Sunday, July 5, 2015

16:00 Registration open
18:00 Welcome reception

Monday, July 6, 2015

**Topic 1: Fundamental issues in nonequilibrium thermodynamics**

Chair: D. Jou

08:45 Welcome
09:00 Mechanics with missing details
    M. Grmela

10:30 Break

11:00 Extended thermodynamics and moment methods: Successes and challenges
    H. Struchtrup

12:30 Lunch

Chair: S. Kjelstrup

14:00 Steepest entropy ascent in nonequilibrium quantum dynamics
    G. P. Beretta

14:25 Local quasi-equilibrium description of multiscale systems
    J. M. Rubi, I. Santamaría-Holek, A. Pérez-Madrid

14:50 Heat flux fluctuations and extended thermodynamics
    D. Jou, M. Criado-Sancho

15:15 Reversibility and irreversibility in non-equilibrium thermodynamics: How to derive Onsager-Casimir reciprocal relations?
    M. Pavelka, V. Klika, M. Grmela

15:40 Break

Chair: A. N. Beris

16:10 Generalized Poisson-Kac processes: Basic properties and implications in extended thermodynamics and transport
    M. Giona, A. Brasiello, S. Crescitelli

16:35 Quantum finite-time availability for parametric oscillators
    K. H. Hoffmann, P. Salamon

17:00 Thermodynamic performances of three-body near-field heat engines

17:25 Objective thermomechanics
    T. Fülöp

17:50 A hyperbolic model for viscous fluids
    I. M. Peshkov, E. Romenski

19:00 Dinner
Tuesday, July 7, 2015

**Topic 2: Fundamental underpinnings of and rigorous mathematical results in nonequilibrium thermodynamics**

Chair: H. C. Öttinger

09:00 Linear response theory, Green-Kubo formulas and Langevin dynamics
G. A. Pavliotis

10:30 Break

11:00 Onsager reciprocity, gradient flows, and large deviations
M. A. Peletier

12:30 Lunch

14:00 Preservation of thermodynamic structure in model reduction
H. C. Öttinger

14:25 Essential equivalence of the GENERIC and Steepest Entropy Ascent models of dissipation for non-equilibrium thermodynamics
A. Montefusco, F. Consonni, G. P. Beretta

14:50 A Hamilton-Jacobi theory of nonequilibrium statistical model reduction
B. Turkington

15:15 Lagrangian formulation of irreversible thermodynamics, and the second law of thermodynamics
K. Glavatskiy

15:40 Break

16:10 Galilean relativistic fluid mechanics
P. Ván

16:35 Formulation and asymptotic limits of the relativistic heat equation and the relativistic kinetic Fokker-Planck equation using GENERIC
M. H. Duong

17:00 Diffusion in liquids: DDFT with hydrodynamic interactions and (giant) fluctuations
A. Donev, E. Vanden-Eijnden

17:25 Threshold effects and fluctuation-response relations in Zero Range Processes
M. Colangeli, E. N. M. Cirillo, A. Muntean

18:00 Poster session

19:00 Dinner
Wednesday, July 8, 2015

**Topic 3: Coarse-graining techniques and truly multiscale simulations**

Chair: V. G. Mavrantzas

09:00 The theory of coarse-graining, also known as non-equilibrium statistical mechanics

P. Español

10:30 *Break*  

Chair: V. G. Mavrantzas

11:00 Towards constitutive equations of complex fluids derived from thermodynamically guided molecular simulations

P. Ilg

12:30 *Lunch*  

Chair: B. Svendsen

14:00 Systematic coarse-graining in nucleation theory

M. Schweizer

14:25 Collective dynamics of dislocations from systematic coarse-graining

M. Kooiman, M. Hütter, M. G. D. Geers

14:50 A population balance based, coarse grained, evolution equation for microstructure in thixotropic colloidal dispersions

P. M. Mwasame, N. J. Wagner, A. N. Beris

15:15 Two-phase flow in microporous materials: From a local to global permeability

I. Savani, M. Vassvik, S. Sinha, A. Hansen, D. Bedeaux, S. Kjelstrup

15:40 *Break*  

Chair: P. Español

16:10 Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble

C. Baig, V. G. Mavrantzas

16:35 Moment closure approximations of the Boltzmann equation based on φ-divergences: Hierarchical multi-scale methods

M. R. A. Abdel-Malik, E. H. van Brummelen

17:00 On the numerical treatment of dissipative particle dynamics and related systems: Equilibrium and nonequilibrium studies

X. Shang, B. Leimkuhler

17:25 Optimizing coarse-grained models for equilibrium and non-equilibrium molecular systems: Force matching and dynamical force matching

E. Kalligiannaki, V. Harmandaris, M. Katsoulakis, P. Plechac

17:50 Relative resolution: A hybrid strategy for molecular modeling

A. Chaimovich, K. Kremer, C. Peter

19:00 *Conference dinner (BBQ)*
Thursday, July 9, 2015

**Topic 4: Role of thermodynamics in modeling the dynamics of complex materials under deformation**  
Chair: M. Grmela

08:45 Introduction to the Willem Prins Lecture  
S. J. Picken

09:00 Nonequilibrium thermodynamics modeling of the flow and deformation of complex materials with internal microstructure  
(*Willem Prins lecture*)  
A. N. Beris

