Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

A Decomposition Approach to Feasibility for Decentralized Operation of Multi-stage Processes

Ekundayo Olorunshe[a], Nilay Shah[a], Benoît Chachuat[a] and Max Mowbray[a]*

[a] The Sargent Centre for Process Systems Engineering, Imperial College London, London, United Kingdom
* Corresponding Author: m.mowbray@imperial.ac.uk

ABSTRACT

The definition of strategies for operation of process networks is a key research focus in process systems engineering. This challenge is commonly formulated as a numerical constraint satisfaction problem, where most practical algorithms are limited to identifying inner approximations to the feasible operational envelope. Sampling-based approaches so far have only been developed for formulations that required coordinated operation of the units within the network. We propose a decomposition approach that enables decentralized operation for acyclic muti-unit processes by sampling. Our methodology leverages problem structure to decompose unit-wise and deploys surrogate models to couple the resultant subproblems. We demonstrate it on a serial, batch chemical reactor network. In future research, we will extend this framework to consider the presence of uncertain unit parameters robustly.

Keywords: Process Operations, Machine Learning, Numerical Methods, Algorithms, Simulation

INTRODUCTION

Constraint Satisfaction and Process Operation

Significant interest within the process systems engineering community has been directed towards the numerical solution of constraint satisfaction problems (CSP) to define process operational strategies. This is underpinned by decision problems such as the feasibility and flexibility index, introduced in the early 1980s [1]. In pharmaceutical manufacturing, recent research has focused on design space characterization [2], as the multidimensional combination and interaction of input variables (e.g., material attributes) and process parameters that have been demonstrated to provide assurance of quality. The design space can be understood as the feasible space (FS) of operational parameters that ensure the process' defining constraints are satisfied.

Most research to date has focused on characterizing the FS within single-unit systems, with comparatively less attention to multi-unit systems [3]. However, manufacturing processes are inherently integrated, making it essential to investigate the interactions between unit operations. Typical approaches to identifying multi-unit FS are underpinned by mathematical programming and sampling [1,3]. The former approach is computationally efficient but has limitations in its application. For example, the problem formulation aims to identify a convex inner approximation to the FS – itself generally nonconvex - and defines a multilevel program. Therefore, identifying global optima is a challenge and significantly conservative solutions can be returned. Instead sampling approaches may aim to build a discrete set of operational parameter values that provide an inner approximation to the FS. Given they rely only on model evaluations they are an approach particularly suited to characterizing nonconvex FS [2].

In the context of multi-unit systems, there are two strategies: centralized (CO) and decentralized (DO) operation. These paradigms govern how decisions are made and how constraints are managed across interconnected units within a network. Effective management of such systems requires careful consideration of these strategies, as each offers distinct advantages and tradeoffs. CO treats the system monolithically, with decisions made by a single entity that has complete visibility of the entire network. This approach enables the best coordination across units. For example, a CO can adjust upstream and downstream parameters jointly to meet constraints, ensuring that the system operates cohesively. However, it often requires complex communication systems and can face bottlenecks when dealing with high-dimensional problems [5]. DO divides the system into smaller, autonomous units that make decisions locally. Each unit operates within its defined FS, independently of upstream or downstream units. This implies the decentralized FS is a subset of the centralized one. This approach reduces the need for communication and enables robust operations, particularly in distributed systems where central coordination is impractical. This autonomy enhances fault tolerance and scalability [5]. However, DO requires local FS to account for all possible interactions between adjacent units, which may lead to significantly reduced flexibility.

Contributions

Two major challenges exist in the identification of decentralized multi-unit FS through sampling. The first is the system dimensionality. Applying the logic of the curse of dimensionality, as the size of the process network grows, the volume of the search space increases exponentially, which can imply a dramatic increase in computational expense. In this research, a decomposition strategy is proposed that formulates a series of unit-wise problems, solved incrementally via sampling. In doing so, the approach exploits network structure, retaining the advantages of sampling solutions and mitigating the curse of dimensionality. The second challenge is ensuring that the solution returned provides an FS of maximum volume. In the discussion below, we outline a methodology that leverages this network structure to enhance sampling efficiency for identification of a solution set of maximum volume. The key contributions include:

1. Developing a class of CSPs built upon a directed acyclic graph (DAG) structure representative of the process network to define a DO strategy.
2. Introducing constraint propagation methods that work relative to a precedence order defined by the DAG structure of the CSP.
3. Applying sampling-based solvers for constraint propagation to identify decentralized FS for multi-unit systems.
4. Formulation of a log marginal likelihood maximisation to optimize the volume of FS solution returned.

The paper is organised as follows. Section 2 introduces the methodology, then Section 3 provides details of case study and results, and conclusions are provided in Section 4. Note that details of sampling approaches to solve relevant CSP are omitted for conciseness. For discussion the reader is directed to [2].

