

# Surrogate modeling of the leaching process in a rare earth elements recovery plant

Dimitrios Fardis<sup>1</sup>, Donghyun Oh<sup>1</sup>, Nick Sahinidis<sup>1,2</sup>, Alejandro Garciadiego<sup>3,4</sup>, Andrew Lee<sup>3,4</sup>



<sup>1</sup> School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

<sup>2</sup> H. Milton School of Industrial and Systems Engineering, Georgia Institute of Technology

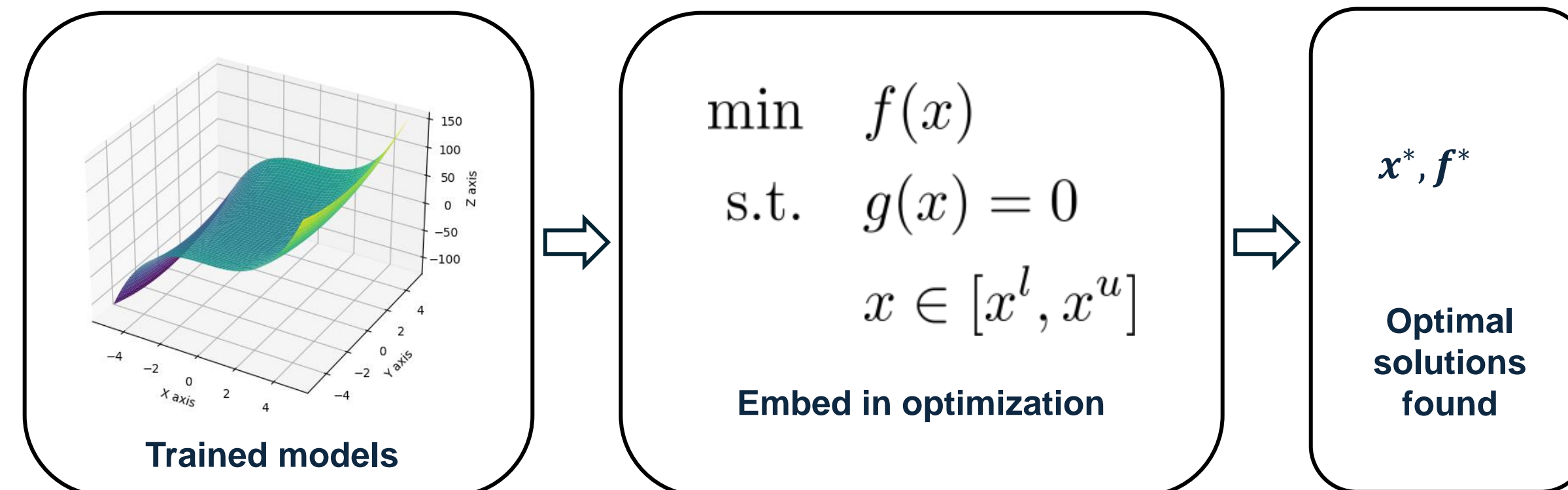
<sup>3</sup> National Energy Technology Laboratory, Pittsburgh, PA 15236, USA

<sup>4</sup> NETL Support Contractor, Pittsburgh, PA 15236, USA

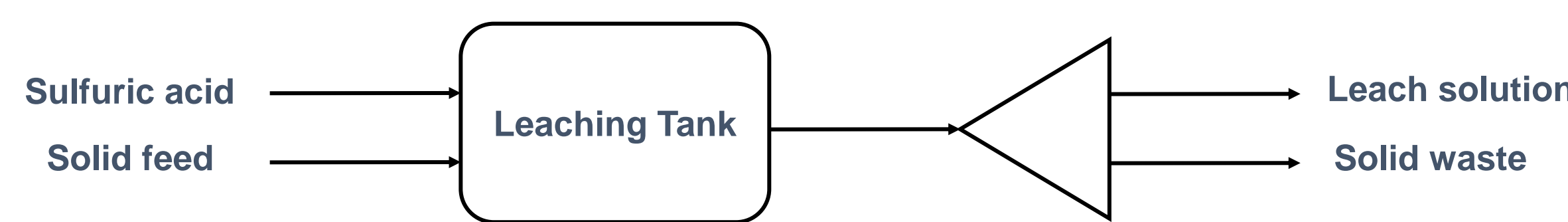


## Surrogate-based optimization

Is it possible to model and optimize chemical processes accurately using simple surrogate models?

