSE) until a desired MSE is reached. The cross-validation technique is developed to quantify the ROM prediction error. The goal of our error quantification framework is to provide a single point estimate as well as its 95% confidence interval to characterize the accuracy of the prediction for any given inputs. An illustrative example of the developed sampling approach is shown below.



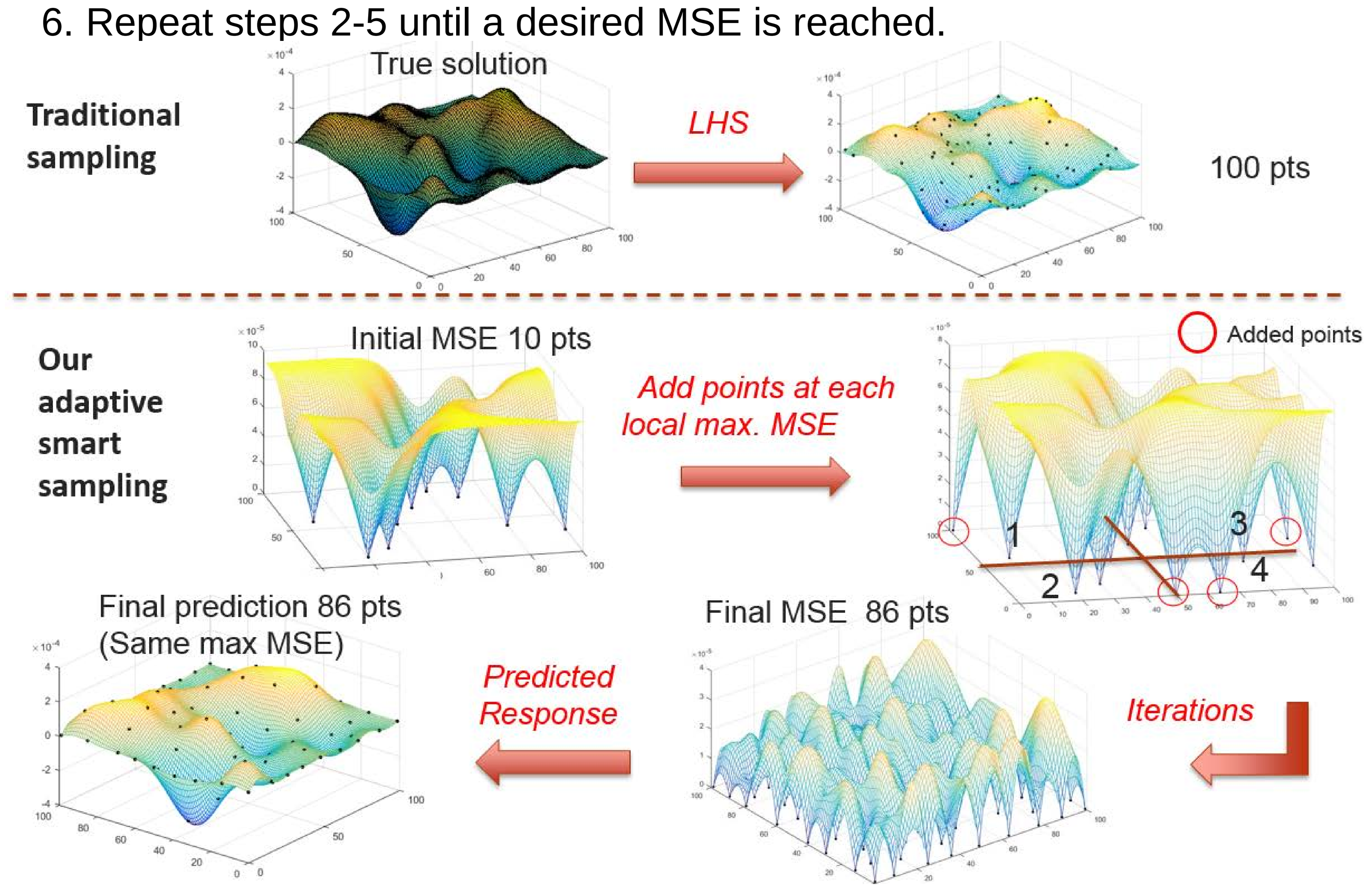
Sampling Method for ROM Approach

ROM SMART SAMPLING

The goal of the smart sampling method is to progressively refine and minimize the Kriging MSE by adding additional sampling points at regions with local maximum MSE. The steps of the adaptive smart sampling routine are outlined below. We demonstrate the advantages of our approach using a 2D Poisson equation as well as a representative NGFC system stack after comparing the results from traditional sampling methods.

