

2016 HiPC Workshop on High Performance Computing and Big Data in Molecular Engineering (HBME)

To be held in conjunction with HiPC 2016 on 19 December 2016, Hyderabad, India

<https://docs.google.com/document/u/1/d/18tj9vPki1SDQVNw17PSX1uIv51VQB-78lv3aF4wHuOk/pub>

Technical Program

HBME : Session 1 (Chair: J. K. Singh)
2:00 - 2:50 PM
Keynote: Transitions to and from jammed states in glasses and sphere packings under shear deformation.
Speaker: Prof. S. Sastry, JNCASR, Bengaluru
2:55 - 3:20 PM
Technical Paper 1 Presentation – HBME01
Title : Towards understanding optimal load balancing of heterogeneous short-range molecular dynamics Presenter: S. Hirschmann, D. Pflüger, C. W. Glass
3:25 - 3:50 PM
Technical Paper 2 Presentation – HBME02
Title: Molecular dynamics simulation of nanoscopic Couette flow and lubricated nano-indentation Authors: S. Stephan, M. P. Lautenschläger, M. T. Horsch, H. Hasse
3:55 - 4:40 PM
Break
HBME : Session 2 (Chair: C. W. Glass)
4:40 - 5:05 PM
Technical Paper 3 Presentation – HBME03
Title: In-silico skin model: A tool for virtual testing of formulations Authors: R. Gupta, B. S. Dwadasi, B. Rai
5:10 - 5:35 PM
Technical Paper 4 Presentation – HBME04
Title: Insight into the nature of evaporation processes enabled by massively parallel molecular dynamics simulations Authors: M. Heinen, R. S. Chatwell, J. Vrabc
5:40 - 6:05 PM
Technical Paper 5 Presentation – HBME05
Title: Round robin study of molecular simulation programs Authors: M. Schappals, H. Hasse