Surrogate-based Multi-Objective Optimization and Uncertainty Quantification Methods for Large, Complex Geophysical Models

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1. Introduction

Motivation

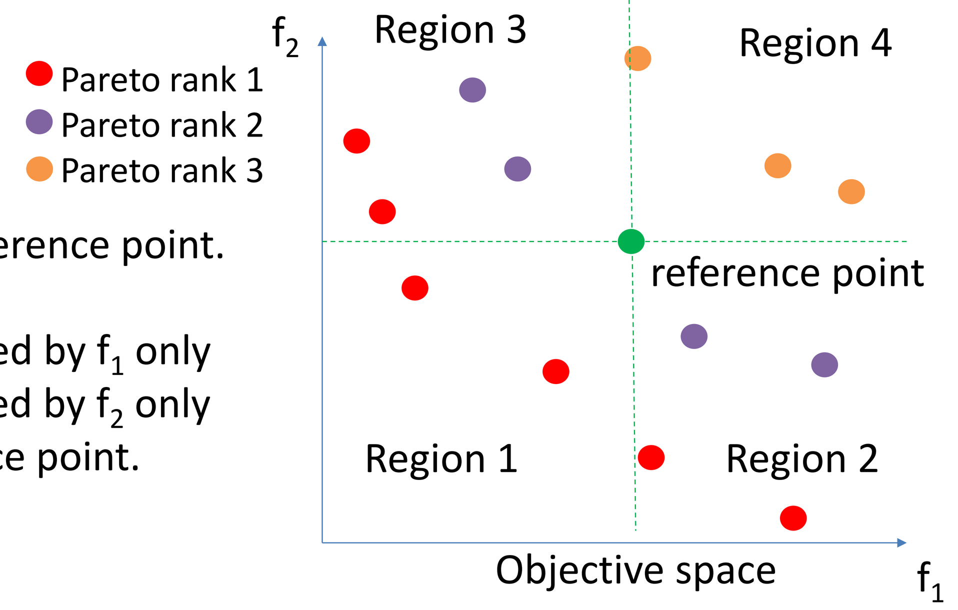
- Parameter calibration can significantly improve the performance of models.
- Large complex geophysical models are expensive to run. (distributed hydrological models, land surface models, weather/climate models, etc.)
- Calibration of multi-physical processes models must be multi-objective.
- Need to simultaneously improve the performance of multiple processes.
- Multi-objective optimization and MCMC cost a huge (10^5-10^6) number of model evaluations.
- How to reduce the number of model evaluations for Multi-objective optimization and MCMC?

Research highlights

- Surrogate-based multi-objective optimization (MO-ASMO).
  Multi-Objective – Adaptive Surrogate Modelling based Optimization
- Surrogate-based MCMC (MC-ASMO).
  Markov-Chain – Adaptive Surrogate Modelling based Optimization
- Novel adaptive sampling approaches for surrogate model.
- Special technology for simultaneously improving all objectives.
- Demonstrate the effectiveness and efficiency of MO-ASMO/MC-ASMO with test problems.
- Applied to a land surface model CoLM.

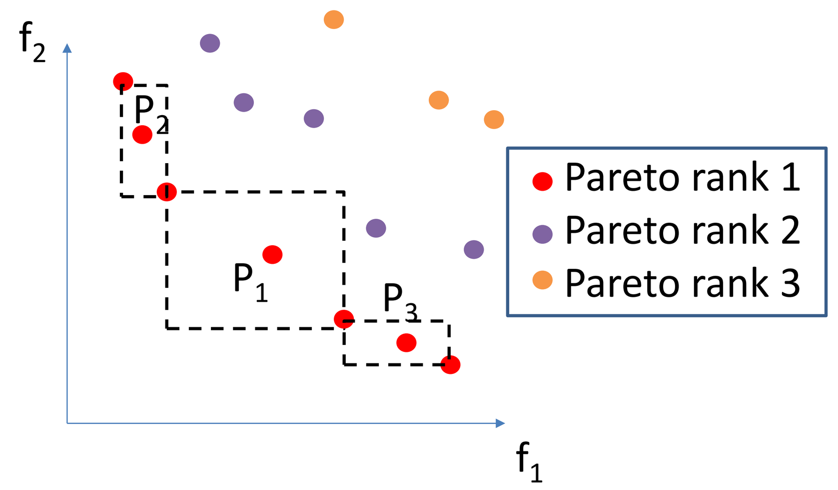
2. MO-ASMO: Surrogate-based Optimization

Pareto frontier:
cannot improve one objective without degrading another.