METHODOLOGY

Problem Statement

The problem setup assumes a network of interconnected unit operations. This can be represented on a DAG, $\mathcal{G} \coloneqq (\mathcal{N}, \mathcal{E})$, where $\mathcal{N}$ is the set of units, denoted as $\mathcal{N} \coloneqq \{1, \dots, N\}$, and $\mathcal{E}$ represents the edges, which denote the order of connection between units, with $(i, j) \in \mathcal{E}$ indicating a connection from unit i to unit j. The connectivity of the graph may also be expressed using an asymmetric adjacency matrix $A \in \{0,1\}^{N \times N}$, where $A_{i,j} = 1$ indicates a directed flow between unit i and unit j. The following data and restrictions are assumed for simplicity of presentation:

- A set of upstream units, $\mathcal{N}_i^{in} \subset \mathcal{N}$, with $card(\mathcal{N}_i^{in}) \leq 1$, which provide feed streams to unit $i \in \mathcal{N}$.
- A set of downstream units, $\mathcal{N}_i^{out} \subset \mathcal{N}$, with $card(\mathcal{N}_i^{out}) \leq 1$, which receive product streams from unit $i \in \mathcal{N}$.
- The attributes, $\boldsymbol{u}_i^j \in \mathbb{R}^{n_{u_{ij}}}$, of any feed stream connected to unit i from upstream unit $j \in \mathcal{N}_i^{in}$.
- The attributes, $\boldsymbol{y}_i^k \in \mathbb{R}^{n_{y_{ik}}}$, of any product stream from unit i connected to downstream unit $k \in \mathcal{N}_i^{out}$.
- The properties of the product streams of unit i defined as,

$$\boldsymbol{y}_i^k = \boldsymbol{F}_i^k\,(\boldsymbol{v}_i, \boldsymbol{u}_i), \tag{1}$$

where $\boldsymbol{v}_i \in \mathbb{R}^{n_{v_i}}$ are process parameters local to unit i, and $\boldsymbol{u}_i \coloneqq \left(\boldsymbol{u}_i^j\right)_{j \in \mathcal{N}_i^{in}} \in \mathbb{R}^{n_{u_i}}$ denotes the concatenation of all inlet stream properties to unit i.

- The connection between the stream properties at the outlet of unit i and those at the inlet of the downstream unit $k \in \mathcal{N}_i^{out}$, related by,

$$\boldsymbol{u}_k^i = \mathbf{C}_k^i(\boldsymbol{y}_k^i)\,. \tag{2}$$

- The inequality constraint functions imposed on each unit in the process train, expressed,

$$\mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \coloneqq \boldsymbol{g}_i(\boldsymbol{v}_i, \boldsymbol{u}_i, \boldsymbol{y}_i) \preccurlyeq \mathbf{0}. \tag{3}$$

Using the data associated with the setup, the centralized problem formulation is defined [3],

$$\mathbb{V}_{\mathrm{CO}} \coloneqq \left\{ \boldsymbol{v} \in \mathcal{K}_v \middle| \begin{array}{c} \forall i \in \mathcal{N}, \exists\, (\boldsymbol{u}_i, \boldsymbol{y}_i) \in \mathbb{R}^{n_{u_i}} \times \mathbb{R}^{n_{y_i}} : \\ \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \boldsymbol{y}_i^k = \mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i), \forall k \in \mathcal{N}_i^{out} \\ \boldsymbol{u}_k^i = \mathbf{C}_k^i(\boldsymbol{y}_k^i), \forall k \in \mathcal{N}_i^{out} \end{array} \right\}, \tag{4}$$

with $\mathcal{K}_v \coloneqq \prod_{i \in \mathcal{N}} \mathcal{K}_{v_i} \subset \mathbb{R}^{n_v}$ denoting a compact set defined through prior knowledge. In [3], a solution approach is provided by approximately solving unit-wise subproblems,

$$\mathbb{VU}_{i,CO} := \left\{ (\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathcal{K}_{vu_i} \;\middle|\; \begin{array}{c} \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \forall k \in \mathcal{N}_i^{out}, \exists(\boldsymbol{v}_k, \boldsymbol{u}_k) \in \mathbb{VU}_{k,CO}: \\ \boldsymbol{u}_k^i = \mathbf{C}_k^i\left(\mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i)\right) \\ \forall j \in \mathcal{N}_i^{in}, \exists(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,CO}: \\ \boldsymbol{u}_i^j = \mathbf{C}_i^j\left(\mathbf{F}_j^i(\boldsymbol{v}_j, \boldsymbol{u}_j)\right) \end{array} \right\}. \quad (5)$$

An exact solution to these subproblems ensures that the unit-wise parameters, $(\boldsymbol{v}_i, \boldsymbol{u}_i)$, i) satisfy constraints defined on the unit, ii) produce output stream properties that in turn provide feasible input stream properties to downstream units $k \in \mathcal{N}_i^{out}$, and iii) all input variables $\boldsymbol{u}_i$ are produced as a result of feasible operation of upstream units $j \in \mathcal{N}_i^{in}$.

