# Discrete Simulation of Fluid Dynamics Conference



July 17-21, 2023 The University of New Mexico, Albuquerque, NM

Sponsored by the UNM Department of Chemical and Biological Engineering and Los Alamos National Laboratory







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### About

### **Discrete Simulation of Fluid Dynamics (DSFD)**

The DSFD series of conferences originated with the 1986 Los Alamos conference organized by Gary D. Doolen. Since that time, the DSFD conferences have emerged as the premiere forum for researchers in the field, and many exciting discoveries in lattice models of fluid dynamics have been first announced at DSFD conferences.

Topics emphasized at these meetings include lattice Boltzmann schemes, dissipative particle dynamics, smoothed-particle hydrodynamics, direct simulation Monte Carlo, molecular dynamics, quantum Monte Carlo methods, multiparticle collision dynamics, and hybrid methods. There will be sessions on advances in both theory and computation, on engineering applications of discrete fluid algorithms, and on fundamental issues in mathematical modeling, numerical analysis, statistical mechanics, kinetic theory, and hydrodynamics and their applications in microscopic, nanoscale and multiscale physics for emerging technologies. Other topics of interest include theoretical and experimental work on interfacial phenomena, droplets, free-surface flow, and micro- and nanofluidics.

#### Scientific committee

Santosh Ansumali Jawaharlal Nehru Centre for Advanced

Scientific Research, Bangalore, India

Bruce Boghosian Tufts University, Boston, USA

Jean-Pierre Boon Free University of Brussels, Belgium
Bastien Chopard University of Geneva, Switzerland
Paul Dellar University of Oxford, United Kingdom
Jens Harting Helmholtz Institute Erlangen-Nürnberg

for Renewable Energy, Germany

Takaji Inamuro University of Kyoto, Japan

Ilya Karlin Chairman, ETH Zurich, Switzerland Paulo Cesar Philippi Federal University of Santa Caterina,

Florianopolis, Brazil

Marisol Ripoll Research Centre J"ulich, Germany

Xiaowen Shan Commercial Aircraft Corporation of China,

Beijing, China

Sauro Succi CNR, Rome, Italy

Alexander Wagner North Dakota State University, Fargo, USA

### Local organizing committee

Qinjun Kang
Sang M. Han
Nick Carroll
Daniel Livescu
Hari Viswanathan
Christoph Junghans
Philip H. Stauffer
Hongkyu Yoon
Alexander Wagner
Aleksandra Pachalieva
Adam Quintana
Michael Woodward

Los Alamos National Laboratory
The University of New Mexico
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Los Alamos National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
North Dakota State University
Los Alamos National Laboratory
The University of New Mexico
Los Alamos National Laboratory

#### **Sponsors**







### **About Albuquerque**

Albuquerque is a vibrant and diverse city. Residents love the warm climate, low cost of living, gorgeous sunshine, unique cuisine, and endless cultural attractions. Learn more about why Lobos love calling Albuquerque home.

### **Quick Facts about Albuquerque**

- We have 310 days of sunshine but still manage to have all four seasons.
- We sit at 5,312 of elevation; we are truly a mile-high city!
- Our average commute time to work is 26 minutes. We are a big city but easy to navigate!
- The Rio Grande River flows through our city and provides unique ecosystems to explore and study.
- Rumor has it the breakfast burrito is said to have found its humble tasty beginnings at our International Balloon Fiesta in the 1970s.

#### What to do in Albuquerque?

- "Visit Albuquerque. Find Home." https://unmfirst.unm.edu/why-choose-us/why-albuquerque.html
- "Albuquerque is a hidden travel gem."

  https://www.newmexico.org/places-to-visit/regions/central/albuquerque/bucket-list/
- "50 Reasons To Love Albuquerque"

  https://www.newmexicomagazine.org/blog/post/50-reasons-to-love-albuque
  rque/
- "Welcome to Albuquerque" https://www.visitalbuquerque.org/

