

Collocation and Large-Scale Nonlinear Programming for Dynamic Optimization in Chemical Engineering

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Dynamic optimization strategies based on collocation methods have been applied over a wide number of engineering applications. They include offline applications like optimal control, trajectory planning, nonlinear parameter estimation and optimization of reactors and batch processes, as well as on-line applications such as nonlinear model predictive control, nonlinear state estimation and dynamic, real-time optimization. Here we discuss recent advances for the simultaneous collocation approach and emphasize the characteristics, benefits and challenges related to these strategies. These relate to convergence and stability properties, treatment of inequality constraints and limiting performance behavior for challenging dynamic optimization problems. Moreover, we discuss the realization of these methods through large-scale NLP strategies. Using full-space barrier methods, these allow the efficient calculation of gradient and Hessian information and the exploitation of sparsity. This leads to fast solutions and sensitivity calculations. Finally, these developments will be illustrated on several chemical engineering case studies.