The decentralized FS is a subset, $\mathbb{V}_{DO} \subseteq \mathbb{V}_{CO}$, of the centralized. A decentralized unit-wise subproblem may also be defined,

$$\mathbb{VU}_{i,DO} := \left\{ (\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathcal{K}_{vu_i} \;\middle|\; \begin{array}{c} \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \forall k \in \mathcal{N}_i^{out}, \exists(\boldsymbol{v}_k, \boldsymbol{u}_k) \in \mathbb{VU}_{k,DO}: \\ \boldsymbol{u}_k^i = \mathbf{C}_k^i\left(\mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i)\right) \\ \forall j \in \mathcal{N}_i^{in}, \forall(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}: \\ \boldsymbol{u}_i^j = \mathbf{C}_i^j\left(\mathbf{F}_j^i(\boldsymbol{v}_j, \boldsymbol{u}_j)\right) \end{array} \right\}. \quad (6)$$

This subproblem (6) differs subtly from (5) and ensures that the unit-wise parameter values $\boldsymbol{v}_i$, i) satisfy constraints defined on the unit, and ii) produce output stream properties that in turn provide feasible input stream properties to downstream units $k \in \mathcal{N}_i^{out}$ for all input variables values $\boldsymbol{u}_i$ produced as a result of feasible operation of upstream units $j \in \mathcal{N}_i^{in}$. Solving these unit-wise subproblems and taking the Cartesian product, $\mathbb{V}_{DO} \coloneqq \prod_{i\in\mathcal{N}} \mathbb{V}_{i,DO}$ of the projection of the sets, $\mathbb{VU}_{i,DO}$ onto the subspace of unit-wise process parameters, $\mathbb{V}_{i,DO}$, yields the decentralized FS.

In practice, solving (6) is challenged as solution to any given unit requires knowledge of the solution to all other unit subproblems, i.e. one must already know a solution $\mathbb{V}_{DO}$. In the following, a sampling-based graph decomposition methodology is proposed that aims to identify a solution that maximizes a measure of the volume of $\mathbb{V}_{DO}$ with a minimum number of model evaluations.

A Decomposition Approach

In this section, a sampling-based solution algorithm that acts with respect to a precedence ordering defined on the graph, $\mathcal{G}$, is presented. The algorithm provides incremental solution of unit-wise subproblems $i \in \mathcal{N}$, which provide approximations to,

$$\mathbb{V}_{i,DO} := \left\{ \boldsymbol{v}_i \in \boldsymbol{\mathcal{K}}_{v_i} \;\middle|\; \forall k \in \mathcal{N}\backslash\{i\}, \exists \boldsymbol{v}_k \in \mathcal{K}_{v_k}: (\boldsymbol{v}_j)_{j\in\mathcal{N}} \in \mathbb{V}_{DO} \right\},$$

where $\mathbb{V}_{DO} \coloneqq \prod_{i\in\mathcal{N}} \mathbb{V}_{i,DO}$. Our main hypothesis is that a) solving this sequence of subproblems is more sample efficient than solving the problem directly, b) that doing so enables tuning of the solution set identified, and c) the solution yielded may be less conservative than other approaches by inheriting the advantages of sampling.

Subproblem relaxations and propagations

In the following, two subproblem relaxations are presented that represent two separate steps of the methodology. The first is referred to as the backward propagation; and the second, the forward propagation. They are applied sequentially to approximate (6).

The backward propagation has previously been presented in [3], and so its presentation is brief. The subproblem relaxation deletes constraints enforcing feasible operation upstream,

$$\mathbb{VU}_{i,DO}^{(\mathrm{b})} := \left\{ (\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathcal{K}_{vu_i}^{(\mathrm{b})} \;\middle|\; \begin{array}{c} \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \forall k \in \mathcal{N}_i^{out}, \exists(\boldsymbol{v}_k, \boldsymbol{u}_k) \in \mathbb{VU}_{k,DO}^{(\mathrm{b})}: \\ \boldsymbol{u}_k^i = \mathbf{C}_k^i\left(\mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i)\right) \end{array} \right\} \quad (7)$$

with constraints only considering operational viability of the unit and those downstream. The search space $\mathcal{K}_{vu_i}^{(\mathrm{b})} \coloneqq \mathcal{K}_{v_i} \times \mathcal{K}_{u_i}^{(b)}$ is estimated via an initialization procedure presented later in this paper. As discussed in [3], the relaxation admits an initial leaf unit problem that may be solved, given $\mathcal{N}_i^{out} = \emptyset$. As a result, the solution is according to the reverse of the precedence ordering. In principle the cartesian product set, $\mathbb{V}_{DO}^{(b)} = \prod_{i\in\mathcal{N}} \mathbb{V}_{i,DO}^{(b)}$ could be used as a search space reduction for identification of (4) as discussed in [3].

