THE FUTURE OF CONTROL OF PROCESS SYSTEMS

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Abstract

This paper provides a perspective on the major challenges and directions on academic process control research over the next 5-10 years, and its industrial implementation. Large scale systems control and identification, nonlinear model-based and model-free control, and controller performance monitoring and diagnosis are discussed as major directions for future research, along with control technology and industry workforce challenges and opportunities.

Keywords

Process systems, control theory, control technology, optimization

Introduction

This perspective will focus on assessment of the current state-of-the-art and promising future research and development directions on the control of process systems (chemical and petrochemical plants, oil refineries, biorefineries, pharmaceutical manufacturing plants, etc.). As we look back, the following major themes of academic process control research emerged over the last three decades:

- Nonlinear Control
- Model Predictive Control (MPC)
- Integration of operations and control

The advances have been impressive. Model-based nonlinear controller synthesis and estimation have reached a level of technical maturity that was hard to imagine 30 years ago. Optimization is firmly embedded in advanced process control (APC) methods. Process and controller performance monitoring methods have proliferated.

On the other hand, linear MPC technology continues to be the backbone of industrial control technology for more than three decades. There has been progress towards incorporating nonlinear components in plant-wide dynamic models, incorporating more efficient solvers for optimization problems at the advanced control layer, and implementing improved identification/estimation and controller performance monitoring methods. However, nonlinear modeling at a plant-wide scale remains a far-reaching goal, and so does the implementation of centralized nonlinear MPC technology. The quest for new technologies that will lead the next wave of innovation and enable step changes rather than incremental improvements is wide open.

Evidently, the gap between academic research and industrial needs persists and may even be growing. Academic research aims to push the technical boundaries towards improving performance and providing robustness and safety guarantees; it does so by employing increasingly sophisticated mathematical methods and formulations. Industry may be less interested in getting that next couple of percent of optimality and instead focused on how to

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implement and sustain these solutions in an automated fashion and reduced reliance on available experts.

Moving forward, major business and industry trends include:

- Increased emphasis on environmental sustainability, which puts greater demands on process control systems to enforce environmental regulations, with minimum overhead cost.
- Supply chain uncertainty putting a greater emphasis on automation to maintain optimality under dynamic conditions in raw material quality and availability.
- The (re-)emergence of artificial intelligence and machine learning which holds renewed promise for improved data utilization across industrial applications.

These trends further reinforce what have been the key drivers for process control research and development over the last few decades:

- Scale
- Nonlinearity
- Data

Large scale and complexity continue to be key features of industrial scale process control problems, due to material and energy integration within a plant, increased integration of operations (planning, scheduling, real-time optimization) with control, and integration at the business/enterprise level (systems-of-systems). Dealing with them requires the solution of large-scale optimization problems, often with discrete and continuous variables. The solution of such problems at scale remains a challenge.

Nonlinearity becomes especially important when the plant operates over a wide range of conditions, for example due to transitions between different operating conditions dictated by supply chain decisions. Such transitions will become more prevalent as the timescales between planning/scheduling and real-time control continue to converge. This should increase in the future as supply chain challenges are likely to remain.

Finally, the big data revolution we are currently witnessing across science, technology, and society at-large is bound to challenge our thinking on the role of data in automatic control and motivate intense research in this direction. More data may become available through improved sensing capabilities but the quality and information carried by the data may not justify the additional cost of obtaining it. Several additional questions arise: What will be the role of data in process modeling? How can data fuse with fundamental models for control and optimization? How can we quantify stability, performance, and robustness (the cornerstones of control) within a data-driven (or data-assisted) modeling and control framework? How are we taking advantage of the strides being made in Artificial Intelligence to improve the robustness and sustainability of control systems? These questions will undoubtedly frame future research in the next 5-10 years.

This paper will provide a perspective on future developments that have the potential to address these challenges. As exemplified by the merging of the FOCAPO/CPC series over the last 10 years, the continued *fusion of optimization and control* will be a key enabler to this end. Examples where such a fusion is essential from a control perspective include the solution of plant-wide control problems and the explicit handling of uncertainties in robust or stochastic MPC formulations. Another major enabler in our view will be the adoption of *modular, distributed* modeling, optimization, and control architectures and platforms, which can help mitigate the challenges of large scale, provide flexibility, agility, and robustness, and ultimately enable a transition from process automation to process autonomy.

