

# WG on Theoretical & Computational Methods

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# Possible Topics/Directions

- Rigorous Mathematical Formulations
  - Coarse-Graining Formulations, e.g. Mori-Zwanzig; memory
  - Statistical Thermodynamics; beyond Mean Field theory
  - Theorem-proving using simulations
- Uncertainty & Stochastics
  - Model uncertainty vs parametric uncertainty
  - Hybrid deterministic-stochastic systems
  - Inference in stochastic networks
- Data-Driven Multi-Fidelity Stochastic Simulation
  - Machine learning & Kriging-coKriging
- Numerical Methods
  - Taxonomy of methods used in MSM
  - More emphasis on mesoscopic methods (SPH, DPD, LBM,...)

## **Incorporating Cellular Substructure into Reaction-Diffusion Models**

**Presenter:** Samuel Isaacson, Boston University

**Webinar Date:** Monday, November 9, 2015 - 2:30pm

## **Stochastic Simulation at Your Service**

**Presenter:** Linda R. Petzold, University of California Santa Barbara

**Webinar Date:** Monday, December 14, 2015 - 3:00pm

## **Theory, Algorithms and Applications of Dissipative Particle Dynamics**

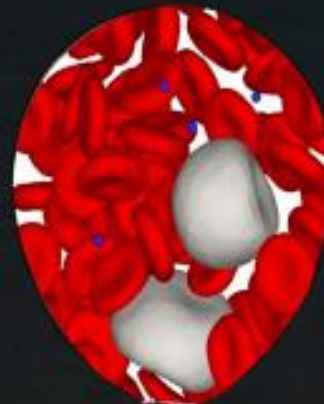
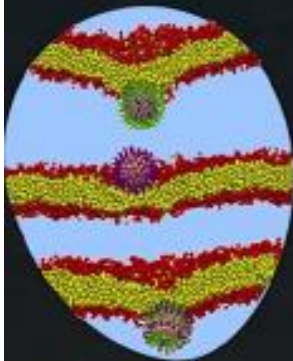
**Meeting Date:** Monday, September 21-23, 2015

**Meeting Location:** Shanghai University

# Theory, Algorithms and Applications of Dissipative Particle Dynamics

September 21-23, 2015

Shanghai University, 149 Yanchang Rd., Shanghai 200072, China



Marco Ellero  
Dmitry A. Fedosov  
Hongxia Guo  
Jiaping Lin  
Zhongyuan Lu

## Invited Speakers

Swansea University, UK  
Forschungszentrum Jülich, Germany  
Beijing Institute of Chemistry, CAS, China  
E. China Univ. Sci. & Technol., China  
Jilin University, China