Demonstration of smart sampling using a 2D Poisson equation:

1. Initialize small number of sampling points.
2. Run Kriging regression to obtain MSE.
3. Divide the entire domain into several sub-domains.
4. Find the maximum MSE in each sub-domain.
5. Add those critical points to expand the sampling pool.
6. Repeat steps 2-5 until a desired MSE is reached.



Demonstration of smart sampling using default NGFC system

Traditional Sampling:

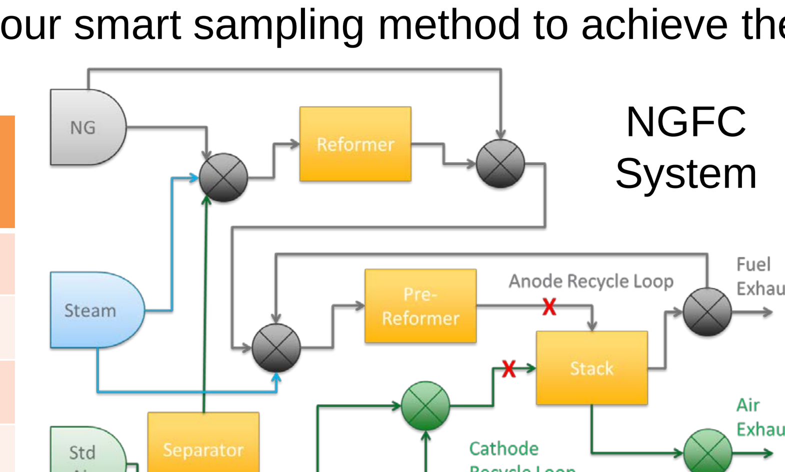
1. Build response surface using 11k successful 8D SOFC-MP cases to predict stack voltage.
2. Run additional 1k SOFC-MP simulations as validation cases.
3. Find maximum Kriging MSE (3e-4) for the entire 1k validation cases.

Adaptive Smart Sampling:

1. Start with 2k out of the 11k successful 8D SOFC-MP cases, build Kriging regression to predict stack voltage.
2. Find max. MSE for the 1k validation cases.
3. Sort MSE for the 11k cases.
4. Add another 2000 points from the original 11k cases with max MSE.
5. Repeat until MSE for validation cases is less than 3e-4.

Results: Comparing with traditional method using11k samples, less than 8k samples are needed when applying our smart sampling method to achieve the same maximum MSE.

