White Paper

OptiRamp® Real-Time Simulation Technology

Process Virtualization for Large-Scale Optimization and Diagnostics

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Introduction

Computing algorithms for simulation and optimization is essential to the design and operation of continuous processes, such as natural gas compressor networks or power generation systems. Statistics and Control, Inc. (S&C) builds on the improvements in computation methods and substantial increases in computing power to provide its clients a high-fidelity method, referred to as OptiRamp® Real-Time Simulation Technology (RTST), that allows for effective analysis and designing current operating processes at scale. RTST handles large-scale calculations through its use of state-of-the-art parallel distributed processing techniques developed with an open-source architecture suitable for big data ecosystems. RTST uses a highly scalable, fault-tolerant distributed data system to perform vast quantities of statistical operations in real time. The patented OptiRamp suite of tools provides value to organizations by assimilating real-time data through its RTST computational engine and empowering S&C clients to make rapid process decisions to optimize the operation of large-scale processes. This white paper provides an overview of the OptiRamp process virtualization concept, describes how OptiRamp RTST is used for large-scale production process optimization and diagnostics (illustrated through the application of a large-scale compressor network), and presents benefits of such technology over standard static model approaches when applied to large, multidimensional models.

OptiRamp Process Virtualization

Optimal operation of large-scale processes poses a formidable computation problem due to ever-changing process characteristics resulting in highly complex multi-dimensional relationships that need to be described by the process models. Typically, original equipment manufacturers (OEMs) provide process operators with data and specifications used to construct initial static process models of all necessary equipment and components, which provides a good start for process modeling; however, over time, as process conditions change and equipment degrades (as quickly as a month from commissioning), these models no longer describe the intricate relationships across all process components and operators lose visibility into the overall technological process.

S&C offers large-scale process operators a highly accurate view into the technological process by constructing and continuously updating dynamic process models through the creation of a real-time virtual process, which continuously runs in parallel to the actual process and mimics its
behavior in real time with high accuracy. The OptiRamp process virtualization concept is illustrated in Figure 1.

Creating a concurrent virtual process serves two major purposes: auto-tuning and accuracy analysis (see the left side of Figure 1) and prediction, optimization, diagnostics, and control (right side of Figure 1). In auto-tuning and accuracy analysis, the virtual process adjusts the initial models by aligning simulated variable values to real-time process values through auto-tuning. Auto-tuning minimizes the variance between real-time and simulated values and adjusts model coefficients accordingly. At every time scan, the current process values are compared with simulated data to determine overall model accuracy. When predefined accuracy is achieved, the operator can set process and economic objectives and initiate the Optimization algorithm. For additional information about how accuracy is achieve, refer to the OptiRamp Accuracy Submodule white paper.

Process simulation occurs concurrently with the real process, and all calculations are performed during the computation stages of OptiRamp signal processing. Process variable values are generated in accordance with established relationships among process variables, including laws of conservation of mass and energy, fluid properties, and state equations. RTST inputs are the current operating mode and OEM-configured process models, e.g., compressor characteristics at different speeds, piping diagrams, etc. Simulated variables are generated for every time scan corresponding to measured variable values. The simulation algorithm uses particle filtering methods based on dynamic state space models described by equation (1).

\[
\begin{align*}
\{w_t &= f(w_{t-1}) \\
\{ x_t &= g(w_t) \}
\end{align*}
\] (1)
where \( f \) and \( g \) are estimated using polynomial regression, \( w_t \) is a vector of state parameters at time \( t \), and \( x_t \) is a vector of observed (measured) variables at time \( t \). Then \( w_t \) is estimated using Sequential Monte Carlo (SMC) sampling (from a simulated distribution).

SMC is a method of estimating model parameters by simulating many weighted samples that asymptotically approximate the desired parameter’s posterior distribution. For completeness purposes, the SMC theoretical background is provided below.

