Sample n-1 points in the parameter space using surface evolver (n around 200 for starting). X denotes the parameter space (1x nparameters)

PCA is carried out on the output EFD features generated for the n-1 starting points. Loadings are stored

Data D: (x1:n-1, PC11:n-1) is constructed where x represents the SE parameter values and PC1 denotes the first principal component of the data

Build a GP model where x is treated as input and PC1 as output

Optimizing the GPR:

FOR I = 1:Nsampling

* Sample nth point using the acquisition function defined over the GPR model. Point xn is sampled using the rule: .
  + Sample the parameter space using LHS for 100000 points (x)
  + Estimate the acquisition function at the points
  + Select the x for which the acquisition function is maximum
* Use surface evolver to get SE-EFDn for the newly sampled parameter values xn using the acquisition function
* Transform the SE-EFDn to PC1 using the loadings of PCA and add noise to the model
* Add the samples to the existing data and update the GP

END

Expected Improvement is chosen as the acquisition function

Where,

References:

http://krasserm.github.io/2018/03/21/bayesian-optimization/