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Author Petra Wennerström		
Title (English) A new constant pressure algorithm and periodic boundary conditions in molecular dynamics free energy calculations		
Title (Swedish)		
Abstract Periodic boundary conditions were implemented in a already existing molecular dynamics software. In addition a new constant pressure algorithm was implemented. The new algorithm is a combination of molecular dynamics and Monte Carlo volume sampling. The results are promising but the algorithm needs more testing.		
Keywords Molecular dynamics, periodic boundary conditions, isothermal- isobaric ensemble, Monte Carlo, constant pressure.		
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