Let \( \{ \pi_n \}_{1}^{p} \) be a sequence of probability measures (e.g., posterior distribution of the parameter in question given information until time \( n \)) defined on a measurable space \( (E, \varepsilon) \). The SMC method generates a large collection of \( N \) weighted random samples \( \{ W_n^{(i)} , X_n^{(i)} \} \) with \( i = 1, \ldots, N, \)

\( W_n^{(i)} > 0 \) and \( \sum_{i=1}^{N} W_n^{(i)} = 1 \) such that equation (2) holds whenever \( N \to \infty \).

\[
\sum_{i=1}^{N} W_n^{(i)} \varphi(X_n^{(i)}) \to \int_{E} \varphi(x) \pi_n(x) dx ,
\]

where \( \varphi \) is any \( \pi_n \)-integrable real-valued function defined on \( E \), i.e., the empirical distribution of \( \{ W_n^{(i)} , X_n^{(i)} \} \) converges asymptotically to \( \pi_n \). These weighted samples are usually referred to as particles and, hence, SMC is often called a particle filter.

For best results, OptiRamp uses the sequential SMC sampler algorithm proposed by Doucet, et al. in 2006. The algorithm consists of three steps: initialization, resampling, and sampling.

During initialization, the algorithm sets \( n = 1 \) for \( i = 1, \ldots, N \) and samples \( X_1^{(i)} \sim \eta_1 \), where \( \eta_n \) is the importance distribution defined by equation (3).

\[
\eta_n(dx) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_n^{(i)}}(dx) ,
\]

where \( dx \) is the dominating measure and \( \delta \) is the Dirac measure. Next, initialization evaluates \( w_1(X_1^{(i)}) \) according to equation (4) and normalizes these weights to obtain \( \{ W_1^{(i)} \} \).

\[
w_n(x) = \gamma_n(x) / \eta_n(x) ,
\]

where \( \gamma_n(x) \) is a positive, real-valued function known as pointwise. The algorithm iteratively completes resampling and sampling steps. During resampling, the algorithm evaluates whether \( \left\{ \sum_{i=1}^{N} W_n^{(i)} \right\}^{-1} < T \) (with \( T \) being a given threshold), resamples the particles, and sets \( W_n^{(i)} = 1/N \). During sampling, the algorithm sets \( n = n + 1 \) (stops if \( n = p + 1 \)), samples \( X_n^{(i)} \sim K_n \left( X_n^{(i)} ; \right) \) (where \( K_n \) is an ergodic Markov kernel), and normalizes equation (5).

\[
W_n^{(i)} = W_{n-1}^{(i)} \tilde{w}_n \left( X_n^{(i)} \right) / \sum_{j=1}^{N} W_{n-1}^{(j)} \tilde{w}_n \left( X_n^{(j)} \right) ,
\]
where $\tilde{w}_n(X_{n-1:n}^{(i)})$ is the normalizing coefficient.

Finally, RTST minimizes the difference between smoothed measured variable values and corresponding simulated values. Specifically, let $y(t)$ be the simulated value corresponding to $\hat{x}(t)$. Then set $x(t) - y(t)$. The algorithm then optimizes objective function (6)

$$\sum_t (\hat{x}(t) - y(t))^2 \rightarrow \min$$

by applying Ordinary Least Squares line-of-best fit techniques. Ultimately, simulation parameters are adjusted and process model is tuned to reflect predefined accuracy criteria.

The next two sections provide detailed descriptions of how RTST is applied for large-scale process optimization and diagnostics.

**RTST for Large-Scale Process Optimization**

One of the best illustrations of *OptiRamp* RTST is its application in large-scale pipeline compressor networks with hundreds of individual units, where each unit may be single- or multi-stage compressors, with complex connections and interactions across all units. Gas pipelines are complex dynamic systems with elements distributed over large distances from each other and from control centers. Changes in operating modes of each element affect the entire pipeline system. Therefore, an important aspect in complex gas transportation system optimization is a mathematical description of the whole system, including all levels of the optimization object.