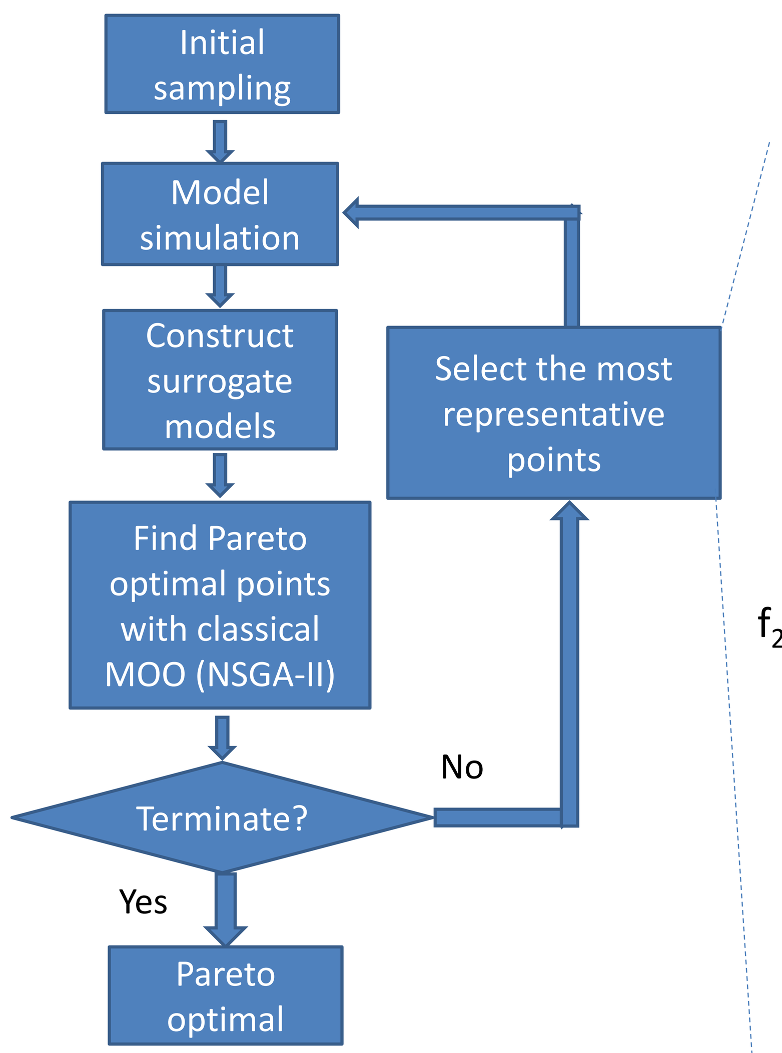


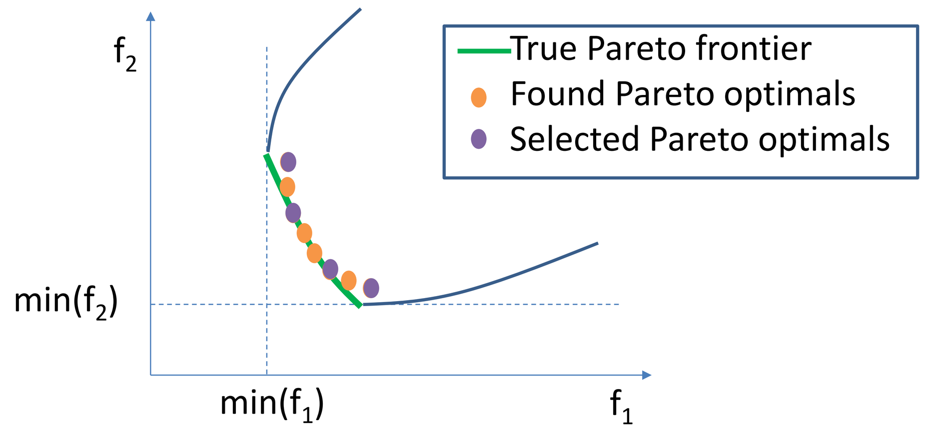
Region 1: Non-dominated region of the reference point. Superior to the reference point.
Region 2: Non-dominated region. Dominated by f_1 only
Region 3: Non-dominated region. Dominated by f_2 only
Region 4: Dominated region of the reference point. Inferior to the reference point.