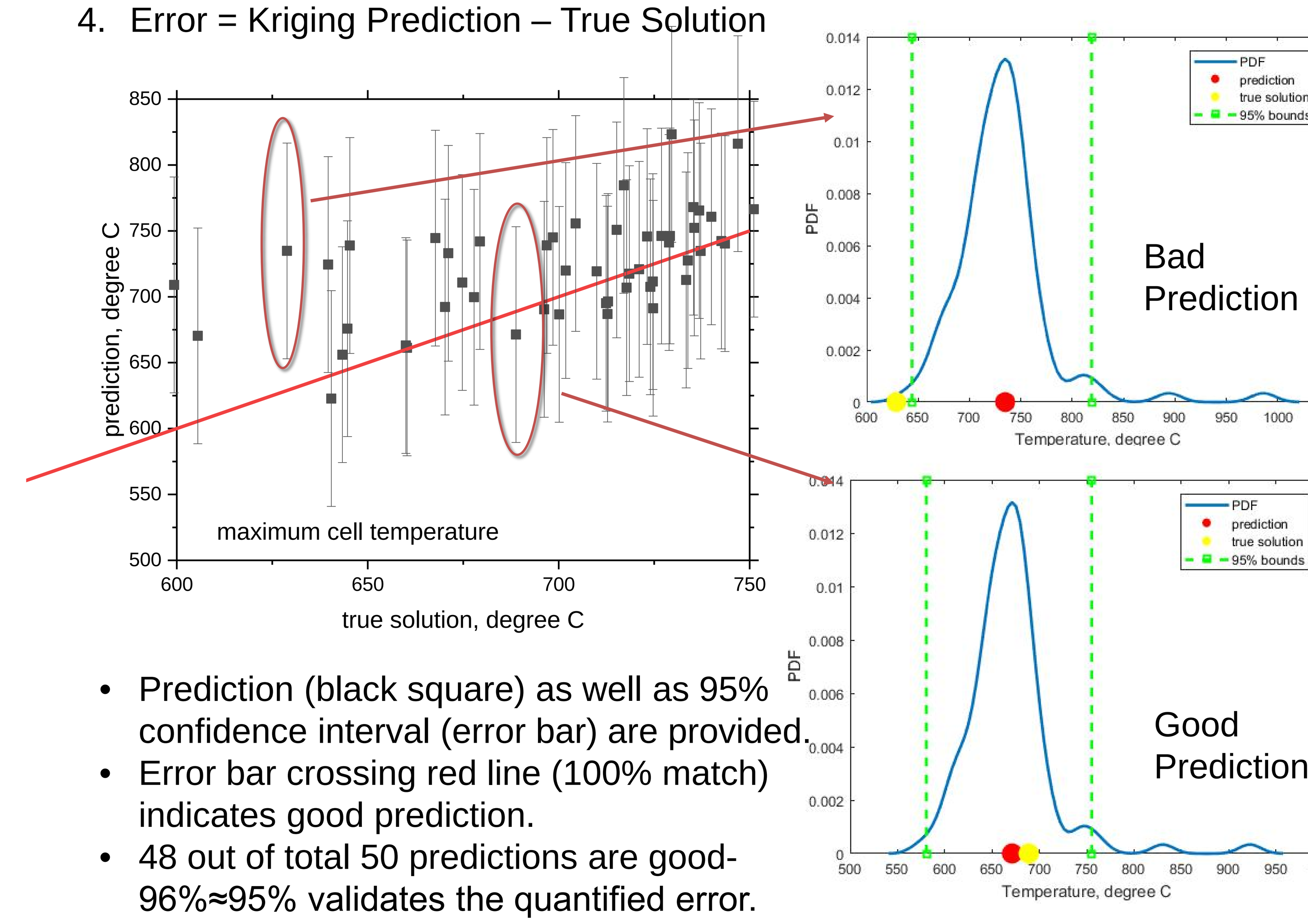
Number of samples	Maximum MSE	MSE Ratio
2000	1.46e-3	487%
4000	4.24e-4	141%
6000	3.77e-4	126%
8000	2.87e-4	96%