One of the key factors in natural gas pipeline network operation is network linepack. The desired operation of the network derived from estimated receipts and deliveries is expressed in terms of the linepack profile that must be maintained. Compressor stations in the pipeline network are then operated in a manner to generate this linepack profile. Generally, operating points selected for compressor station units are based on experience and experimentation and are, therefore, not optimal. In large-scale processes, it becomes impossible to use traditional methods of calculation (static models) to find optimal operating modes, hence, the use of real-time simulation is imperative to provide network operators real-time recommendations for various control aspects—such as properly sizing the control element (e.g., recycle valves in single-stage compressors), especially during various operating modes (during system start-up, shutdown, or variance within the gas composition)—to predict the operating point movement (trajectory on an $N$-dimensional surface) under various transient conditions, and to analyze the operating mode behavior sensitivity to determine the optimal operating mode subject to various boundary conditions (e.g., compressor operating point between the surge limit line and the choke line).

Traditional methods use static mathematical models of the gas transportation process. The processes observed in pipeline network inlets and outlets integrally include all pipeline and compressor parameters in a stable environment. A static mathematical model is a collection of equations in steady-state working conditions that describe the interdependencies between process variables. Some of these variables are independent inputs that include disturbances and
manipulated variables. Others are outputs that must be computed using the mathematical model based on a set of inputs. For complex systems, such as a pipeline network, most outputs are derived not only from inputs but also from other computed outputs. To model the desired operating mode, the user (or system) must assume a certain set of input parameters. Very often, it is impossible for a complex system to assume an appropriate set of inputs that would produce such set of outputs that exist within a defined process operating envelope and that respects all process limits, targets, and constraints. If the operating mode is modeled outside of the allowable operating envelope, then this mode obviously cannot be used for process optimization and analysis.

Process Simulation

Let $i$ be the index of all compressors in the network, let $j$ be the nested index of stages of each compressor (with $j = 1$ for single-stage compressors), and let $k$ be the index of dependencies across the network. The search for these dependencies deploys machine learning techniques, such as neural networks and ensemble modeling, and is outside of the scope of this white paper.

The following key parameters are then defined for the compressor network:

1. $P_{si,j}$ — Suction pressure for $i^{th}$ compressor at $j^{th}$ stage
2. $P_{di,j}$ — Discharge pressure for $i^{th}$ compressor at $j^{th}$ stage
3. $\Delta P_{oij}$ — Differential pressure for $i^{th}$ compressor at $j^{th}$ stage
4. $T_{si,j}$ — Suction temperature for $i^{th}$ compressor at $j^{th}$ stage
5. $T_{di,j}$ — Discharge temperature for $i^{th}$ compressor at $j^{th}$ stage
6. $N_i$ — Rotation speed for $i^{th}$ compressor
7. $\alpha_{ij}$ — Recycle valve position for $i^{th}$ compressor at $j^{th}$ stage
8. $\beta_i$ — Throttle valve position or guide vane position for $i^{th}$ compressor, if $N_i$ is constant
9. $C_{ij}$ — % contents of different gases for $i^{th}$ compressor at $j^{th}$ stage, if real time gas composition is measured
10. $\Gamma$ — Vector of network parameters, including ambient temperatures throughout the network, pressures in nodes and common collectors, etc.

In steady-state, the network can be described by a series of static multidimensional dependencies indicated by a set of implicit functions $F_k$ shown in equation (7).

$$F_k(P_{si,j}, P_{di,j}, T_{si,j}, T_{di,j}, \Delta P_{oij}, N_i, \alpha_{ij}, \beta_i, C_{ij}, \Gamma) = 0$$

$F_k$ can either be built based on OEM data and specifications or can be created using OptiRamp Modeling. However, the challenge is to describe the system in a transient state, which for a large network is nearly a perpetual occurrence (changing environmental conditions, demand, business requirements, etc.) and a formidable computation problem as well.

