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An Efficient Real-Time Dynamic Optimization Architecture for the Control of Non-Isothermal Tubular Reactors.

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Abstract
In this work we present the development of an efficient model-based real time dynamic optimization (DO) architecture for the control of distributed parameter systems (DPS). The approach takes advantage of the dissipative nature of this class of systems to obtain reduced order models (ROM) which are then used by the optimization modules to compute in real time the optimal operation policy. The DO module is based on the combination of the control vector parameterization (CVP) approach and a suitable NLP solver selected among several local and global possibilities.

Keywords: Real-Time Optimization, Distributed Process Systems and Low Order Models.

1. Introduction

Model Predictive Control (MPC) emerged in process industry as a technology which simultaneously was able to provide optimal operation while offering a systematic way of handling constraints and solving the strong coupling between inputs and outputs. Essentially, a model predictive controller requires a reliable representation of the process (a model) to explore future scenarios plus an optimization algorithm to search over a given horizon the best possible applicable operation policy maximizing or minimizing a given objective function. Despite the success of this technology in process industry, a number of crucial issues related with the harmonious coordination of its different components (models, optimisers, observers etc) and efficient prediction models still remain (Cannon, 2004).
In fact, the latter issue is particularly critical in DPS where descriptions are obtained from microscopic conservation laws for mass and energy balances, what results into highly coupled nonlinear sets of partial differential equations (PDEs). In this way, and despite some work done in MPC for distributed process systems (Chen, 2003 and

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Dufour, 2004), research efforts are needed to efficiently deal with the high dimensionality of the problem.

In this paper, we take advantage of the dissipative nature of the process systems to obtain low order finite dimensional representations of the original set of PDEs, suitable for fast on line optimization. In particular, the Finite Element structure (FEM) is exploited to obtain ROMs of the systems based on the use of the Galerkin projection on a set of spectral eigenfunctions and proper orthogonal functions (PODs), already used by Bendersky and Christofides (2000) in optimal control, thus allowing the comparison of their predictive capabilities, simulation and re-calculation costs. This new methodology is evaluated in the control of a non-isothermal tubular reactor.

2. Nonlinear Model Predictive Control

In general, the model predictive control problem is formulated so as to solve in real time a finite horizon open-loop optimal control problem subject to system dynamics and constraints involving states and controls.

2.1. Open loop optimal control problem. Mathematical formulation.

The open loop optimal control problem can be formulated as the computation of time (and usually also spatial in DPS), varying control profiles in order to minimize a certain performance index:

$$J(v(t,\xi),u(t,\xi),t)=\theta(v(t_f,\xi))+\int_0^{t_f} L(v(t,\xi),u(t,\xi),t)dt \tag{1}$$

where L can arise from productivity, economical or ecological considerations. The objective function we will consider in this work fits into the standard MPC stability objective, of the form:

$$L(v,u)=(v-v^s)^T Q(v-v^s)+(u-u^s)^T R(u-u^s) \tag{2}$$

where v^s and u^s are setpoints, and Q and R positive definite symmetric weighting matrices. Equation (1) is subject to the system dynamics (PDEs) of the form:

$$(v(t,\xi))_t=\ell(v(t,\xi))+F(v(t,\xi),u(t,\xi)) \tag{3}$$

where $\ell(\cdot)$ represents a linear parabolic operator defined on a given spatial domain Ω with smooth boundary. $F(v(t,\xi),u(t,\xi))$ is a nonlinear vector field depending on the state variables (v) and on the control variables (u). Initial and boundary conditions must be imposed on the system so as to guarantee that a unique solution exists. Other restrictions such as bounds for both the control variables and alternative process constraints (path, point and/or final time) can be included as well.

2.3. Solution approach: Control Vector Parameterization.

The high dimensionality of DPS nonlinear systems makes the MPC problem particularly challenging. This issue was partially overcome, however, in the recent years by developments in efficient CVP methods adapted to distributed systems (Balsa-Canto et al. 2004a). The CVP approach transforms the original infinite dimensional problem in a nonlinear programming problem (NLP) by means of the discretization of the control variables into a number (ρ) of elements, and approximating the control values using low order polynomials (Vassiliadis, 1993).

The solution of the resulting NLP problem can be obtained through standard, global or local, NLP solvers: local methods, although efficient, may converge to local solutions in the case of multimodal problems while global methods, although more robust, usually require large computational effort.

In addition, it is worth mentioning that the evaluation of the objective function demands the solution of a set of PDEs (Eqn. 3) that the traditional techniques transform into a large scale set of ordinary differential equations (ODEs) unsuitable for MPC. Therefore ROM models described in section 3 arise as the alternative.