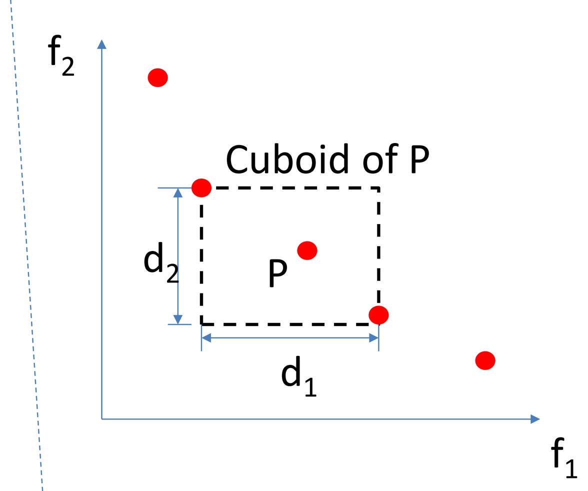
Non-dominated sorting:
- First sort with Pareto rank
- Then sort with the **crowding distance.** i.e. $P_1 > P_2 > P_3$. Larger distance means better diversity.



Flowchart of MO-ASMO

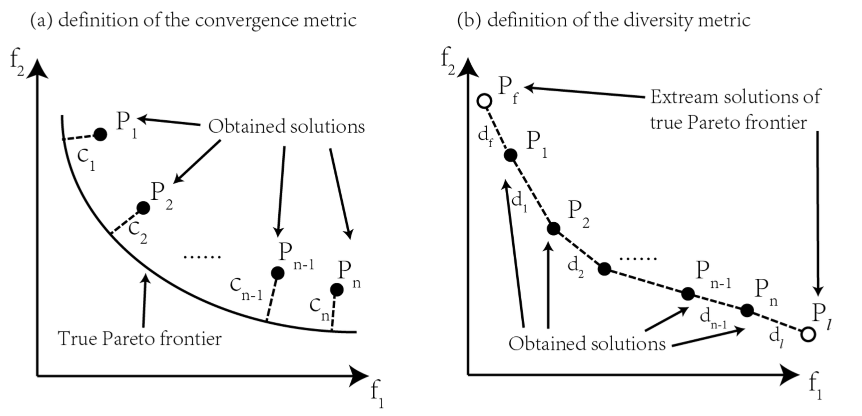




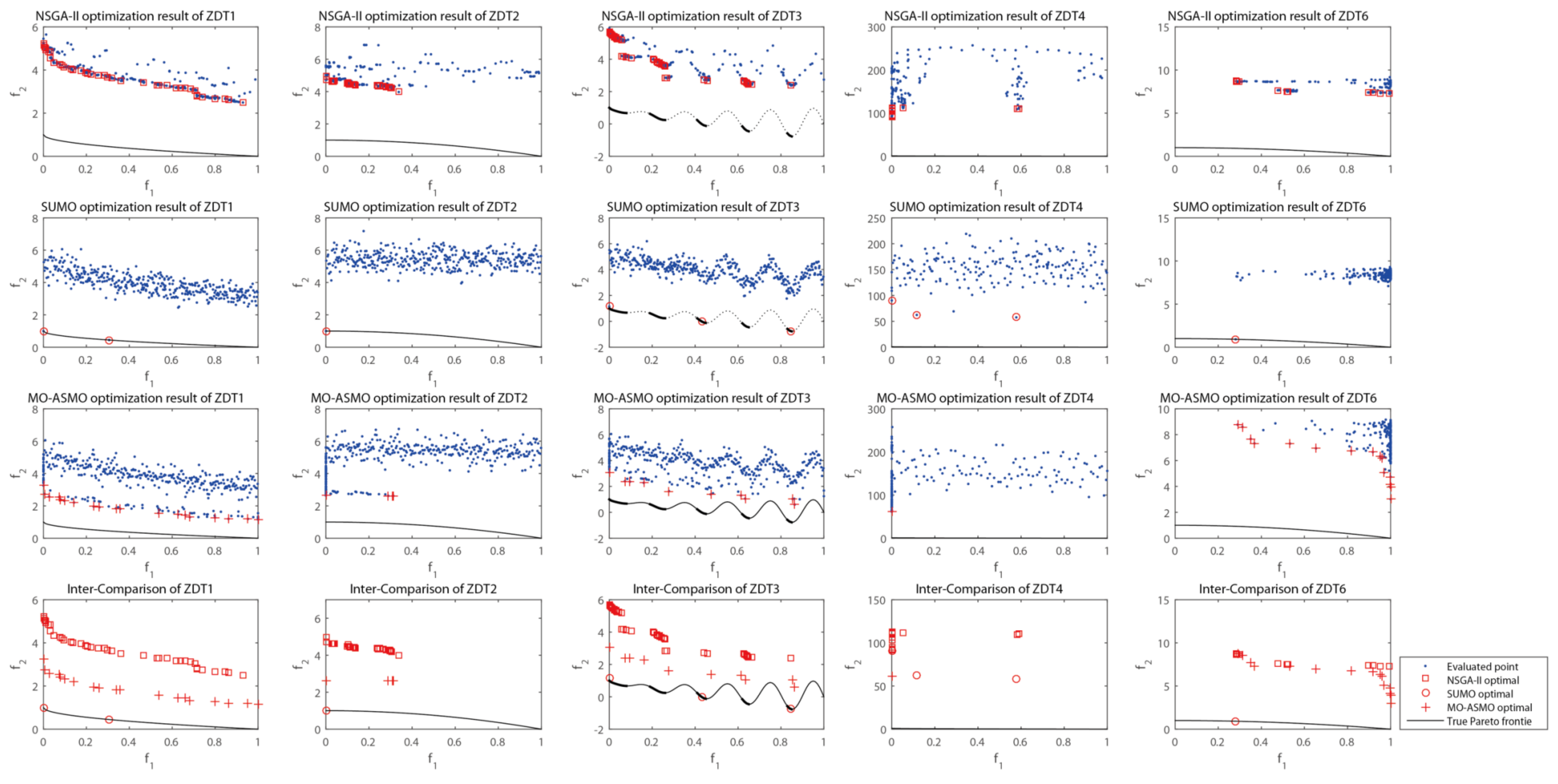


Crowding distance:
Sum of the edge length of the cuboid.
$D = d_1 + d_2$
Select the optimal points with largest crowding distance as the most representative points.

