

nMOLDYN - Feature #2207

Limit number of frames to optimize prime factors

18/12/2014 11:20 AM - Christensen, Sebastian

Status:	New	Start date:	18/12/2014
Priority:	Normal	Due date:	
Assignee:		% Done:	0%
Category:		Estimated time:	0.00 hour
Target version:		Spent time:	0.00 hour
Description			
<p>I was calculating the dynamic incoherent scattering factor for a simulation with 8693 frames. But that was extremely slow - estimated time 24 days. Then I realized that the DISF calculation probably uses FTT and 8693 is a prime number. If I included 1 frame less the largest prime factor was reduced by $8692=2*2*41*53$ and the calculation time was 7 hours.</p> <p>Maybe this is trivial for experienced users. But it would be nice to have a feature which offered to optimize the number of frames for low prime factors if they exceed a certain limit</p>			