Utilizing the intermediate results in estimation of $\mathbb{VU}_{i,DO}^{(b)}$, the forward propagation is defined,

$$\mathbb{VU}_{i,DO}^{(\mathrm{f})} := \left\{ (\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathbb{VU}_{i,DO}^{(\mathrm{b})} \;\middle|\; \begin{array}{c} \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \forall k \in \mathcal{N}_i^{out}, \exists(\boldsymbol{v}_k, \boldsymbol{u}_k) \in \mathbb{VU}_{k,DO}^{(\mathrm{b})}: \\ \boldsymbol{u}_k^i = \mathbf{C}_k^i\left(\mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i)\right) \\ \forall j \in \mathcal{N}_i^{in}, \forall(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}^{(\mathrm{f})}: \\ \boldsymbol{u}_i^j = \mathbf{C}_i^j\left(\mathbf{F}_j^i(\boldsymbol{v}_j, \boldsymbol{u}_j)\right) \end{array} \right\}. \quad (8)$$

In addition to the properties of (7), (8) enforces that the selection of $\boldsymbol{v}_i$ be feasible given any unit input stream property from feasible upstream operation $j \in \mathcal{N}_i^{in}$. In contrast to (7), however, these subproblems are solved according to the precedence ordering of $\mathcal{G}$ proceeding from the root node forward. A solution may then be identified as $\mathbb{V}_{DO} = \prod_{i\in\mathcal{N}} \mathbb{V}_{i,DO}^{(\mathrm{f})}$.

Approximate solutions for general problems

Due to the general assumptions made in problem definition, identifying closed forms for these approximations is highly challenging. Instead, as in [3], adaptive sampling schemes are deployed to gain a discrete inner-approximation $\overline{\mathbb{VU}}_{i,DO}^{(d)} \subset \mathbb{VU}_{i,DO}^{(d)} \quad \forall\, d \in \{b, f\}$.

Parameterizations may then be identified to tackle (7) and (8).

Parameterizing the extended feasible space

As in [3] binary classifiers, $\bar{\mathbf{G}}_i: \mathbb{R}^{n_{v_i}} \times \mathbb{R}^{n_{u_i}} \to \mathbb{R}$ are learned to parameterize $\mathbb{VU}_{i,DO}^{(d)}$, as follows,

$$\mathbb{VU}_{i,DO}^{(\mathrm{d})} \approx \left\{(\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathcal{K}_{vu_i}^{(\mathrm{d})} \middle| 0 \geq \bar{\mathbf{G}}_i^{(\mathrm{d})}(\boldsymbol{v}_i, \boldsymbol{u}_i)\right\},$$

using training data generated in sampling the solution, $\overline{\mathbb{VU}}_{i,DO}^{(d)}$. Having detailed means to approximate the relaxations, discussion moves to outline a three-step solution methodology based on defining subproblems amenable to sampling solutions.

Step 0: Initialization of the unit-wise search spaces

First, estimate of $\mathcal{K}_{u_i}^{(b)}\ \forall i \in \mathcal{N}$ is gained through a box-outer approximation to data generated from a sampling-based initialization procedure. The data is generated by forward simulation of the process network under parameter values, $\boldsymbol{v}$, sampled from $\mathcal{K}_v$ according to a Latin hypercube design.

Step 1: Backward Propagation

Then, as in [3], approximation is made to (7). The existence conditions in (7) are recast as auxiliary optimization problems,

$$\mathbb{VU}_{i,DO}^{(\mathrm{b})} \approx \left\{(\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathcal{K}_{vu_i}^{(\mathrm{b})} \middle| \begin{array}{c} \mathbf{0} \succcurlyeq \mathbf{G}_i(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ \forall k \in \mathcal{N}_i^{out}:\ 0 \geq \min\limits_{\boldsymbol{v}_k, \boldsymbol{u}_k} \bar{\mathbf{G}}_k^{(\mathrm{b})}(\boldsymbol{v}_k, \boldsymbol{u}_k) \\ s.t.\ \boldsymbol{u}_k^i = \mathbf{C}_k^i\left(\mathbf{F}_i^k(\boldsymbol{v}_i, \boldsymbol{u}_i)\right) \end{array}\right\}.$$

The solution set is sampled, $\overline{\mathbb{VU}}_{i,DO}^{(b)} \subset \mathbb{VU}_{i,DO}^{(b)}$, through evaluation of the process model and constraints $\mathbf{G}_i(\cdot)$ and solution of a box-constrained nonlinear program (NLP). It is worth noting that the equality constraint is reduced into the objective, as $\boldsymbol{u}_k^i$ is provided through evaluation of the process model; additionally, the surrogate constraints $\bar{\mathbf{G}}_k^{(\mathrm{b})}(\cdot)$ are available from the solution of units $k \in \mathcal{N}_i^{out}$.