2.4. Feedback implementation in DPS.

Real time implementation of the optimal control policy needs to consider the effect of unmeasured disturbances not being part of the prediction model. To that purpose, feedback is implemented by regularly measuring the current state of the process. In our case and to overcome the considerable computational delays in the optimization step, the following feed-back logic is proposed: First the open-loop optimal control problem is solved off line and the result (u_0*) is applied to the real system. The measurement obtained at each sampling time t_k is fed to the ROM to estimate the initial conditions at t_k+t_s, (where t_s is the computational delay). These conditions are the ones employed by the optimizer to compute the new control profile to be implemented in the real plant This profile will initialize the next optimization.

3. Low order finite dimensional representation

The conventional approach (e.g. FEM and finite differences) to simulate DPS is based on spatial discretization schemes which approximate the original PDEs (Eq. 3) by a large set of algebraic equations and ODEs. However, the solution of the resulting system is computationally involved thus conditioning the efficiency of dynamic optimization algorithms. Alternatively, one can make use of the dissipative nature of DPS (Courant and Hilbert, 1937) to represent the solution as an infinite series expansion of the form:

$$v(t,\xi)=\sum_{i=1}^{\infty}c_i(t)\varphi_i(\xi) \tag{4}$$

where each element of the set of basis functions $\left\{\varphi_i(\xi)\right\}_{i=1}^{\infty}$ is calculated as the solution of the following integral equation: $\int_\Omega R\varphi_i d\xi=\lambda_i\varphi_i$. Depending on the nature of the kernel R, two different methods are considered: 1.- *Spectral decomposition* where R is the Green function associated with the spatial operator and 2.- *Proper orthogonal decomposition (POD)* where R is a two point correlation matrix constructed form empirical data (Alonso et al., 2004). A key feature of dissipative systems is that any point of the system domain will evolve to a low dimensional hyperplane where it will remain (Alonso and Ydstie, 2001) what allows the extraction of a low dimensional dynamic manifold capturing the relevant dynamic behaviour of the system. In this way, the solution can be approximated as a truncated series expansion of the form:

$u(t,\xi) \cong \tilde{u}(t,\xi) = \sum_{i=1}^{k} c_i(t)\varphi_i(\xi)$. The projection of the original PDE, on the basis functions, results into the following set of ODEs:

$$c_t = Ac + f(c); \qquad \tilde{u} = [\varphi_1,\ldots,\varphi_k]c \tag{5}$$

where A and f(c) are the projections of the linear and nonlinear parts of the PDE system on the basis functions. In this work, a methodology which efficiently exploits the underlying algebraic FEM structure is used to implement the previous projections (Vilas et al., 2004). If the PDE is highly nonlinear, state transformations as those proposed by Balsa-Canto et. al. (2004b) would reduce the class of nonlinearities to polynomial type thus facilitating the projection. In addition, the number of decision variables can be drastically reduced by expanding the control in terms of the ROM basis functions, this being especially attractive in dealing with 2D or 3D problems.

Finally, it must be noted that the although the selection of the basis function class is problem dependent, spectral projection methods are more systematic than PODs. In fact, POD's accuracy depends at a high extent on the number and quality of the experimental data used, what calls for recursive POD update algorithms to preserve prediction accuracy (Annaswamy et al., 2002).

4. Case study: Tubular Chemical Reactor

The methodology proposed is applied to a nonlinear distributed chemical reactor which consists of two highly nonlinear coupled PDEs describing temperature (v_2) and concentration (v_1) (the detailed mathematical problem may be found in Padhy and Balakrishnan, 2003). The control variable $u(t,\xi)$ is the cooling water temperature and it has been assumed that actuators and sensors are on the entire domain.

4.1. Process simulation. FEM vs ROM.

FEM has been used to simulate the reactor dynamics (122 ODEs) and results obtained where compared with ROMs predictions. Figures 1 and 2 illustrate the comparisons between FEM and ROMs based on the spectral decomposition (8 ODEs) and PODs (8 ODEs), respectively. LSODE was used to solve the ODE systems.