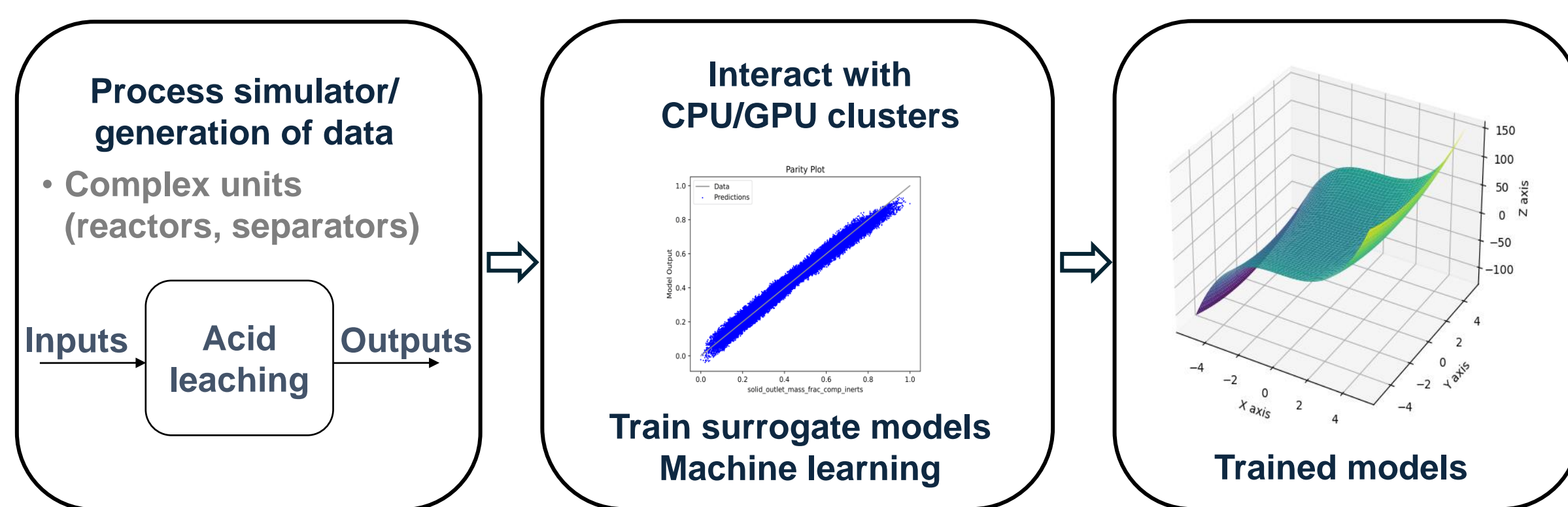


In this context, we identify the most appropriate surrogates to simplify the leaching flowsheet of rare earths:



## Surface approximation

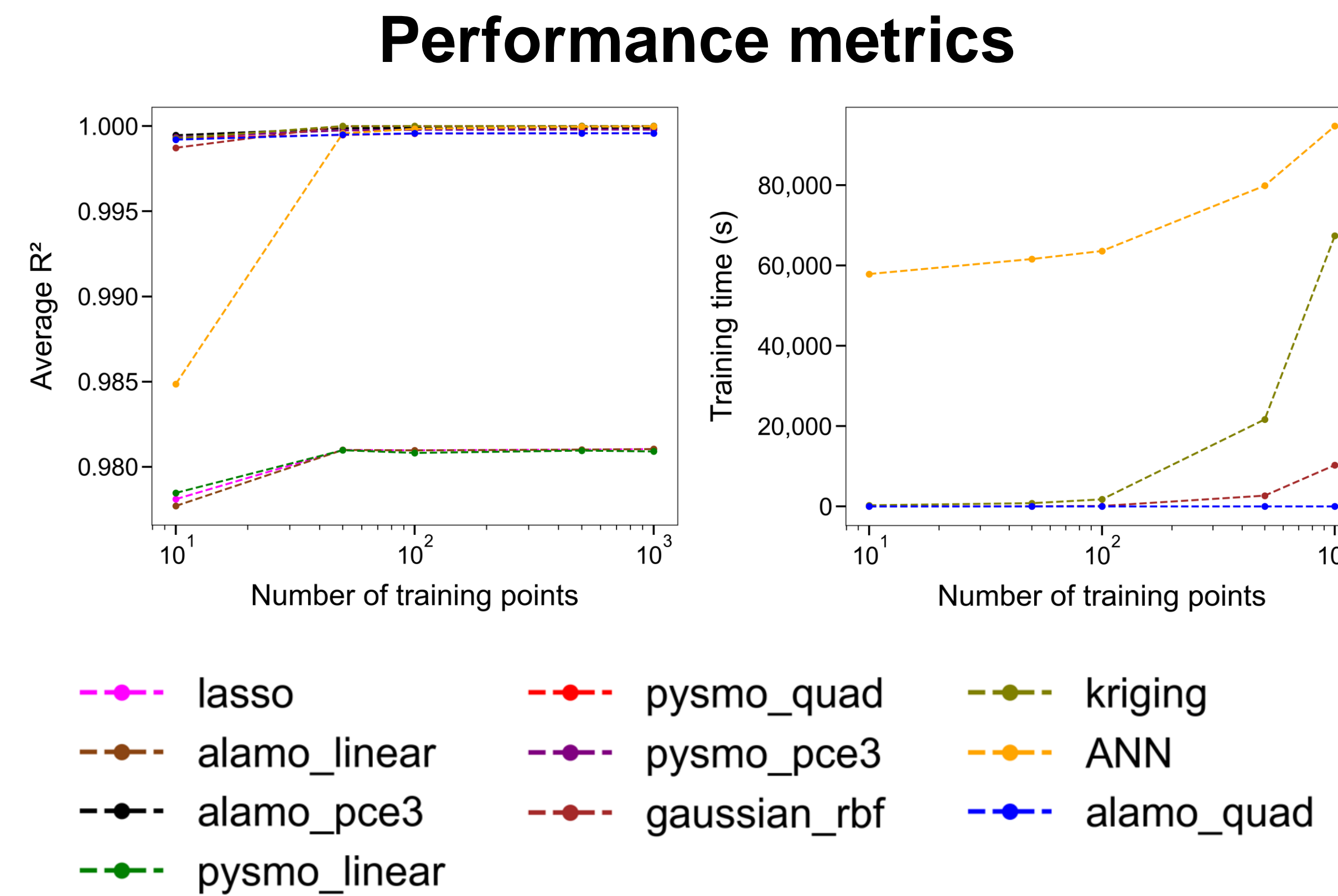
What surrogate modeling techniques are the most appropriate for the leaching process?