OptiRamp solves this problem by applying RTST concepts at scale. Specifically, RTST builds transfer functions for the system dynamic elements. This process includes introducing new
variables—variances in dynamic elements (denoted by $\Delta$ for each parameter) derived using the transfer functions in equation (8).

$$\Delta\theta = \theta(H(s)),$$

(8)

where $\theta$ is any parameter from the list above and $H(s)$ is a transfer function. OptiRamp then converts the known, static, multidimensional models into dynamic multi-dimensional models according to the set of dependencies indicated by a set of implicit functions $G_k$ given by equation (9):

$$G_k(P_{sij}, \Delta P_{sij}, P_{dij}, \Delta P_{dij}, T_{sij}, \Delta T_{sij}, T_{dij}, \Delta T_{dij},$$

$$\Delta P_{oij}, \Delta \Delta P_{oij}, N_i, \Delta N_i, \alpha_{ij}, \Delta \alpha_{ij}, \beta_i, \Delta \beta_i, C_{ij}, \Gamma, \Delta \Gamma) = 0$$

(9)

Note, the dimensionality of such dynamic models increases dramatically relative to their static counterparts. RTST handles these large-scale simulations through its use of SMC applied on state-of-the-art massively parallel and distributed processing techniques on a highly scalable, fault-tolerant distributed data operating system.

**Process Optimization**

A key application of RTST and the resultant dynamic process models is the ability of the system to optimize the current operational process either through direct control actions or through recommendations to the compressor network operator. In the optimization problem, the objective function is typically fuel economy or process efficiency, while the constraints are properties of each network unit (e.g., surge control). At scale, there could be tens of thousands of constraints.

Let $k = k_{fuel}$ be the index of dependency $G_{k_{fuel}}$ describing the relationship of consumed fuel from the other network variables. Then let $G_{k_{fuel}}$ be the explicit function corresponding to the implicit function $G_{k_{fuel}}$. Then, for example, the fuel optimization problem for a compressor network driven by gas turbines can be stated using expressions (10), (11), and (12).

Minimize

$$G_{k_{fuel}}(P_{sij}, \Delta P_{sij}, P_{dij}, \Delta P_{dij}, T_{sij}, \Delta T_{sij}, T_{dij}, \Delta T_{dij},$$

$$\Delta P_{oij}, \Delta \Delta P_{oij}, N_i, \Delta N_i, \alpha_{ij}, \Delta \alpha_{ij}, \beta_i, \Delta \beta_i, C_{ij}, \Gamma, \Delta \Gamma)$$

(10)

Subject to

$$G_z(P_{sij}, \Delta P_{sij}, P_{dij}, \Delta P_{dij}, T_{sij}, \Delta T_{sij}, T_{dij}, \Delta T_{dij},$$

$$\Delta P_{oij}, \Delta \Delta P_{oij}, N_i, \Delta N_i, \alpha_{ij}, \Delta \alpha_{ij}, \beta_i, \Delta \beta_i, C_{ij}, \Gamma, \Delta \Gamma) = 0,$$

(11)

where $z$ varies across all indices excluding $k_{fuel}$ and the following non-negativity limits:

$$\{P_{sij}, \Delta P_{sij}, P_{dij}, \Delta P_{dij}, T_{sij}, \Delta T_{sij}, T_{dij}, \Delta T_{dij},$$

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\[
\Delta P_{oi}, \Delta \Delta P_{oi}, N_i, \Delta N_i, \alpha_{ij}, \Delta \alpha_{ij}, \beta_i, \Delta \beta_i, C_{ij}, \Gamma, \Delta \Gamma \geq 0
\]  
(12)

The optimization problem can be stated similarly for gas/steam turbine- and electric motor-driven compressors for a combination of such scenarios. Referring to equation (9) above, each \( G_k \) can be thought of as a multidimensional surface. To optimize the process, the objective function (e.g., process efficiency) values must be evaluated and compared across at least two operating points. For the large-scale, multidimensional surface \( G_k \), it is often impossible to assume correct input conditions that correspond precisely to an operating point on this surface because static models cannot find the correct set of input values on that surface; thus, the operating point is often calculated to be outside of the surface, rendering the value of such calculation essentially null.

Figure 2 illustrates this concept and the corresponding RTST solution on a three-dimensional model. The benefit from RTST is that it will start the system from the correct initial condition on the hypersurface illustrated on Figure 2 and will transfer the operating point along the modeled surface in small increments, where the overall trajectory is built on the modeled surface such that each new operating point will also be located on the surface. This method will be true for all operating points and will align with the actual process. Therefore, RTST provides a method for finding appropriate operating points for large-scale, multidimensional models. The critical aspect and value add from S&C’s RTST solution is that this process works across large hyperplanes \( G_k \) describing the behavior of a large-scale compressor network.
It is important to note, that when RTST moves the operating point along the trajectory on the hypersurface, it also satisfies all constraints (such as material balance and non-negativity limits) and tests the objective function for optimal criterion.