Performance metrics for multi-objective optimization:
Convergence: Fitness to the true Pareto frontier.
Diversity: Solutions are far away from each other and uniformly cover the Pareto frontier.
(for 2D problem only)



Demonstrating the effectiveness and efficiency of MO-ASMO with ZDT test problems

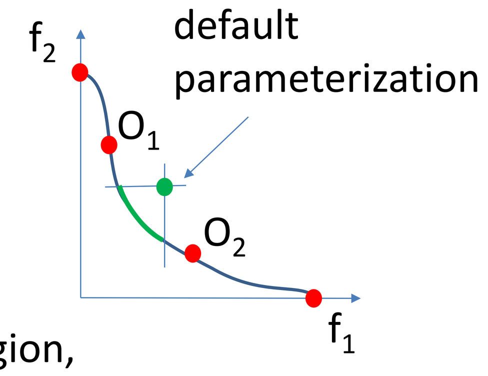


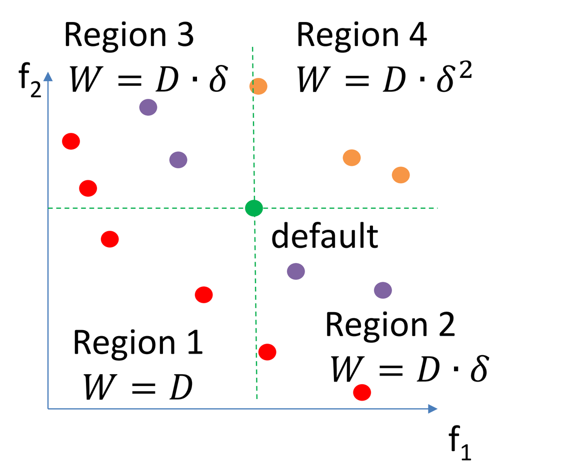
Simultaneously improve all objectives with weighted crowding distance