Techniques investigated:

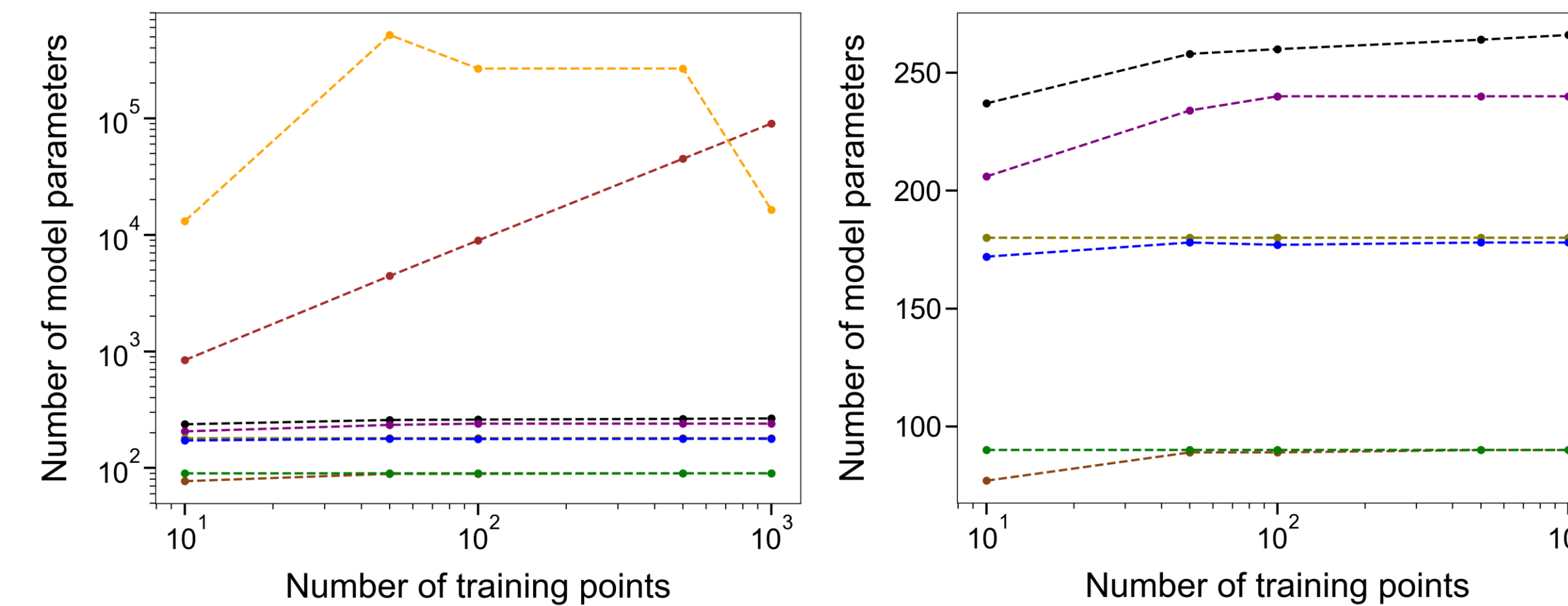
- ANNs
- LASSO regression
- ALAMO (linear, quadratic and PCE-3 models)
- Polynomials, RBFs, kriging using PySMO