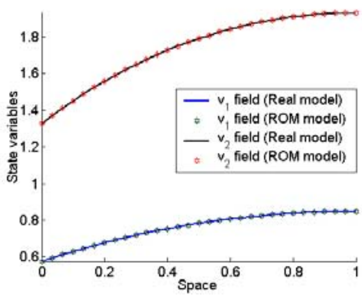

Figure 1 .Comparison between real and spectral basis models

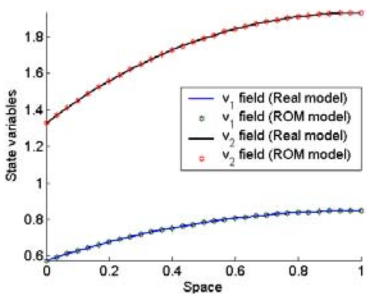

Figure 2. Comparison between real and POD models

From the figures it becomes clear that both low order models present good predictive capabilities. However, because the computational effort is larger for the POD model, spectral decomposition was the choice selected for the on line optimization.

4.1. NMPC implementation and results.

The main objective, stated as in Eqns. (1)-(2), is to reach the reference (set point) trajectories for the state variables in an optimal way. The references used in this case (v_1^{ref} and v_2^{ref}) correspond to the open-loop stationary state. Details on the reference states, weighting matrices in the objective function, reactor residence time, can be found in Padhy and Balakrishnan (2003). The control variable was approximated using 4 eigenfunctions, and each of the four time dependent coefficients was approximated using 15 steps along the residence time (large enough to maintain the close-loop stability). Thus resulting into a NLP problem with 60 decision variables. Regarding the NLP solver, several alternatives were evaluated: two global stochastic/hybrid methods and a collection of local methods where the SOLNP (SQP method, by Ye, 1989) was finally selected due to its ability to reach the optimal solutions with reasonable computational effort.

The behaviour of the real plant is reproduced through FEM simulation on a second computer communicated with the MPC controller through data files. Each five minutes (30 minutes is the reactor residence time) new measurements are introduced in the optimizer (with a previously ROM simulation). Simultaneously, the new optimal control is implemented on the FEM simulation.

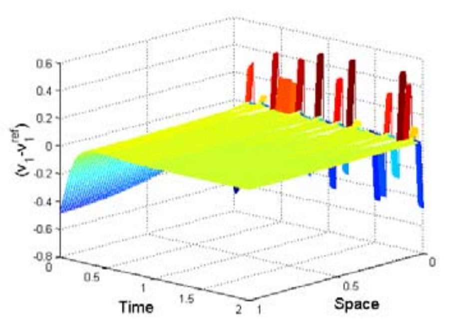

Figure 3 .Concentration deviations with MPC

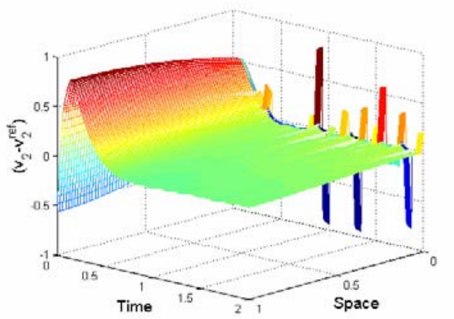

Figure 4. Temperature deviations with MPC

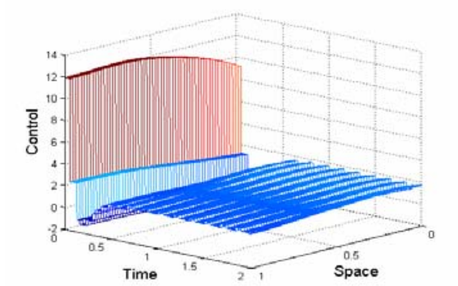

Figure 5. Control with MPC

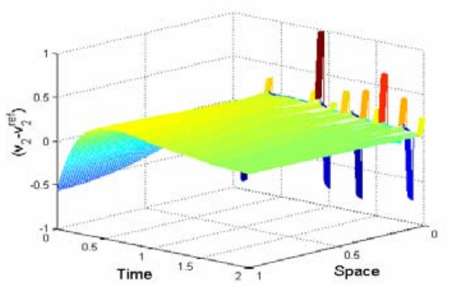

Figure 6. Temperature deviations without MPC

The performance of the open and closed loop plant under perturbations of temperature and concentration in the inlet stream is illustrated through Figures 3-6. As compared with Figure 6 (open loop response), the proposed real-time optimization scheme is able to efficiently reject disturbances and to enforce fast convergence of the reactor temperature and concentration to the desired set points.

5. Conclusions

In this work, ROMs have been proposed as an alternative to standard discretization methods for the online dynamic optimization of DPS, without any linearization around the reference trajectory and, thus, allowing changes in the operations conditions. The methodology was evaluated for the control of a tubular chemical reactor, simulated using FEM approach. The control expansion combined with the CVP method, resulted in a nonlinear optimization problem efficiently solved with an SQP based optimizer (SOLNL).

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