In the backdrop of this discussion is the need to have the proper workforce that will be able to adopt and implement state-of-the-art control solutions in industry. Specifically:

- Expertise to develop and, equally importantly, maintain APC systems remains at a premium. To do so effectively requires both intimate process knowledge and an increasing mathematical expertise.
- An increasingly transient workforce makes it more difficult to cultivate and sustain this expertise in house. In addition, we will likely continue to see a hybrid workforce, which will create new challenges in recruiting and training the workforce that will lead the next wave of innovation.

The next sections further expand on these challenges and present our view towards future developments. We first focus on specific academic research directions that we view as particularly promising and then discuss industrial control technology and workforce training considerations and challenges for the next 5-10 years.

Large-Scale Systems Control and Identification

Due to the integration of mass, energy, and information, optimal decision making over large-scale systems are of increasing importance in modern process systems engineering practice. The pursuit for *scalability* is also a distinctive feature of process control research and an indispensable criterion for the effectiveness of process control methods.

Large-scale processes, or process networks, can be viewed as a collection of topologically interconnected process units from a physical perspective, or interrelated variables and constraints from a computational perspective. To control process networks, it is necessary to decompose the physical process (as represented by its dynamical model) or the mathematical problem of interest into (interacting) *subsystems*. Such a decomposition approach dates to the classical interaction analysis for pairing inputs and outputs into multiple control loops (McAvoy, 1983) developed since 1960s, and D-stability analysis in the context of robust control (Yu & Fan, 1990). It is also embodied in the research on the control of multi-time-scale systems (Baldea & Daoutidis, 2007), where fast dynamics are separable from the slow ones on an approximate inertial manifold, and dissipative systems (Hioe et al., 2013), where the dissipativity of any interconnected system can be inferred from the subsystems' dissipativity.

Distributed optimization and coordination

Distributed control (Christofides et al., 2013) offers a structured and flexible architecture for large-scale process control. On one hand, control is performed based on subsystems, invoking subsystem solvers for the decision making. On the other hand, communication is allowed among the subsystems, so that the optimal decision can be reached with less or no compromise.

In general, one can consider the problem of distributed control in the form of *nonconvex constrained optimization* (e.g., Tang & Daoutidis (2022a)). The formulation involves n blocks of decision variables $x_1, x_2, ..., x_n$ (corresponding to the subsystems) and a small block of auxiliary variables z (arising from the interactions among the subsystems):

$$\begin{aligned} \min \quad & \sum_{i=1}^{n} f_i(x_i) + g(z) \\ \text{s.t.} \quad & A_i x_i + C_i z = b_i \\ & x_i \in \mathbf{X}_i, z \in \mathbf{Z} \end{aligned} \quad . \tag{1}$$

In formulation (1), the set constraints $\mathbf{X}_1$, $\mathbf{X}_2$, ..., $\mathbf{X}_n$ are generally nonconvex, comprising of nonlinear equality and inequality constraints in algebraic expressions, and the objective terms f_1, f_2, ..., f_n can also be nonconvex. The constraints and objective term on z can be assumed to be simple without loss of generality. For problem (1), when z is fixed, the subsystem problems can be separated and solved through dedicated nonlinear programming solvers (or simpler linear/quadratic programming solvers). Therefore, the key question for *distributed optimization* (Boyd, 2011; Yang et al., 2019) is to find a coordination scheme to iterate z so that the subsystem solutions approach an optimal (in fact, what can usually be guaranteed is stationary) solution of the monolithic problem (1).

The first distributed optimization that guarantees the convergence under nonconvex constraints was proposed in Sun & Sun (2019), where a two-layer scheme is used to guarantee the convergence of x through the inner-layer iterations and decay of z through outer-layer iterations. The algorithm was further refined in Tang & Daoutidis (2022a) to improve the computational efficiency, where an Anderson acceleration scheme (Zhang et al., 2020) is used to reduce the inner iterations, and adaptive tolerances are set to terminate the subsystem solver in a timely manner during the intermediate iterations. An alternative single-layer algorithm was proposed in Subramanyam et al. (2021), where a large penalty parameter for $\|z\|^2$ is chosen according to the desired ultimate error and fixed.