Comparing with the default parameterization

O_1: better f_1, worse f_2
O_2: better f_2, worse f_1

We want to find the green region, simultaneously get better f_1 and f_2.

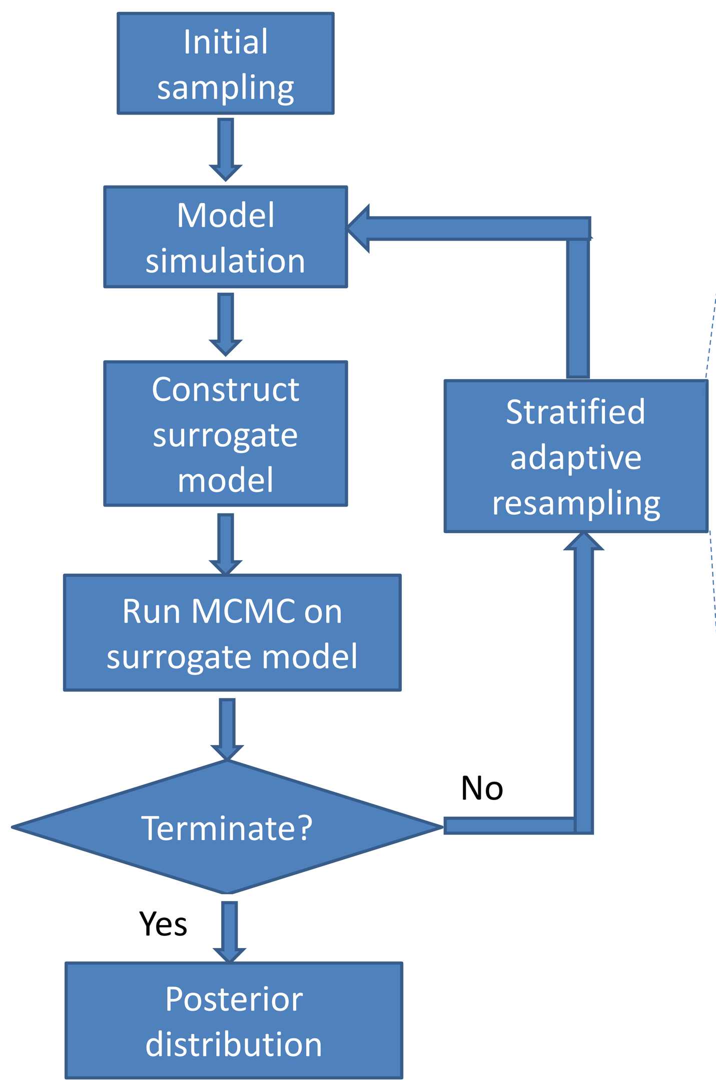




Definition of weighted crowding distance

3. MC-ASMO: Surrogate-based MCMC

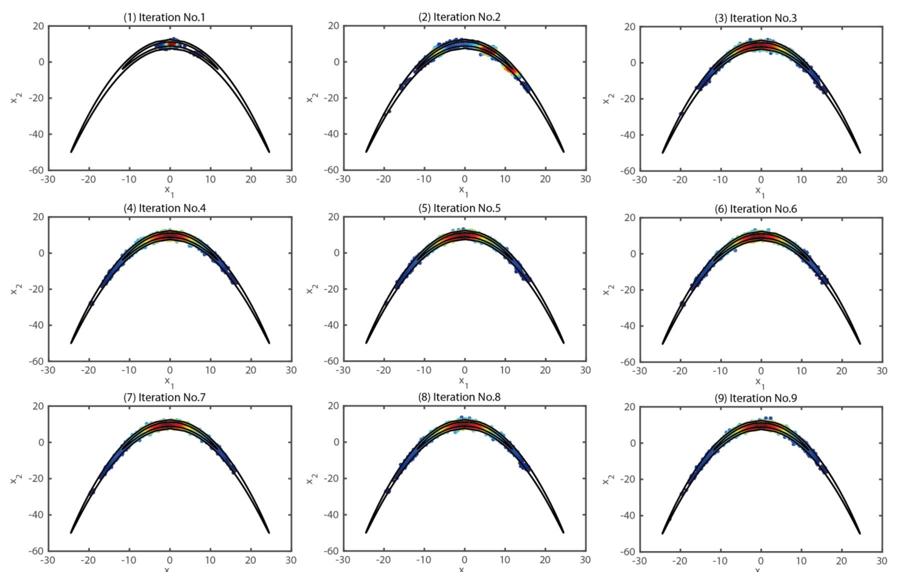
Flowchart of MC-ASMO



Two criteria for stratified adaptive sampling:
1) Similarity to the posterior from surrogate model
2) Keep far always from the evaluated points

Two steps of stratified adaptive sampling:
1) Sort the posterior samples and divide into h bins according to quantiles.
2) In each bin, select one point with largest distance to its evaluated neighbor.

Posterior distribution of banana function obtained by MC-ASMO (with only 1,000 model evaluations)