Step 2: Forward Propagation

With the approximation to (7) completed, approximation to (8) is then made. The robustness conditions in (8) are recast as auxiliary optimization problems. Conveniently evaluation of the existence conditions and constraints in (8) is avoided via the approximation. This removes the requirement for further process model evaluations, and instead only relies on the solution to general NLP defined on surrogates,

$$\mathbb{VU}_{i,DO}^{(\mathrm{f})} \approx \left\{(\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathbb{VU}_{i,DO}^{(\mathrm{b})} \middle| \begin{array}{l} \left.\begin{array}{c} 0 \geq \max\limits_{(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}^{(\mathrm{f})}} \bar{\mathbf{G}}_i^{(\mathrm{b})}(\boldsymbol{v}_i, \boldsymbol{u}_i) \\ s.t.\ \boldsymbol{u}_i^j = \bar{\boldsymbol{F}}_{j\to i}\left(\boldsymbol{v}_j, \boldsymbol{u}_j\right), \forall j \in \mathcal{N}_i^{in} \end{array}\right\}(i) \\ \forall j \in \mathcal{N}_i^{in}: \left.\begin{array}{c} 0 \geq \min\limits_{(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}^{(\mathrm{b})}} \bar{\mathbf{G}}_j^{(\mathrm{b})}(\boldsymbol{v}_j, \boldsymbol{u}_j) \\ s.t.\ \boldsymbol{u}_i^j = \bar{\boldsymbol{F}}_{j\to i}\left(\boldsymbol{v}_j, \boldsymbol{u}_j\right) \end{array}\right\}(ii) \end{array}\right\}$$

where $\bar{\boldsymbol{F}}_{j\to i}(\cdot) \approx \boldsymbol{C}_i^j\left(\mathbf{F}_j^i(\cdot)\right)$ is an ML regressor identified in the backward propagation. Within the formulation above, (i) enforces conditions on $\boldsymbol{v}_i \in \mathbb{V}_{i,DO}^{(\mathrm{f})}$ with (ii) enforcing restrictions on $\boldsymbol{u}_i \in \mathbb{U}_{i,DO}^{(\mathrm{f})}$, such that $\mathbb{VU}_{i,DO}^{(\mathrm{f})} = \mathbb{V}_{i,DO}^{(\mathrm{f})} \times \mathbb{U}_{i,DO}^{(\mathrm{f})}$. Specifically, (i) ensures that the selection of $\boldsymbol{v}_i$ satsfies constraints defined on the unit, and that outlet stream properties ensure feasibility downstream, no matter the operation of units upstream; whereas (ii) enables identification of the set of unit input stream properties arising from feasible operation upstream, identification of which is required for the purpose of decomposition. It is worth noting that the root node problems have no upstream units and so are only constituted by a modified variant of (i),

$$\mathbb{VU}_{i,DO}^{(\mathrm{f})} \approx \left\{(\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathbb{VU}_{i,DO}^{(\mathrm{b})} \middle| 0 \geq \bar{\mathbf{G}}_i^{(\mathrm{b})}(\boldsymbol{v}_i, \boldsymbol{u}_i)\right\} \quad \forall i \in \mathcal{N}^r$$

with $\mathcal{N}^r = \left\{ i \in \mathcal{N} \mid \mathcal{N}_i^{in} = \emptyset \right\}$. As before solution sets are sampled $\overline{\mathbb{VU}}_{i,DO}^{(f)} \subset \mathbb{VU}_{i,DO}^{(f)}$, and a solution returned as $\mathbb{V}_{DO} \approx \prod_{i \in \mathcal{N}} \overline{\mathbb{V}}_{i,DO}^{(f)}$.

Tuning step 2: A classifier backoff strategy

In most cases, multiple solution sets, $\mathbb{V}_{DO}$, exist, corresponding to different allocations of operational flexibility to each unit. Solving step 2 as defined provides greater operational flexibility to upstream units. To balance operational flexibility, we introduce tuning parameters, $\boldsymbol{\epsilon} \in \mathbb{R}_+^N$, in the forward propagation – one for each unit,

$$\mathbb{VU}_{i,DO}^{(\mathrm{f})}(\boldsymbol{\epsilon}) \approx \left\{(\boldsymbol{v}_i, \boldsymbol{u}_i) \in \mathbb{VU}_{i,DO}^{(\mathrm{b})} \middle| \begin{array}{l} \begin{array}{c} 0 \geq \max\limits_{(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}^{(\mathrm{f})}(\boldsymbol{\epsilon})} \bar{\mathbf{G}}_i^{(\mathrm{b})}(\boldsymbol{v}_i, \boldsymbol{u}_i) + \epsilon_i \\ s.t.\ \boldsymbol{u}_i^j = \bar{\boldsymbol{F}}_{j\to i}\left(\boldsymbol{v}_j, \boldsymbol{u}_j\right), \forall j \in \mathcal{N}_i^{in} \end{array} \\ \forall j \in \mathcal{N}_i^{in}: \begin{array}{c} 0 \geq \min\limits_{(\boldsymbol{v}_j, \boldsymbol{u}_j) \in \mathbb{VU}_{j,DO}^{(\mathrm{b})}} \bar{\mathbf{G}}_j^{(\mathrm{b})}(\boldsymbol{v}_j, \boldsymbol{u}_j) + \epsilon_j \\ s.t.\ \boldsymbol{u}_i^j = \bar{\boldsymbol{F}}_{j\to i}\left(\boldsymbol{v}_j, \boldsymbol{u}_j\right) \end{array} \end{array}\right\},$$