Noting that the real-time implementation of MPC usually cannot allow many iterations but instead must be early terminated, the recent work of Tang & Daoutidis (2021) proposed a primal algorithm, where suitably defined ℓ_1 and squared ℓ_2 penalty of z are added to the objective function to define a robust upper estimation of the control-Lyapunov function (called the Lyapunov envelope). The upper bound property is derived from the incremental dissipativity of subsystems. In such a way, the primal iterations that reduce the envelope value can guarantee closed-loop stability even when early terminated. Evidently, there are still only very few algorithms for distributed optimization of nonlinear processes, and the development of well-performing and efficient algorithms will be an important future direction.

The complexity of these algorithms and the narrowing of expertise available to truly understand them may exceed industry's ability to manage them. The self-sustainability of these solutions will become a critical factor in industry's ability to get value from these solutions. As a result, research direction and funding entities should include the adaptability and sustainability of these solutions as key research elements. Tesla does not expect the driver to continuously retune the algorithm in a self-driving car so why should the process industry think differently?

Network structure analysis for decomposition

For distributed control and optimization, one first needs to decompose the system. By representing the dynamic model as a network (i.e., a graph of nodes and edges), extensive works have proposed to decompose the network through detecting the underlying *community structures* in the network topology (Daoutidis et al., 2018; Daoutidis et al., 2019). Specifically, communities refer to the blocks of nodes that interconnect densely inside but loosely in-between (Fortunato & Hric, 2016). Typically, community detection is performed by an approximate algorithm to maximize a modularity or likelihood index, which captures the statistical difference between inter- and intra-community connection propensities (Newman, 2016).

The community detection-based decomposition approaches have been examined by several case studies to benchmark processes (Pourkargar et al., 2019) and extended to take into consideration the restriction on subsystems' observability (Yin & Liu, 2019; Masooleh et al., 2022). Community detection as an effective method of generating high-quality subsystem configurations for distributed control is supported by the studies on sparse optimal control of Laplacian dynamics associated with networks, where the sparsity of the feedback controller is rewarded due to the cost on feedback channels (Lin et al., 2013). It was found that the community structures of modular networks result in lower control cost with a modular controller, and that when the control cost is used as the fitness index, modularity emerges throughout simulated evolution (Constantino et al., 2019; Tang et al., 2019). Such decomposition approaches have also been extended to optimization (Mitrai et al., 2022). We note that the community detection approach has been implemented in the industrial advanced process control software of Shell and Yokogawa and was applied to an industrial-scale crude distillation process (Tang et al., 2023).

On the other hand, the community detection-based methods, as a tractable simplification of the combinatorial problem of finding the decomposition with rigorously certifiable optimal performance, neglect the details of the dynamics and may not guarantee a clear interpretation of the resulting systems. The development of network decomposition approaches that can accommodate prior process knowledge, process uncertainty and controller robustness, user-defined logic rules, or even performance specifications, is highly needed.

Network topology identification

The modeling of large-scale systems is also not trivial. While multi-input-multi-output (MIMO) approaches for system identification can usually be directly deployed on small-scale systems, for large-scale processes, it is difficult to obtain high-quality models without first determining the *topological structure* of the model. Specifically, since each output is typically affected by only a few local inputs, it is desirable to specify a candidate set of inputs, forcing the effect of any other input to be zero, before modeling the detailed dynamics of the system. As seen in the previous subsection, such topology information is also useful for determining the decomposition for distributed control.

The model structure specification based on engineers' manual selection, however, can be time-consuming and error prone. The aim of topology identification algorithms is to determine the unknown network structure of the dynamics automatically based on *data*. The typical representation of the structure is a *linear dynamic graph*, i.e., the edges between the nodes (variables) x_i and x_j correspond to nonzero transfer functions $H_{ij}(z)$ (Materassi & Salapaka, 2012).

$$x_i(t) = \sum_j H_{ij}(z) x_j(t) + e_i(t). \tag{2}$$

Each node x_i is possibly associated with an exogenous excitation signal e_i.