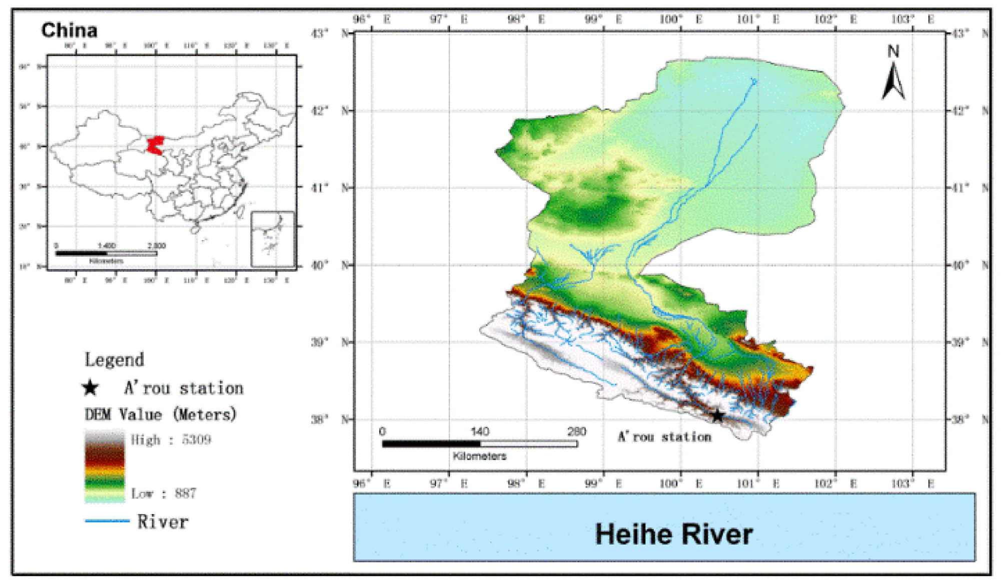
4. Case study

Model: Common Land Model (CoLM)
By Yongjiu Dai, GCESS, BNU

Study area: A'rou station
Heihe river basin, China

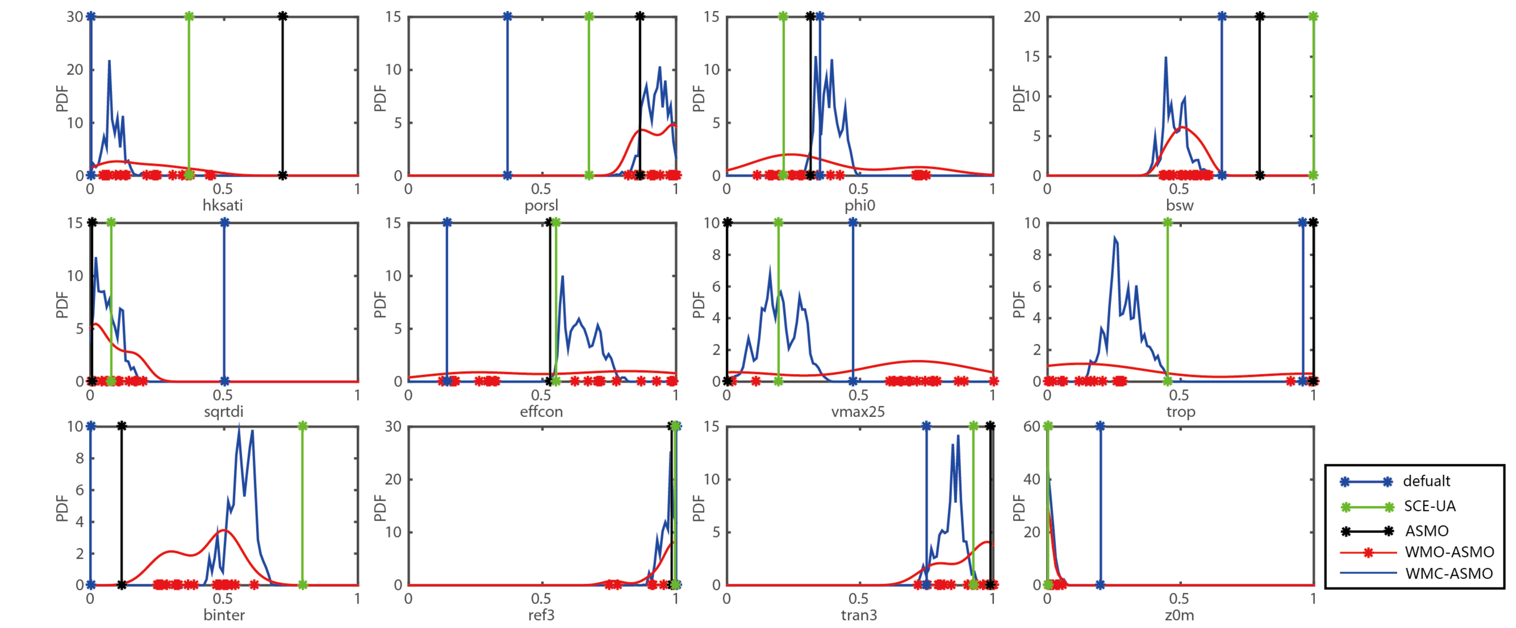
Date: 2008-01-01 to 2009-12-31

40 adjustable parameters, screened out 12 important parameters to tune.
6 objectives functions.