## Evaluation of Surrogate models



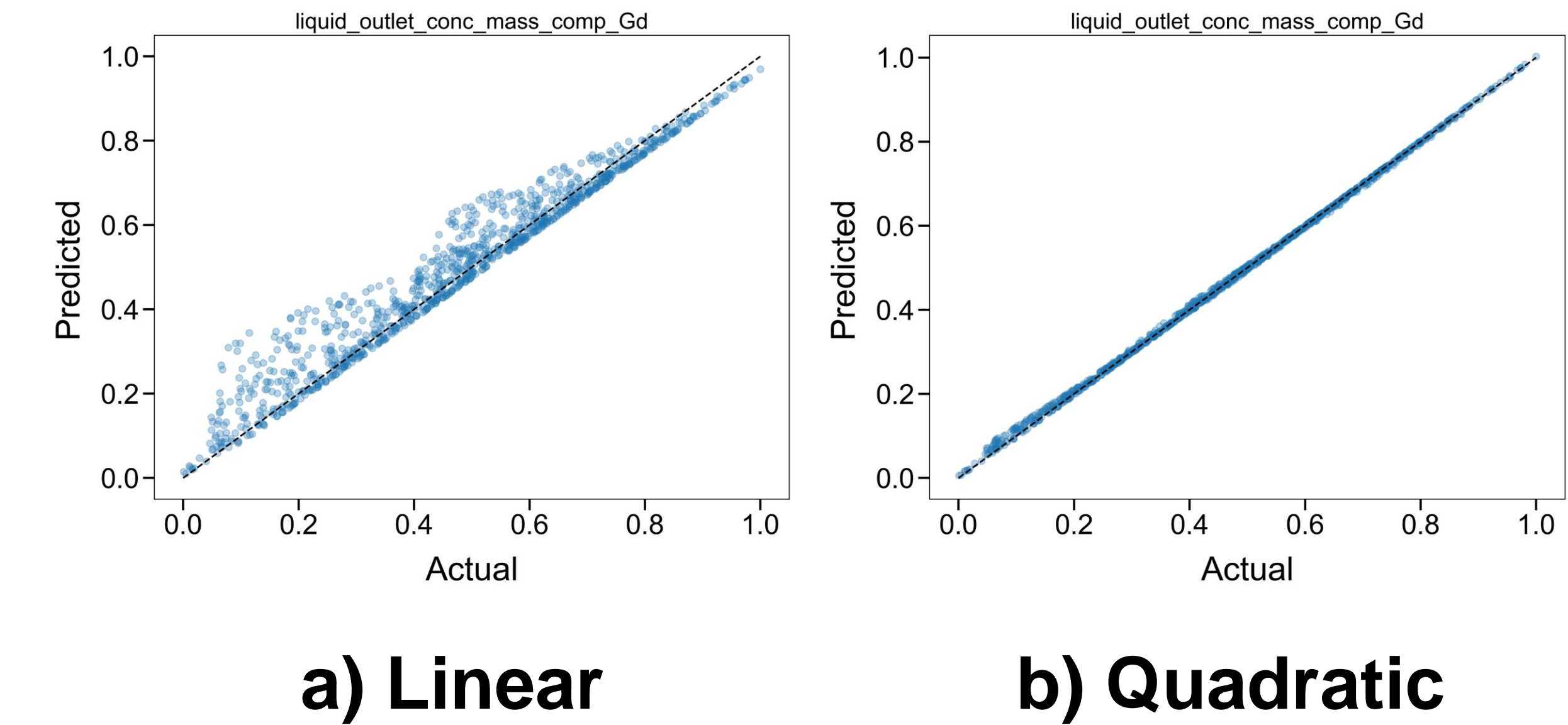
- All models have very good predictive ability
- Training times are 2-6 orders of magnitude larger for complex models