Depending on whether the graph is cyclic and whether there exist unobservable hidden nodes, a variety of methods have been proposed in the literature (Sepehr & Materassi, 2019; Subramanian et al., 2020; Veedu et al., 2021), and theoretical proofs have been given based on conditions on graph-theoretic conditions. Process networks are expected to be cyclic with hidden nodes, which fit into the recent advances in topology identification. However, restrictive assumptions are typically made on the excitation of variables, which may be necessary to uniquely determine the topology but may not be practically satisfied due to the correlations between variables that cannot be independently manipulated. The incorporation of first-principles prior knowledge in topology identification is an important future step.

Nonlinear Model-Based and Model-Free Control

Chemical processes are intrinsically nonlinear. For processes with strongly nonlinear behavior, local linear model approximations are not valid and nonlinear control methods are needed. An early review of nonlinear control algorithms and applications was given in Bequette (1991). With the development of NLP algorithms, nonlinear MPC has become the most representative method in the recent decades (Grüne & Pannek, 2017).

The development of machine learning and data-driven techniques and the integration of them into control theory have resulted in novel methods and perspectives for nonlinear process control. In the next three subsections, we discuss three different types of approaches to handle nonlinearity in dynamics and control, respectively. In short, the three ideas are (i) to model nonlinearity, (ii) to linearize nonlinearity, and (iii) to enclose nonlinearity, with decreasing reliance on the direct characterization of nonlinearity and increasing commonality with linear systems.

Black-box approximation of nonlinearity

Since first-principles nonlinear models are difficult to establish and guarantee to be accurate, it is then a straightforward idea to seek data-driven black-box approximations of the nonlinearity in dynamics, e.g., by allowing the model to have higher-order expansion terms (Doyle III et al., 1995). Neural networks, due to their universal approximation property, have been extensively used for modeling static nonlinearity appended to linear dynamics in Hammerstein-Wiener models (Su & McAvoy, 1993) or the entire nonlinear dynamics as recurrent neural networks (Wu et al., 2019). Many recent works have been devoted to enabling optimization solvers to handle neural networks (Schweidtmann & Mitsos, 2019; Ceccon et al., 2022), which are beneficial for online MPC computation. In a different vein, Gaussian processes, as nonparametric statistical models, can be inferred from data along with an accompanying probabilistic quantification of uncertainty, and hence have the advantage of providing robust stability guarantee in predictive control (Bradford et al., 2020).

Despite the capacity of function approximation, the criticism that black box fitting gives little physical insight has become common. However, this may not be entirely justified, since these approaches are intended to avoid modeling from first principles or keeping the human in the loop. We argue that the essential problem is how to *constrain the input-output behavior* of black-box models to ensure their stability or robustness, or to reconcile them with prior knowledge. Multiple studies (Fazlyab et al., 2019; Pauli et al., 2021) have formulated the problem of constraining Lipschitz constants (incremental gains) of neural networks as semidefinite programming (SDP), which is non-scalable. The recent work of Revay et al. (2021) proposed the recurrent equilibrium network (REN) architecture as the feedback interconnection of a linear dynamics and element-wise activation functions, which can provably incorporate incremental stability and dissipativity constraints without invoking SDP; instead, the constraints are used to define a new unconstrained parameterization of the REN and can be optimized with (stochastic) gradient search.

Linearization of nonlinear dynamics

The idea of treating nonlinear dynamics as a linear one by seeking a *global transformation* of coordinates was extensively used in input-output linearization for nonlinear model-based control (Kravaris & Kantor, 1990). In a data-driven setting, recent control-theoretic research focused on the construction of Koopman operators from data (Brunton & Kutz, 2022). Specifically, the Koopman operator for an autonomous system (assuming to be discrete-time for simplicity) $x(t + 1) = f(x(t))$ is a linear, usually infinite-dimensional operator K defined on the space of state-dependent functions:

$$K(\varphi) = \varphi \circ f, \forall \varphi : \mathbf{X} \to \mathbf{C}. \quad (3)$$

In the above definition, **X** is the set of states, **C** is the set of complex numbers, and ∘ represents composition, i.e., $(\varphi \circ f)(x) = \varphi(f(x))$.