with root node unit problems adjusted appropriately. This implies the solution set is dependent on the parameters, $\mathbb{V}_{DO}(\boldsymbol{\epsilon})$. In the following, we utilize an adaptive sampling scheme, namely nested sampling as in [2] to provide a discrete inner approximation $\overline{\mathbb{VU}}_{i,DO}^{(\mathrm{f})}(\boldsymbol{\epsilon}) \subset \mathbb{VU}_{i,DO}^{(\mathrm{f})}(\boldsymbol{\epsilon})$. Nested sampling was initially proposed to estimate the marginal likelihood in Bayesian estimation problems. In the context of feasibility, the marginal likelihood has an interpretation as a measure of the volume of a set. Here, we exploit this as means of defining an objective for tuning the backoffs,

$$\min_{\boldsymbol{\epsilon}} -\sum_{i\in\mathcal{N}} \log Z_i(\boldsymbol{\epsilon}) \qquad (9)$$

where $Z_i(\boldsymbol{\epsilon}) = \int_{(\boldsymbol{v},\boldsymbol{u})\in K_{vu_i}} l_i\,(\boldsymbol{v}_i, \boldsymbol{u}_i, \boldsymbol{\epsilon}) p(\boldsymbol{v}_i, \boldsymbol{u}_i) d(\boldsymbol{v}_i, \boldsymbol{u}_i)$ is the marginal likelihood associated with the solution to the unit i subproblem, $\mathbb{VU}_{i,DO}^{(f)}(\boldsymbol{\epsilon})$. In implementation, $l_i\colon \mathcal{K}_{vu_i} \times \mathbb{R}_+^{N} \to \mathbb{R}$ is a continuous, non-negative monotonic approximation to the indicator function which assesses set-membership. Here $l_i(\boldsymbol{v}_i, \boldsymbol{u}_i, \boldsymbol{\epsilon}) = \prod_{l\in\{i\}\cup\mathcal{N}_i^{in}} l_{i,l}\,(\boldsymbol{v}_i, \boldsymbol{u}_i, \epsilon_l)$,

$$l_{i,l}(\boldsymbol{v}_i, \boldsymbol{u}_i, \epsilon_l) = \begin{cases} sigmoid(0) & \boldsymbol{if}\ z_{i,l}^*(\boldsymbol{v}_i, \boldsymbol{u}_i, \epsilon_l) \leq 0 \\ sigmoid\left(-z_{i,l}^*(\boldsymbol{v}_i, \boldsymbol{u}_i, \epsilon_l)\right) & \boldsymbol{otherwise} \end{cases}$$

with $sigmoid(\cdot)$ indicating the univariate, scalar sigmoid function, and $z_{i,l}^*(\boldsymbol{v}_i, \boldsymbol{u}_i, \epsilon_l)$ indicating the optimal objective value of the l^{th} auxiliary optimization problem, or the tightened constraint value in the case of the root-node, in the approximate forward propagation, $\mathbb{VU}_{i,DO}^{(f)}(\boldsymbol{\epsilon})$. Given the use of $l_i(\cdot)$ and assessment of the unit-wise subproblems, $\mathbb{VU}_{i,DO}^{(f)}(\boldsymbol{\epsilon})$, rather than the indicator function itself and the unit-wise projections, $\mathbb{V}_{i,DO}^{(f)}(\boldsymbol{\epsilon})$, this yields an approximation to a measure of the FS.

CASE STUDY

Problem formulation

We demonstrate the decomposition approach on a batch chemical reactor network that consists of two batch reactors connected in series. The reaction mechanism characterizing the reactors is the same, and is that described in [3],

$$2A \to^{k_1} B \to^{k_2} C$$

where component B is the desired product. The reactor dynamics are ODEs that describe the evolution of component molar concentrations in continuous time. The system adheres to Arrhenius kinetics, with $k_r(T)$, indicating the temperature (T) dependent rate constant of reaction step $r \in \{1,2\}$. For the definition of these Arrhenius kinetics please refer to the Digital Supplementary. The volume of both reactors is assumed $V = 1$ m^3. Each ODE system is given by,

$$\dot{c}_{A,j}(t) = -2k_1(T_j)c_{A,j}(t)^2$$
$$\dot{c}_{B,j}(t) = \mathrm{k}_1(\mathrm{T_j})\mathrm{c}_{\mathrm{A,j}}(\mathrm{t})^2 - \mathrm{k}_2(\mathrm{T_j})\mathrm{c}_{\mathrm{B,j}}(\mathrm{t})$$
$$\dot{c}_{C,j}(t) = \mathrm{k}_2(\mathrm{T_j})\mathrm{c}_{\mathrm{B,j}}(\mathrm{t})$$

