

## 7th International Workshop on Nonequilibrium Thermodynamics (IWNET 2015)

### 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*

Chair: D. Jou

- 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  
I. Latella, A. Pérez-Madrid, J. M. Rubi, S.-A. Biehs, P. Ben-Abdallah

- 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*
- Chair: H. C. Öttinger
- 11:00 Onsager reciprocity, gradient flows, and large deviations  
M. A. Peletier
- 12:30 *Lunch*
- Chair: H. Struchtrup
- 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*
- Chair: G. P. Beretta
- 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  $\phi$ -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**

Chair: G. J. M. Koper

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

10:30 *Break*

Chair: L. M. C. Sagis

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. Gohlke, M. Landstorfer, R. Müller

12:15 **Discussion**

A. N. Beris (discussion leader)

13:00 *Lunch*

*End of IWNET 2015*

## Poster presentations

### *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. Nedeia, 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

***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