

GROMACS - Task #1785

no pV term written to energy file when pressure coupling is anisotropic

07/26/2015 01:47 PM - Mark Abraham

Status:	New	
Priority:	Low	
Assignee:		
Category:	mdrun	
Target version:	future	
Difficulty:	uncategorized	
Description		
In https://gerrit.gromacs.org/#q.1157b0468907802e29c7dec763ed2e5db99c02922.n.z a fix made explicit that we only write a pV term to the energy file when there is isotropic pressure coupling.		
Whether we can and should write a pV term for non-isotropic coupling is an open question.		