where $c_{i,j}(t)$ $(kmol\ m^{-3})$ describes the molar concentration of component i in reactor j; and T_j, the temperature in reactor j. Each reactor is operated over a time horizon, $t \in [0,\ \tau_j]$, where τ_j is the batch time. The initial concentration of the first reactor is fixed, whereas the initial concentration of the second reactor is the first reactor's composition at the end of operation, subject to separation of C, as presented in [3]. This separation is considered perfect and, therefore, is excluded from the FS identification. The critical operational parameters in the characterization are the temperature and batch time of both reactors, such that $\boldsymbol{v_j} = [T_j, \tau_j]^T$. Inequality constraints are imposed to ensure the molar impurity of component C at the end of the first operation and on that of component B at the end of operating the second batch reactor:

$$\frac{c_{C,1}(\tau_2)}{c_{A,1}(\tau_2) + c_{B,1}(\tau_2) + c_{C,1}(\tau_2)} \leq b_1$$

$$\frac{c_{B,2}(\tau_2)}{c_{A,2}(\tau_2) + c_{B,2}(\tau_2) + c_{C,2}(\tau_2)} \geq b_2$$

with $b_1 = 0.15$ and $b_2 = 0.74$. The search spaces $\mathcal{K}_{v_1}$ and $\mathcal{K}_{v_2}$ are defined such that $\tau_j \in [250{,}800]$ (min) and $T_j \in [250{,}1000]$ (K).

Implementation Details

Full implementation details together with a description of the algorithm are available within Digital Supplementary. The Nested Sampling algorithm was utilised to solve each unit level problem using the DEUS package [2]. Each unit level problem was considered solved when $card\left(\overline{\mathbb{VU}}_i^{(d)}\right) = 2000$. Due to the nature of sampling algorithms a high degree of parallelisation was leveraged.

Initialization and then backward propagation steps were first applied, and neural network SoftMax binary classifiers and regressors with tanh activations were trained to high validation accuracy in solution to the unit level problems using the FLAX python package. Solution to the box-constrained NLP was provided by the L-BFGS-B implementation in OPTAX. The tuning problem (9) was then solved using a Bayesian optimization strategy. This consists of iteratively solving forward propagations using different values of $\boldsymbol{\epsilon}$. The decision bounds, $\boldsymbol{\epsilon} \in [0{,}0.5]^2$, were identified from knowledge of the range of the SoftMax binary classifier. An initial dataset was identified through a Latin hypercube space filling design on $\boldsymbol{\epsilon} \in [0{,}0.5]^2$ for 3 backoff values. In the forward propagations, the general NLP problems that couple the units were solved using IPOPT and formulated in CasADI. The ML surrogates were embedded using the CasADI callback feature, allowing JAX automatic differentiation routines to pass necessary Jacobian information. A Gaussian process model was built, exploited, and re-trained to optimize (8) using the expected improvement acquisition function and a budget of 7 additional samples to the initial dataset.

Results and Discussion

The results of the Bayesian optimization strategy to approximately solve (9) is shown in Fig. 1. Specifically, Fig. 1 shows the improvement in objective per evaluation of the forward propagation. The figure shows that in general the objective is improved in each iteration highlighting the approach's utility in expanding the flexibility or volume of the decentralized FS.

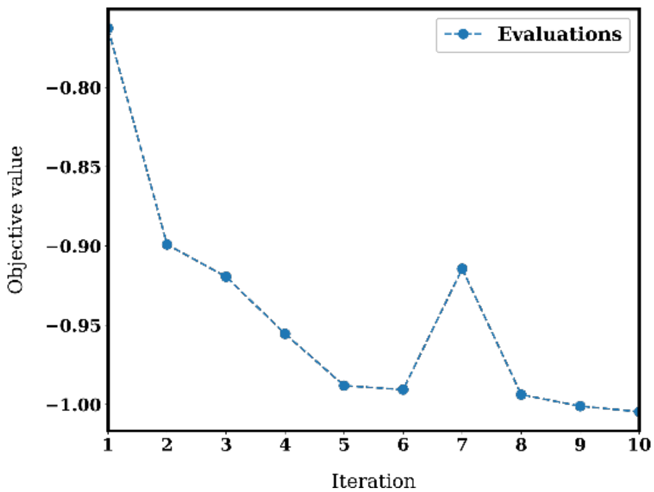

Figure 1: Tuning progress of the decentralized FS through Bayesian optimization.

The decentralized FS with largest volume from the optimization was identified during the 10th sample. The unit-wise projections of the discrete set to approximate (8) are plotted in Fig. 2 in red scatter. Also plotted in Fig. 2 are samples used to initialize the search spaces for the backward propagation (grey) and the centralized FS (blue). The latter was identified using the direct sampling method discussed in [3]. What is notable is that the decentralized FS is a proper subset of the centralized – yielding reduced flexibility. However, this is traded for a more robust operational strategy with lower capital overhead for implementation of control. The quality of the decentralized FS was verified by performing 10000 forward process network evaluations using operational parameters sampled from the approximation to $\mathbb{V}_{DO}$ – all of which yielded feasible operation. It should be emphasised that the approximation was identified using just 18092 evaluations of the unit models in total. Given the identified decentralized FS, $\overline{\mathbb{V}}_{DO} \subset \mathbb{V}_{DO}$, is constituted by 4×10^6 parameter settings this is a significant sample efficiency.