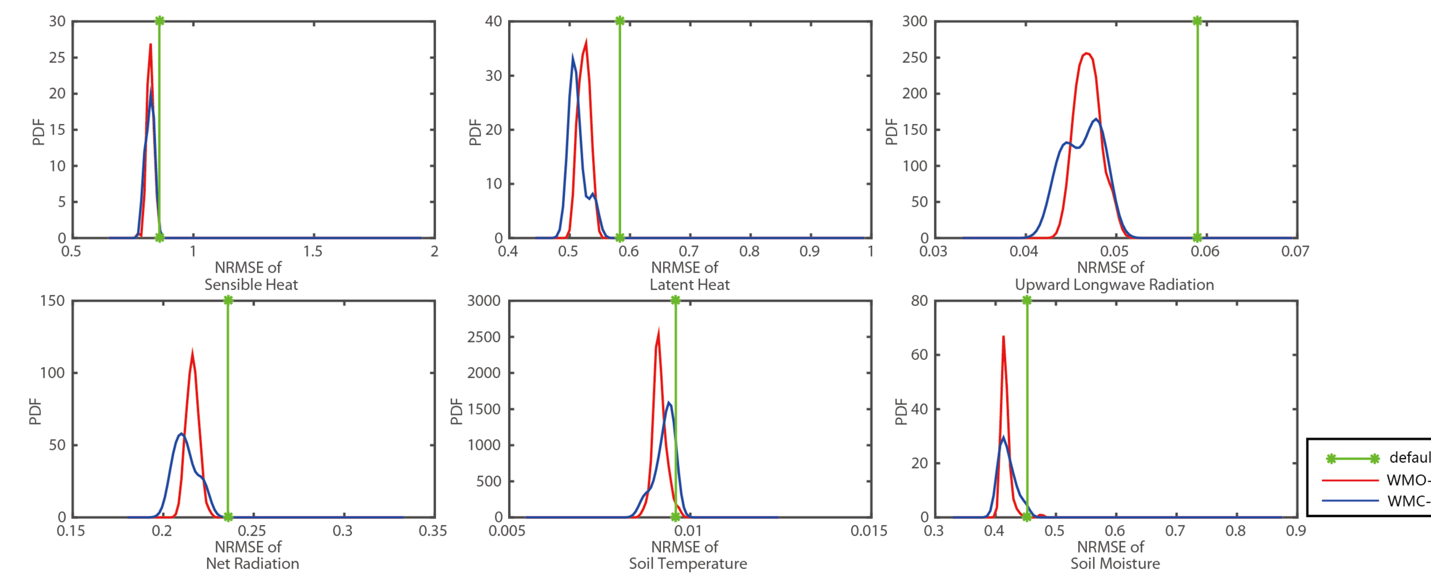


Study area

Calibrate CoLM with WMO-ASMO (500 model evaluations), and with WMC-ASMO (1,000 model evaluations)
[WMO-ASMO: MO-ASMO with weighted crowding distance; WMC-ASMO: MC-ASMO with weighted dominance function]



Pareto optimal points obtained by WMO-ASMO, posterior distribution obtained by WMC-ASMO, as well as optimal point obtained by SCE-UA, ASMO, and the default parameterization.



Posterior distribution of objective functions obtained by WMO-ASMO with 500 model evaluations, and by WMC-ASMO with 1,000 model evaluations.
Simultaneously improving all of the objectives with a small number of model evaluations.

5. Conclusions

- Comparing MO-ASMO vs NSGA-II, MC-ASMO vs DRAM, MO-ASMO and MC-ASMO can reduce the number of model evaluations from 10^5 to 10^2.
- MO-ASMO and MC-ASMO can **simultaneously improve multiple objectives** with the information of default parameter.
- MC-ASMO can draw the posterior distribution like classical MCMC approaches.
- MO-ASMO and MC-ASMO are compatible with various kinds of initial sampling, surrogate modelling, embedded multi-objective optimization and MCMC methods.
- Optimal use of MO-ASMO and MC-ASMO have also been discussed in the original papers.

