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Bachelor / Master Thesis:
Investigations on Different Sampling Strategies in a Hybrid Initialization Approach for Solving Large Nonlinear Algebraic Systems

In order to solve large nonlinear algebraic systems numerically a hybrid initialization method is currently developed at our department. In a first step user provided initial bounds for the iteration variables are tightened to feasible intervals by a box reduction algorithm based on interval arithmetic. This results in sub boxes that potentially contain system's solutions. Secondly, sample points are generated within these boxes and the most promising ones measured by the system's function residuals are used as initial points for state-of-the-art global optimization methods.

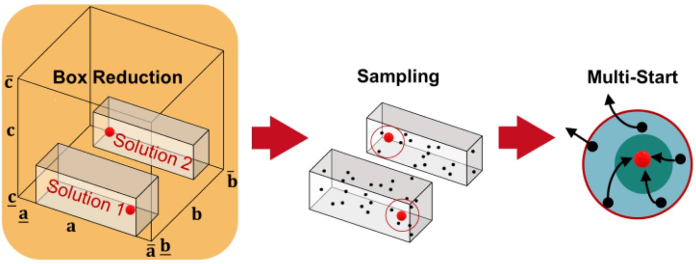

Figure 1 Hybrid approach for initialization

This method has been successfully applied on relatively small and simple examples (up to a system dimension of 120). A drawback in higher dimensional systems is that their reduced boxes are still comparably large which results either in a low point density and rather bad initial points for the multi-start procedure or in intractable computational costs to achieve a suifficient point density.

In this master thesis different approaches shall be investigated to improve the currently used sampling method. One idea is to use linear algebraic decomposition methods to identify independent sub systems in the overall system and generate only sampling points within their individual boundaries. Alternatively, the decomposition methods could be used for the identification of "tearing variables", i.e. variables with the highest number of occurrences in the system's equations. Subsequently only the space spanned by the bounds of the tearing variables is sampled and the system is solved for all other variables at the constant sample points. This generates consistent initial points for the multi-start procedure.

Large equation systems related to chemical engineering problems have already been implemented in MOSAICmodeling and will be provided for this Thesis. The linear decomposition methods are already part of the existing Python package related to the described hybrid approach. Modifications of the present sampling method need to be implemented in Python.

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