## Model complexity

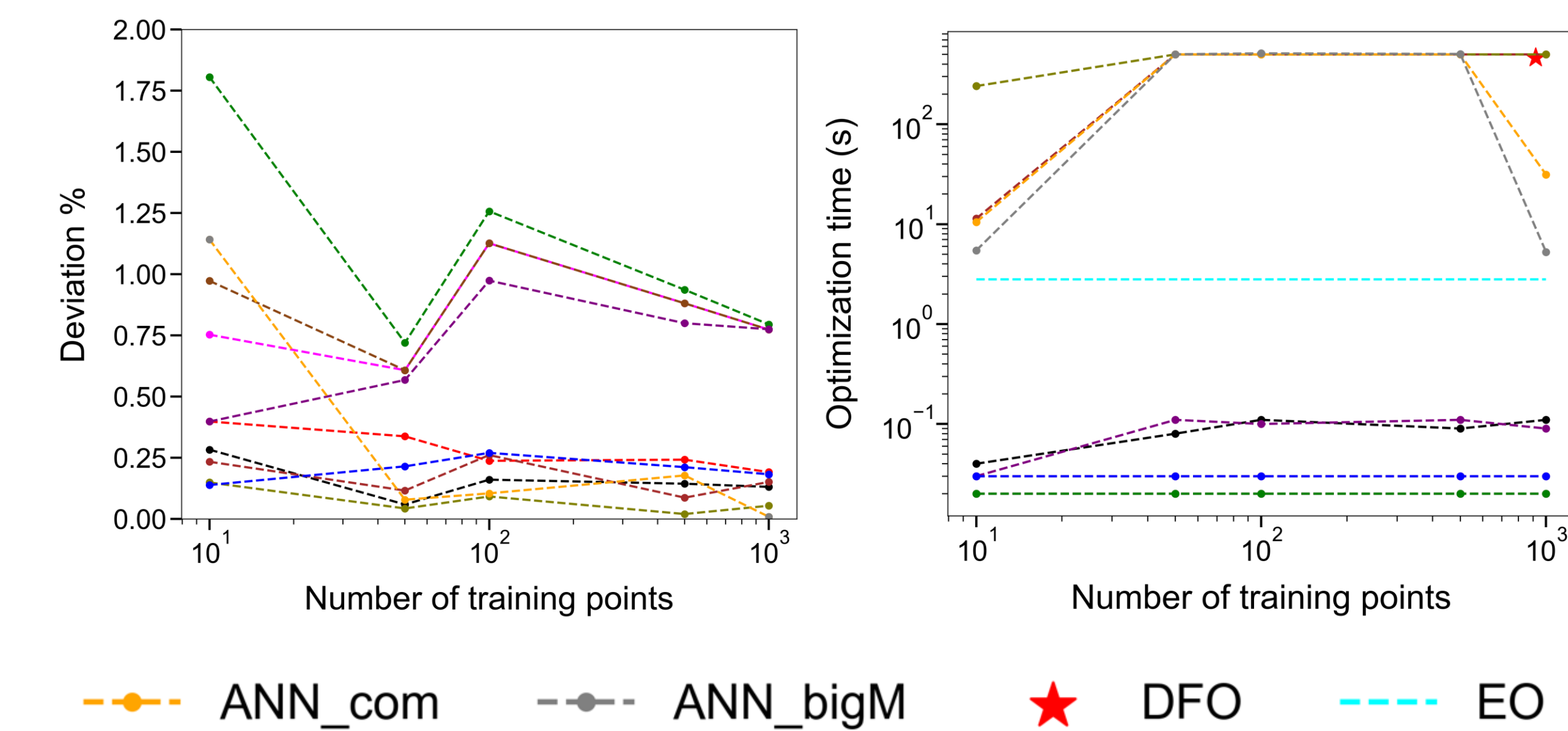


- ANNs and RBFs include up to three orders of magnitude more model parameters than the polynomials
- The inherent complexity of kriging models is not depicted by the number of parameters

## Linear vs. Quadratic ALAMO models



## Optimization results



- Correct solution point with little deviation in the objective
- DFO requires 1 order of magnitude more measurements and 3 orders of magnitude more CPU time than SBO
- SBO is two orders of magnitude faster than EO

## Conclusions

- ANNs, kriging, RBFs are not practical
- Quadratic surrogate models are the most appropriate
- DFO and EO are up to 3 orders of magnitude more expensive than SBO
- Future work will address more complex processes and additional surrogate modeling frameworks

**Acknowledgement:** The authors graciously acknowledge funding from the U.S. Department of Energy's Process Optimization and Modeling for Minerals Sustainability (PROMMIS) Initiative, supported Office of Fossil Energy and Carbon Management

**Disclaimer:** This presentation was funded by the United States Department of Energy, National Energy Technology Laboratory an agency of the United States Government, through a support contract. Neither the United States Government nor any agency thereof, nor any of its employees, nor the support contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, or any of their contractors.