References

MO-ASMO: Gong, W., Q. Duan, J. Li, C. Wang, Z. Di, A. Ye, C. Miao, and Y. Dai (2016), Multiobjective adaptive surrogate modeling-based optimization for parameter estimation of large, complex geophysical models, Water Resour. Res., doi:10.1002/2015WR018230.
MC-ASMO: Gong, W., Q. Duan (2016), Stratified Adaptive Resampling Strategy for Surrogate-based Markov Chain Monte Carlo, Water Resour. Res., (in prepare).
Initial sampling: Gong, W., Q. Y. Duan, J. D. Li, C. Wang, Z. H. Di, A. Z. Ye, C. Y. Miao, and Y. J. Dai (2015a), An Intercomparison of Sampling Methods for Uncertainty Quantification of Environmental Dynamic Models, J. Environ. Inform., (in press), doi:10.3808/jei.201500310.
Surrogate modeling: Gong, W., Q. Duan, J. Li, C. Wang, Z. Di, Y. Dai, A. Ye, and C. Miao (2015b), Multi-objective parameter optimization of common land model using adaptive surrogate modeling, Hydrol Earth Syst Sci, 19(5), 2409–2425, doi:10.5194/hess-19-2409-2015.
Parameter screening: Li, J., Q. Y. Duan, W. Gong, A. Ye, Y. Dai, C. Miao, Z. Di, C. Tong, and Y. Sun (2013), Assessing parameter importance of the Common Land Model based on qualitative and quantitative sensitivity analysis, Hydrol Earth Syst Sci, 17(8), 3279–3293, doi:10.5194/hess-17-3279-2013.