To find a tractable, finite-dimensional approximation of K, one may use a finite number of linear, polynomial, and/or radial basis functions of states x or measurable output snapshots $y(t)$, $y(t - 1)$, ..., $y(t - L)$ as the observer functions to seek a linear dynamics. The methods using output snapshots are called dynamic mode decomposition (DMD) or extended DMD if nonlinear transformations are used (Williams et al., 2015). Noting that the existence of disturbances poses a robustness issue in the identification of Koopman operator, Huang & Vaidya (2018) formulated the DMD problem under bounded disturbances as a robust optimization (min-max) problem and converted it into a least-squares one under Frobenius norm regularization. To ensure that the finite-dimensional linear dynamics is closed, data-driven construction of the eigenfunctions of Koopman operator was proposed (Kaiser et al., 2021).

The data-driven construction of the Koopman operator or its eigenfunctions, however, apparently suffers from the "curse of dimensionality" due to its goal of linearizing the dynamics globally. Despite preliminary discussions for systems with special structures (Schlosser & Korda, 2021), the practical use of Koopman operator theory on large-scale systems remains an open question.

Model-free characterization of system behavior

If we consider the question of whether a complete and accurate model is indeed necessary for control, the answer may be negative. First, correct models barely exist. In a famous quote of George E. P. Box that people often refer to, "All models are wrong, but some are useful". Second, in terms of validating nonlinear or more complex physical models, you're practically limited by the measurements you have available. Does a fully nonlinear model of a distillation tower have value if we only have measurements at the top and bottom to validate the model? Third, it is possible to obtain the controller or control decisions based on some properties or information from the system without a full model. Such control-relevant information can be learned from the analysis of process data that reflects the underlying dynamics, possibly complex. We refer to this paradigm of learning-based control as *model-free control* (Tang & Daoutidis, 2022b).

For nonlinear systems, the dynamic behaviors can be characterized based on inputs and outputs in terms of L_2-gain, passivity, and in general, dissipativity (Kottenstette et al., 2014). Dissipativity refers to the existence of a input- and output-dependent supply rate function $s(u, y)$ that bounds the rate of change of a storage function $V(x)$, i.e., $\mathrm{d}V(x)/\mathrm{d}t \leq s(u, y)$. While under suitable input and output variable selections, first-principles thermodynamic analysis can be used to derive the dissipativity property (Alonso & Ydstie, 2001; Hangos et al., 2001), it is more convenient and generic to learn dissipativity from data, i.e., trajectory samples. Dissipativity learning for linear systems has been discussed based on Hankel matrices (Koch et al., 2021). Essentially, dissipativity captures an *enclosure* of the system's nonlinearity. The simplest case of a dissipative nonlinear system is a sector nonlinearity as in Lur'e systems (Brogliato et al., 2020).

In Tang and Daoutidis (2019, 2021), the framework of dissipativity learning control (DLC) was proposed. DLC entails the following steps.

(i) A linear parameterization of the supply rate is used, e.g., by restricting $s(u, y)$ to be a quadratic function so that it is parameterized by a symmetric matrix. The resulting parameters M are called *dissipativity parameters* and their range **M** need to be inferred from data.

(ii) The remaining part in $s(u, y)$ depending on u and y, integrated on any given trajectory, are called the *dual dissipativity parameters* Γ. With trajectory samples, the range of Γ, denoted as **G**, can be estimated through machine learning techniques.

(iii) According to the definition of dissipativity, **M** = **G*** (dual cone of **G**) can be subsequently estimated and used as the information for controller synthesis.

So far, the DLC framework is restricted to small-scale processes and simple forms of controllers, and the learning of dissipativity requires large offline trajectory samples with zero initial conditions. An online estimation scheme was recently proposed in Welikala et al. (2022), where the dissipativity parameter is in a one-dimensional simplified form. We believe that model-free control, due to its potential to largely reduce the effort of modeling, is a promising direction for further development. Extensions of model-free control methods and comparison studies versus identification-based control are needed to facilitate their practical implementation.

Controller Performance Monitoring and Diagnosis

Monitoring of controller performance and diagnosing the cause for performance deterioration is a practically important part of control technology, which provides the information about controllers under abnormal conditions, facilitates in-time controller maintenance, and improves the system reliability (Gao et al., 2016). The classical approach of Harris (1989) to score the control loops, by comparing the variance of the measured data and that under an ideal minimum variance controller (MVC) as the benchmark, has been widely used in practice. For multivariable systems, Yu and Qin (2008) proposed a rigorous statistical approach to identify the subspaces of severe performance deterioration and correlate them to individual variables or control loops. Generally, a wide range of machine learning techniques can be used for this purpose (Qin & Chiang, 2019).