CONCLUSION

In this research, a decomposition strategy has been presented to sample decentralized feasible spaces for multi-unit process networks. The methodology leverages DAG formulations of process networks, adaptive sampling and machine learning surrogates to define constraint propagation methods that return inner-approximations to the feasible space efficiently. The methodology was applied to a serial batch reactor network and demonstrated to be effective in identifying a subset of the centralized FS to enable decentralized operation. Future work will consider robust formulations to account for uncertain model parameters.

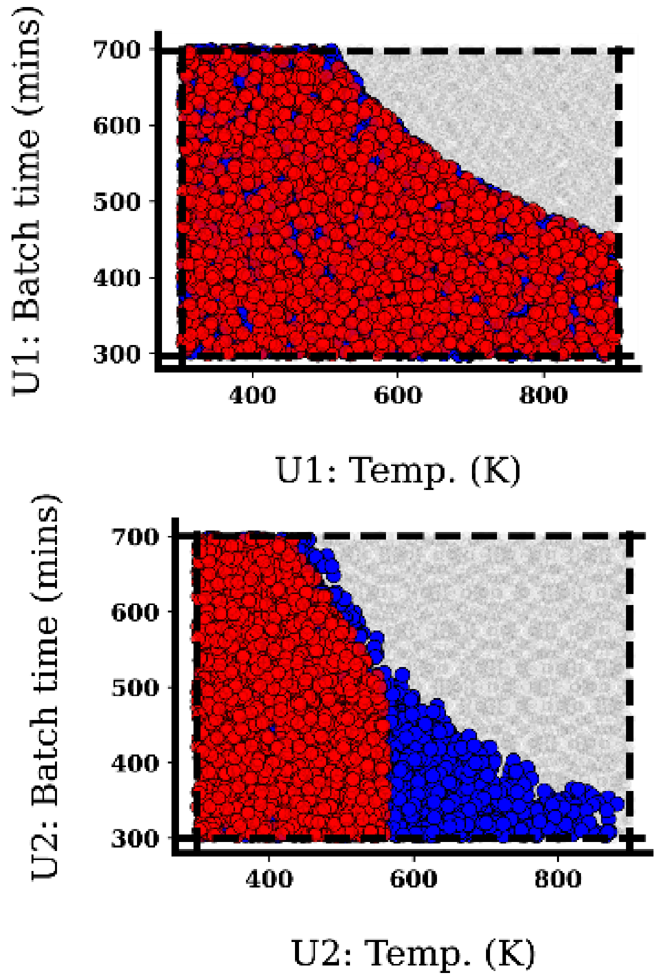

Figure 2: The optimized decentralized FS (red scatter), centralized FS projections (blue scatter), and samples used to initialise the search space (grey scatter).

DIGITAL SUPPLEMENTARY MATERIAL

Digital supplementary is provided by a Python software package, **μF**, available at: https://github.com/mawbray/mu.F. The DEUS package for solving numerical constraint satisfaction problems through Nested Sampling is available at https://github.com/omega-icl/deus.

ACKNOWLEDGEMENTS

This work is co-funded by Eli Lilly & Company through the Pharmaceutical Systems Engineering Lab (PharmaSEL) and by the Engineering and Physical Sciences Research Council (EPSRC) as part of its Prosperity Partnership Programme under grant EP/T518207/1. EO would like to acknowledge the support of Petroleum Technology Development Fund (PTDF) under grant number PTDF/ED/OSS/MSC/EMO/5672.

REFERENCES

1. Halemane, K. P. & Grossmann, I. E. (1983) Optimal process design under uncertainty. AIChE Journal. 29 (3), 425–433.
2. Kusumo, K. P., Gomoescu, L., Paulen, R., García Muñoz, S., Pantelides, C. C., Shah, N. & Chachuat, B. (2019) Bayesian approach to probabilistic design space characterization: A nested sampling strategy. Industrial & Engineering Chemistry Research. 59 (6), 2396–2408.
3. Mowbray, M., Kontoravdi, C., Shah, N., & Chachuat, B. (2024). A Decomposition Approach to Characterizing Feasibility in Acyclic Multi-Unit Processes. IFAC-PapersOnLine, 58(14), 216-221.
4. Harwood, S. M. & Barton, P. I. (2017) How to solve a design centering problem. *Mathematical Methods of Operations Research.* 86 215–254.
5. Samyudia, Y., Lee, P. L., Cameron, I. T., & Green, M. (1995). A new approach to decentralized control design. *Chemical Engineering Science*, *50*(11), 1695-1706.