Therefore, when RTST moves from the initial operating point to a more efficient one, RTST corrects the trajectory into a more efficient direction. The final destination can then be compared with the initial operating point based on the objective function value since both points are on the modeled hypersurface. Hence, RTST is used to solve this large-scale optimization problem posed above. In comparison, as illustrated by the red point in Figure 2, the operating point calculated by the static models will lie outside of the hypersurface, making it impossible to compare two scenarios for the optimization problem.

**RTST for Large-Scale Process Diagnostics**

Predictive maintenance scheduling is an economically beneficial practice across various types of process equipment. Even under the best possible operating conditions, the performance of gas turbines and process compressors is subjected to deterioration due to compressor fouling and corrosion, inlet filter clogging, thermal fatigue, and oxidization of hot-gas path components such as combustion liners and turbine blades. The performance degradation attributed to compressor fouling is mainly due to deposits formed on the compressor blades by particles carried in by the air that are not large enough (typically a few microns in diameter) to be blocked by the inlet filter. Depending on the environment, these particles may range from dust and soot particles to water droplets or even insects. These deposits result in a reduction of compressor mass flow rate, efficiency, and pressure ratio, which in turn causes a drop in the gas turbine’s power output while increasing its heat rate. Typically, for a base load machine, the degradation can be 0.2% to 0.3% of the nominal rating after a month in operation.

*OptiRamp* Performance Diagnostics uses RTST to provide operators with a real-time view of process conditions and proactively notifies operators about abnormal equipment conditions that may occur based on the system of predictions.

Like the calculations mentioned in the previous sections, RTST compares measured and simulated operating points and adjusts model coefficients in order to minimize the difference between “measured” and “predicted” values according to equation (6). The challenge is like the one above in that RTST must compare the measured point that is outside the hypersurface $G_k$ with the simulated point that is on the modeled hypersurface. Again, RTST allows the system to move from a measured point to predicted one with small increments and adjusts model coefficients while running.

This means that RTST recalculates $G_k$ coefficients over time to create a series of implicit functions $G_k(t)$. Large-scale process diagnostics can then be performed using a trigger, $D_k$, described by equation (13).

$$
D_k = \begin{cases} 
1, & \text{if } |\widetilde{G}_k(t_n) - \widetilde{G}_k(t_{n-1})| \geq \varepsilon \\
0, & \text{if } |\widetilde{G}_k(t_n) - \widetilde{G}_k(t_{n-1})| < \varepsilon 
\end{cases} \quad (13)
$$
where $\varepsilon > 0$ is parametrically defined. When $D_k = 1$, i.e., when the new hypersurface is sufficiently far from the initial hypersurface, OptiRamp provides a trigger to the process operator indicating that the equipment present in hypersurface $G_k$ is due for maintenance. The collection of $G_k$ hypersurfaces observed to experience degradation and the magnitude of all such degradations are connected to specific mechanical sources of such degradation, e.g., issues with turbine or the driver; furthermore, these dependencies can be identified using tools like predictive modeling (logistic regression and neural networks) applied to historical maintenance events and hypersurface coefficient changes. This discussion is outside of the scope of this white paper. Refer to the OptiRamp Performance Diagnostics white paper for additional information about diagnostics.
About Statistics & Control, Inc.

S&C—an engineering consulting and technology company headquartered in West Des Moines, IA—solves complex challenges for customers through its unique technology and its highly seasoned team of professionals. The company has a global portfolio spanning the energy, oil and gas, utility, and digital oil field industry sectors. S&C provides clients with turbomachinery control solutions that easily integrate with the existing system as well as OptiRamp® solutions, which focus on process and power analytics to optimize processes and, in turn, reduce costs and increase reliability. S&C also provides consulting, dynamic system studies, modeling, automation, training and OTS, and support services.