It can be argued that the suitability of monitoring and diagnosis approaches depend on the method used by the controller to be monitored and diagnosed. As pointed out in the review of Gao et al. (2016), for model-based control such as MPC, the *detection of plant-model mismatch* is central to monitoring and diagnosis. The key question in such a detection task is to distinguish or separate the effect of plant-model mismatch from that of *disturbances* (and noises) in the closed-loop data. In the literature, diverse approaches have been proposed to this end, e.g., by (i) assuming prior knowledge of disturbance characteristics and obtaining a statistic that shows significance of a nonzero mismatch (Sun et al., 2013) or by (ii) correlating the input and output measurements with exogenous setpoint signals, thus removing the disturbance terms (Badwe et al., 2009). The latter type of approach is conceptually close to closed-loop identification (Van den Hof, 1998). However, in mismatch detection it is usually not required to re-identify a corrected model; instead, it suffices to judge whether the actual dynamics significantly differs from the nominal model.

An accompanying problem with mismatch detection is the modeling of disturbances and noises. In addition to their use in offset-free MPC (Pannocchia et al., 2015), system identification, and filter design, the disturbance and noise models are necessary for mismatch detection when the exogenous signals to decorrelate disturbances and noises are absent. However, the question of how to optimally determine their models based on historical data has not been well answered, although there exist methods for estimating the involved parameters under given model structures (Odelson et al., 2006; Rajamani et al., 2009). Recently, Caspari et al. (2021) proposed a semi-infinite programming formulation for optimizing the structure of disturbance models with maximum observable set subject to the rank condition for observability, which was applied to a small CSTR unit.

A final point is that the self-tuning and sustainability aspects of the developed monitoring methods will be critical in order for industry to take full advantage of these methods. These systems in practice need to work 99% of the time and do so without human intervention.

Control Technology and Industry Workforce

We close this paper with some thoughts and open questions on the future of control systems technology and the role of automation and human involvement in this future.

- *Workforce availability*: The COVID-19 epidemic has led to major supply chain disruptions and changes in workforce modalities. We expect these impacts to persist and bring forth challenges in workforce availability in industry, both at the level of engineers as well as that of operators. A key question that is critical to the future of control technology development and deployment is whether the process industries will be able to continue to attract and retain the best engineering talent available.

- *Lowering the maintenance burdens*: New advances in control technology are often justified by a demonstrated reduced deviation from the setpoint in the face of setpoint changes or disturbances. However, there is a need for metrics on the maintainability of these solutions in the face of changing feedstocks, failing sensors, differing demands, and other practical factors that impact industrial processes. As part of this, we lack concrete measures on the level of human intervention required to makes these solutions continuously derive value in the field. Yet without such measures, there is a risk of letting academic advances go to waste.

- *Automation vs. human intervention:* As planning and scheduling decisions are integrated with control systems, human decision-making is increasingly brought into the loop (pun intended). At the same time, automation and ultimately autonomy are major goals of industry. So how do we quantify the right balance between automation and human intervention? Making the control algorithm work symbiotically with the human (who is not an MPC expert) will be critical to success.

- *The role of AI*: Given the hype on big data and the increasing penetration of AI and machine learning in industry, it is natural to ask how best to take advantage of these advancements in control technology. In previous sections, we discussed aspects of this question, especially related to the role of data in deriving models for control and designing feedback control laws. The development of new AI-driven virtual sensors, which take advantage of audio, video, and other forms of signals as additional information to improve performance, and their integration with the control algorithms will also be vital.

- *Scaling down APC systems*: A lot of the discussion in this paper focused on the future of process control for established, large companies. However, major technological innovation is often seen in smaller companies (with a few hundred employees). If we want to raise the impact of process control, we must scale its deployment down to companies beyond the Fortune 500, which may not have large teams of control engineering experts. The development of APC systems and modules that are more portable and easier to implement on novel process systems will be necessary to make process control a more readily accessible technology.

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