

# Self-Optimizing High Shear Wet Granulation with DeepMPC

Marino Sergi<sup>1,\*</sup>, Carolina Gastone<sup>1</sup> and Erica Franceschinis<sup>2</sup>

<sup>1</sup> Eigengran srl - 10129 Torino - Italy

<sup>2</sup> Department of Pharmaceutical and Pharmacological Sciences  
University of Padova - 35131 Padua - Italy

\* Correspondence: [marino@eigengran.it](mailto:marino@eigengran.it)

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## Abstract

In this paper, we present the development of a self-optimizing high shear wet granulation process using **DeepMPC**, a deep reinforcement learning-based Model Predictive Control technique. DeepMPC is a control approach that combines the benefits of **Deep Learning** and **Model Predictive Control (MPC)**.

The development of self-optimizing high shear wet granulation processes is a key area of research in the pharmaceutical industry, particularly in the context of Pharma 4.0 and the use of advanced technologies such as Artificial Intelligence (AI) and the Internet of Things (IoT) to improve drug development and manufacturing processes. One promising approach to self-optimization in this context is the use of DeepMPC, which involves using machine learning algorithms to build models of the granulation process, which can then be used to predict the outcome of different process conditions and optimize the process in real-time.

However, a key challenge in the development of self-optimizing high shear wet granulation processes is the limited availability of sensor data. To overcome this challenge, this paper proposes the use of sensor data fusion and online learning to enhance the performance of DeepMPC. Sensor data fusion involves combining data from multiple sensors to improve the accuracy and reliability of the measurement, and online learning algorithms can continuously update the models developed using DeepMPC based on new sensor data as it becomes available. The proposed approach involves the integration of Process Analytical Technology (PAT) sensors, such as Near-Infrared Spectroscopy (NIRS) and (first-order) torque.

In addition to sensor data fusion and online learning, this paper also discusses the importance of nonlinear dynamics modeling in the development of self-optimizing high shear wet granulation processes. Nonlinear dynamics refer to the complex, non-linear relationships between different process variables, which can make it difficult to predict the outcome of different process conditions. To address this challenge, deep learning algorithms can be used to model the nonlinear dynamics of the granulation process and improve the accuracy of the predictions. One approach that has shown promise in this context is the use of **Recurrent Neural Network (RNN)**, which are capable of modeling complex, high-dimensional data and can be trained using reinforcement learning techniques to optimize the control policy based on real-time process data. By using deep learning algorithms to model the nonlinear dynamics of the granulation process, it is possible to improve the accuracy of the predictions and optimize the process more effectively.

Finally, this paper discusses the potential use of **Deep Reinforcement Learning (DRL)** to optimize the granulation process in real-time based on the sensor data and models developed using DeepMPC. DRL involves the use of deep learning algorithms to enable an AI system to learn from the interactions between an agent and its environment. In this case, the agent is the DeepMPC controller and the environment is the high shear wet granulation process. We demonstrate the use of DRL to enable the DeepMPC controller to adapt to changes in the process and improve its control performance over time. This represents a key aspect of cognitive control, as the controller is able to learn and adapt to the dynamic nature of the process.

Overall, this paper presents a comprehensive approach to the development of self-optimizing high shear wet granulation processes that is in line with PAT guidelines and incorporates a range of engineering advances, including sensor data fusion, online learning, nonlinear dynamics modeling, and deep reinforcement learning. These approaches can help to overcome the challenges posed by limited sensor data and enable real-time optimization of the granulation process, leading to improved efficiency and product quality in the pharmaceutical industry.