10:30 Break  
Chair: M. Grmela

11:00 Role of thermodynamics in modeling the behavior of complex solids  
B. Svendsen

12:30 Lunch  
Chair: P. Ilg

14:00 Modeling of coupled flow-diffusion effects in shear banding, rodlike, micellar solutions  
N. Germann, A. N. Beris, P. L. Cook

14:25 A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics  
P. S. Stephanou, V. G. Mavrantzas, G. C. Georgiou

14:50 Statistical mechanics-based modeling of finite anisotropic viscoplastic deformation  
M. Hütter, T. Tervoort

15:15 Two-scale model to describe the viscoelastic behavior of filled elastomers  
M. Semkiv, M. Hütter

15:40 Rheology of supercooled liquids: Constitutive modeling guided by nonequilibrium thermodynamics  
I. Füreder, P. Ilg

16:05 Break

**Topic 5: Heterogeneous systems, interfaces, system-boundaries and small systems**  
Chair: G. J. M. Koper

16:30 Modeling interfacial dynamics in soft interface dominated materials  
L. M. C. Sagis

18:00 **Poster session**

19:00 **Dinner**
Friday, July 10, 2015

09:00  Small and large system thermodynamics
       S. K. Schnell, D. Bedeaux, S. Kjelstrup

10:30  Break

11:00  Non-equilibrium molecular self-assembly
       G. J. M. Koper

11:25  Seebeck coefficients of cells with alkali carbonates and gas electrodes
       M. T. Børset, X. Kang, O. S. Burheim, G. M. Haarberg, S. Kjelstrup

11:50  Revision of the Poisson-Nernst-Planck equations in the context of thermodynamic consistency
       W. Dreyer, C. Guhlke, M. Landstorfer, R. Müller

12:15  Discussion
       A. N. Beris (discussion leader)

13:00  Lunch

End of IWNET 2015
**Topic 1: Fundamental issues in nonequilibrium thermodynamics**

P1-1  Fluctuation-dissipation theorem and energetics for stochastic systems possessing finite propagation velocity
  A. Brasiello, M. Giona, S. Crescitelli

P1-2  Verification of Onsager’s reciprocal relations for sedimentation and electroacoustics: Application to colloids
  C. Chassagne, S. Gourdin-Bertin, O. Bernard, D. Bedeaux

P1-3  Verification of Onsager relationship in ion vibration potential (IVP) theories making use of the Newtonian equation of motion: Insights in the forces associated to diffusion and pressure gradients
  S. Gourdin-Bertin, C. Chassagne, O. Bernard, M. Jardat

P1-4  Analyzing superheating-supercooling cycles using a two-phase thermodynamics model
  H. Zhang, S. V. Nedea, D. M. J. Smeulders

**Topic 2: Fundamental underpinnings of and rigorous mathematical results in nonequilibrium thermodynamics**

P2-1  The absence of viscosity in the self-propelled Vicsek fluid: A numerical effort
  O. Chepizhko, M. Polovyi, V. Kulinskii

P2-2  Convergence of solutions and fluctuations: A large deviations approach
  M. H. Duong, A. Lamacz, M. A. Peletier, U. Sharma

**Topic 3: Coarse-graining techniques and truly multiscale simulations**

P3-1  A bottom-up model of adsorption and transport in multiscale porous media
  A. Botan, R. Pellenq, F.-J. Ulm, B. Coasne

P3-2  Multiscale simulations of PNIPAM polymer chains in aqueous solution
  V. Botan, R. Faller, K. Leonhard

P3-3  Algorithms for the long-time simulation of steady nonequilibrium flow
  M. Dobson

P3-4  TBA

P3-5  MD simulations revealing generic effects polymers have on the process of mineralization
  M. Radu, K. Kremer
**Topic 4: Role of thermodynamics in modeling the dynamics of complex materials under deformation**

P4-1  Linear rheology in non-equilibrium states of a polymer melt  
E. A. Andablo-Reyes, E. L. de Boer, D. Romano, S. Rastogi

P4-2  Challenges for statistical mechanics and thermodynamical treatments of dislocation systems  
T. Hochrainer

P4-3  Multiscale numerical modeling of deformation and breakup of viscoelastic droplets under confinement  
A. Scagliarini, A. Gupta, M. Sbragaglia, M. Sega

P4-4  Micromechanics of spongy-particle systems: Modeling approach  
M. E. A. Zakhari, G. W. M. Peters, M. Hütter

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**Topic 5: Heterogeneous systems, interfaces, system-boundaries and small systems**

P5-1  Modeling the volume change kinetics of microgels  
R. Keidel, A. Bardow

P5-2  Atomistic simulation of a semicrystalline polyether  
N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge

P5-3  The application of the global isomorphism to the surface tension of the liquid-vapor interface of the Lennard-Jones fluids  
V. Kulinskii, A. Maslechko

P5-4  Multi-phase modeling of non-isothermal reactive flow in fluidized bed reactors  
V. Orava, O. Souček, P. Čendula

P5-5  Solid oxide fuel cells efficiency prediction  
P. Vágner, M. Pavelka, F. Maršík

P5-6  Modelling and analysis of entropy production in light exposed heterogeneous semiconductor structures  
F. Vázquez, J. E. Nájera-Carpio, A. Figueroa