## PANDA-NN: improved algorithm for contact angle determination in slit pores and interface classification

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Surface phenomena determine the behaviour of fluids in porous media and on wetted surfaces. Proper accounting of these phenomena is the basis of accurate continuum models [1]. The contact angle is a key quantity that quantitatively characterizes surface phenomena. Previously, a model was proposed that classifies the interface surfaces in slit pores [2] and offers a completely new approach for determining the contact angle from a one-dimensional density profile named PANDA [3]. An improved version of this algorithm is proposed, considering the presence of a non-zero wetting layer. The enhanced algorithm is validated on numerical data obtained from molecular dynamics calculations and demonstrates high accuracy. Additionally, a deep neural network based on the PointNet++ architecture [4] is trained to classify the interface surface based on the point cloud. These improvements have resulted in a fully complete algorithm with minimal hyperparameters.

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