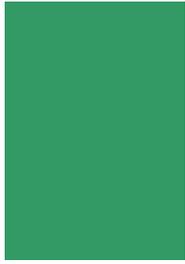


	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 AM	Arrival to ORNL from hotel - badge office				
8:15 AM					
8:30 AM		Arrival to ORNL from hotel	Arrival to ORNL from hotel	Arrival to ORNL from hotel	Arrival to ORNL from hotel
8:45 AM					
9:00 AM		DL_POLY and Parallelism (Smith)	DL_POLY Electrostatics (Smith)	Cray X-1 architecture and programming review (CCS staff)	Final Q&A with Bill Smith
9:15 AM					
9:30 AM	Welcome and Introduction (Cummings + Luijten)			IBM Blue Gene architecture and programming review (CCS staff)	
9:45 AM					
10:00 AM	The DL_POLY Package (Smith)	User experiences with DL_POLY (TBD)	User experiences with DL_POLY (TBD)		
10:15 AM					
10:30 AM		Coffee break	Coffee break	Coffee break	Coffee break
10:45 AM					
11:00 AM	Coffee break	Tutorial session - practical aspects of using DL_POLY	Tutorial session - modifying DL_POLY	Tour of CCS, SNS and CNMS	Future computational nanoscience activities at the CNMS (Cummings)
11:15 AM					
11:30 AM	Using DL_POLY (Smith)				
11:45 AM					
12:00 PM					Adjourn
12:15 PM					
12:30 PM					

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experiences with DL_POLY (User)	session - practical aspects of using DL_POLY	Tutorial session - modifying DL_POLY	General Q&A with Bill Smith	Vectorizing DL_POLY - meetings between Bill Smith, Cummings and CCS staff
experiences with DL_POLY (TBD)				
Coffee break	Coffee break	Coffee break	Coffee break	
The DL_POLY GUI (Smith)	ORNL Vision for Computational Nanoscience (Cummings)	Discussion of DL_POLY2 vs DL_POLY3 (Smith)	Examples of MD in nanoscience (participants)	
	Moderated discussion of DL_POLY role		Examples of MD in nanoscience (participants)	
Access to ORNL computers (R. Fahey)			Examples of MD in nanoscience (participants)	

**Adjourn      Adjourn      Adjourn      Adjourn**



8:00 PM

8:15 PM

8:30 PM

