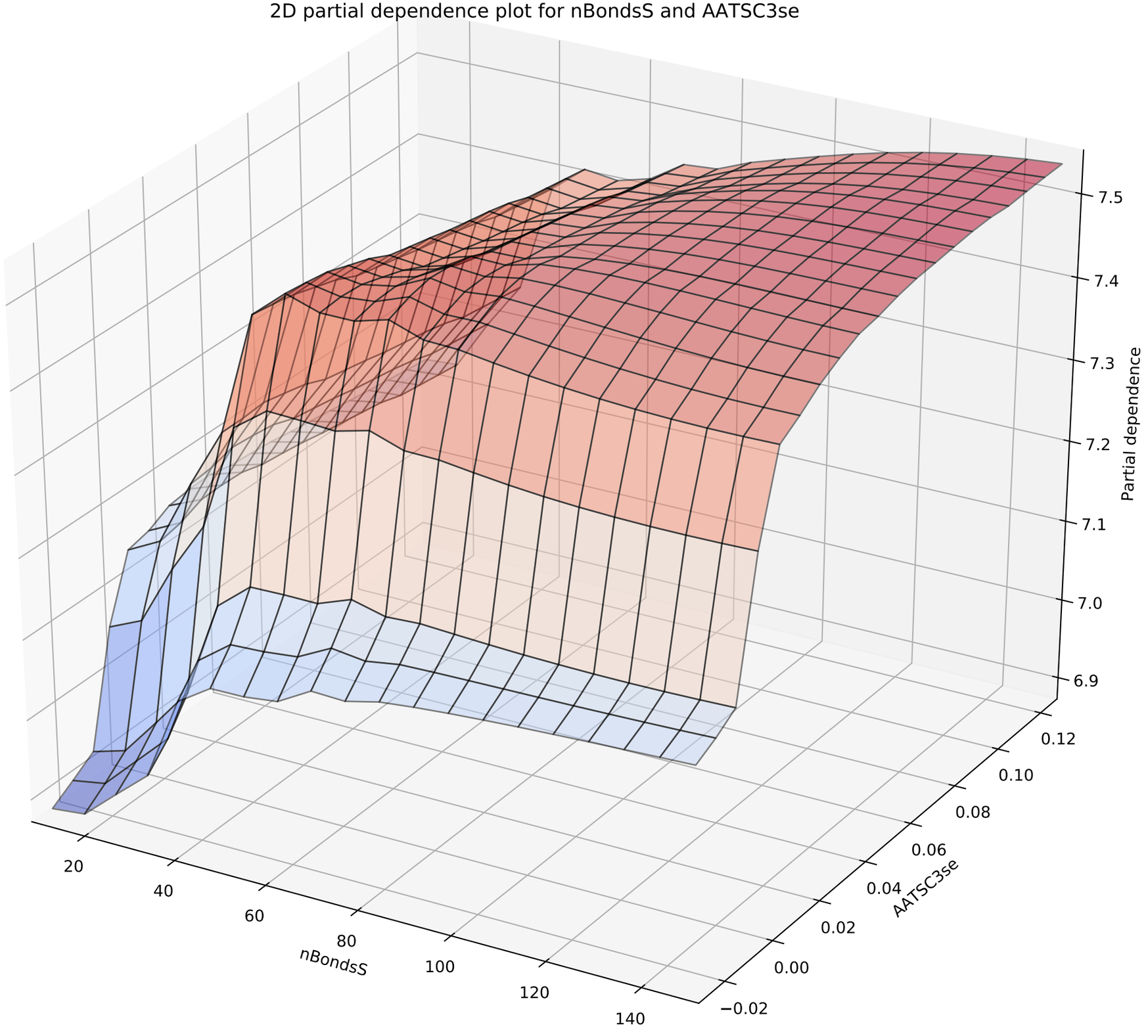

2D partial dependence plot for nBondsS and AATSC3se
nBondsS
20
40
60
80
100
120
140
AATSC3se
−0.02
0.00
0.02
0.04
0.06
0.08
0.10
0.12
Partial dependence
6.9
7.0
7.1
7.2
7.3
7.4
7.5