ROM ERROR QUANTIFICATION

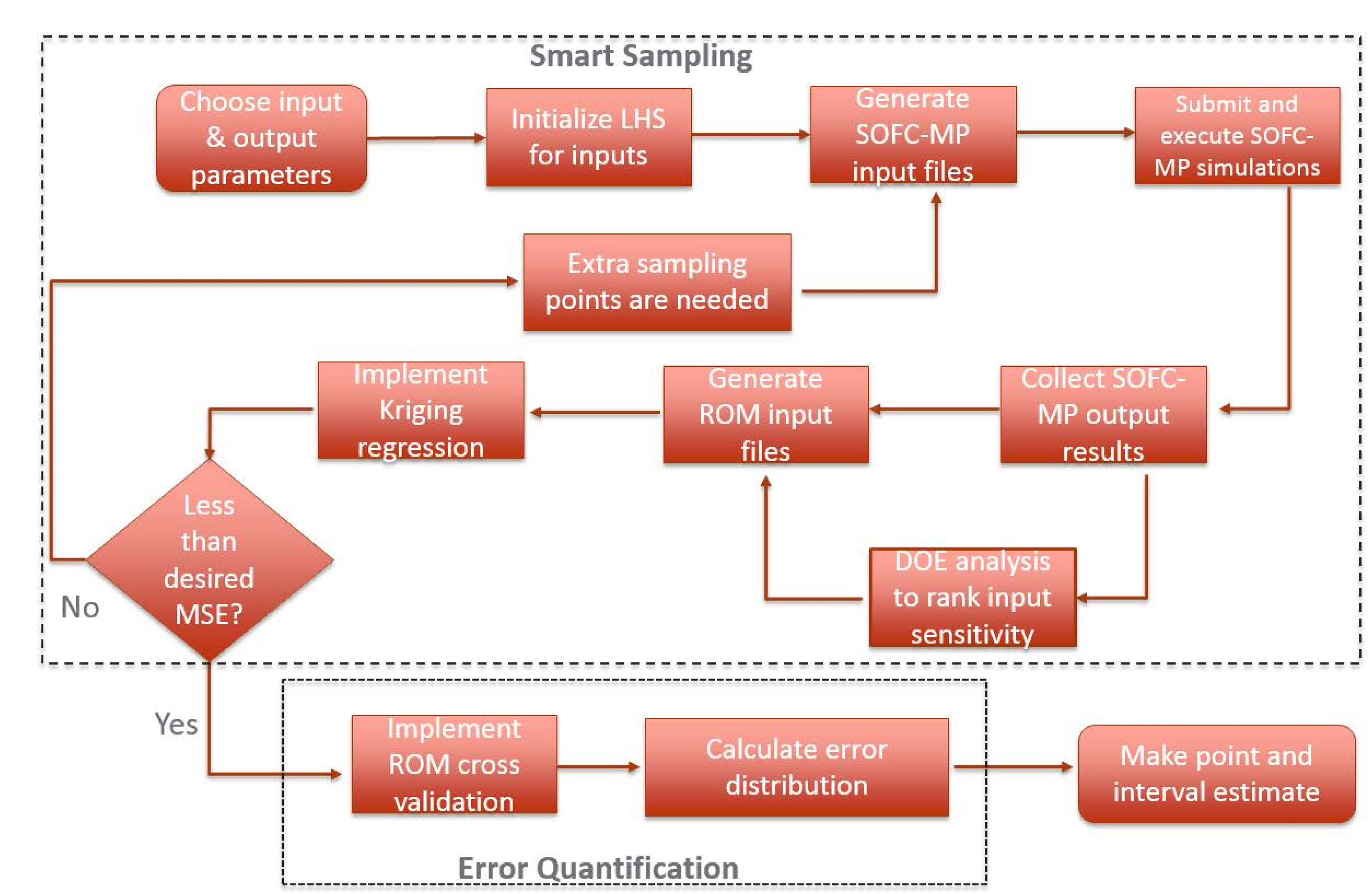
The goal of error quantification is to characterize the prediction error by implementing the 'leave one out' cross-validation technique. The major steps are briefly introduced next. The results are demonstrated for a default NGFC system with 50 additional SOFC-MP runs for prediction evaluation.

1. Divide data into training and validation datasets.
2. Implement Kriging regressions using training dataset.
3. Calculate error distribution using validation dataset.
4. Error = Kriging Prediction – True Solution



- Prediction (black square) as well as 95% confidence interval (error bar) are provided.
- Error bar crossing red line (100% match) indicates good prediction.
- 48 out of total 50 predictions are good-96%≈95% validates the quantified error.

ROM FRAMEWORK FLOWCHART



CONCLUSIONS AND FUTURE WORK

- Kriging regression used to build a ROM.
- Smart sampling approach used to progressively reduce MSE.
- A cross-validation algorithm used to quantify prediction error.
- **Next Step**: Incorporate entire smart sampling and error quantification processes for SOFC stacks into the user interface for automation.

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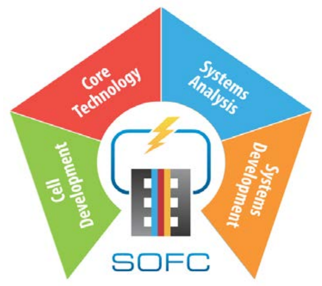

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