#### Museums

 The National Museum of Nuclear Science & History https://www.nuclearmuseum.org/

• Indian Pueblo Cultural Center

https://indianpueblo.org/

• Explora Science Center and Children's Museum

https://www.explora.us/

• New Mexico Museum of Natural History and Science

https://www.nmnaturalhistory.org/

Albuquerque Museum

https://www.cabq.gov/artsculture/albuquerque-museum

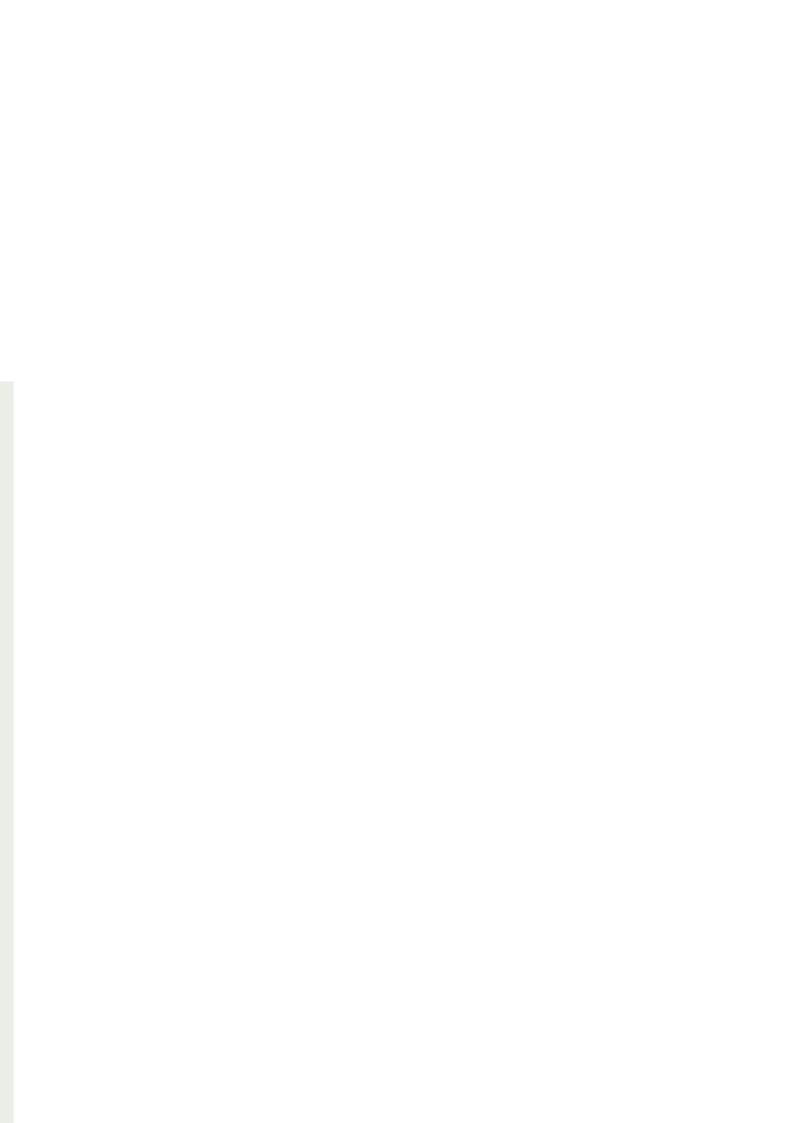
• Anderson-Abruzzo International Balloon Museum

https://balloonmuseum.com/

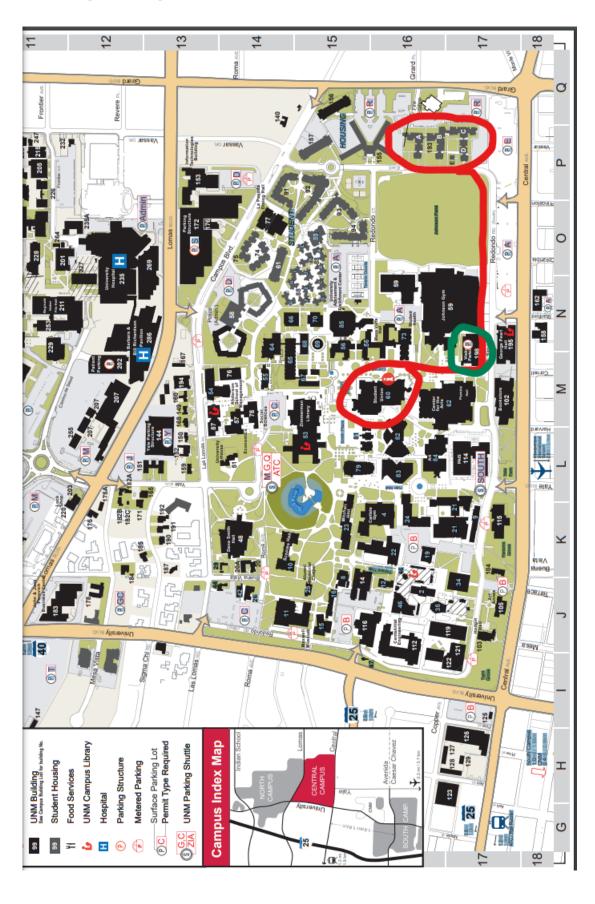
• Unser Racing Museum

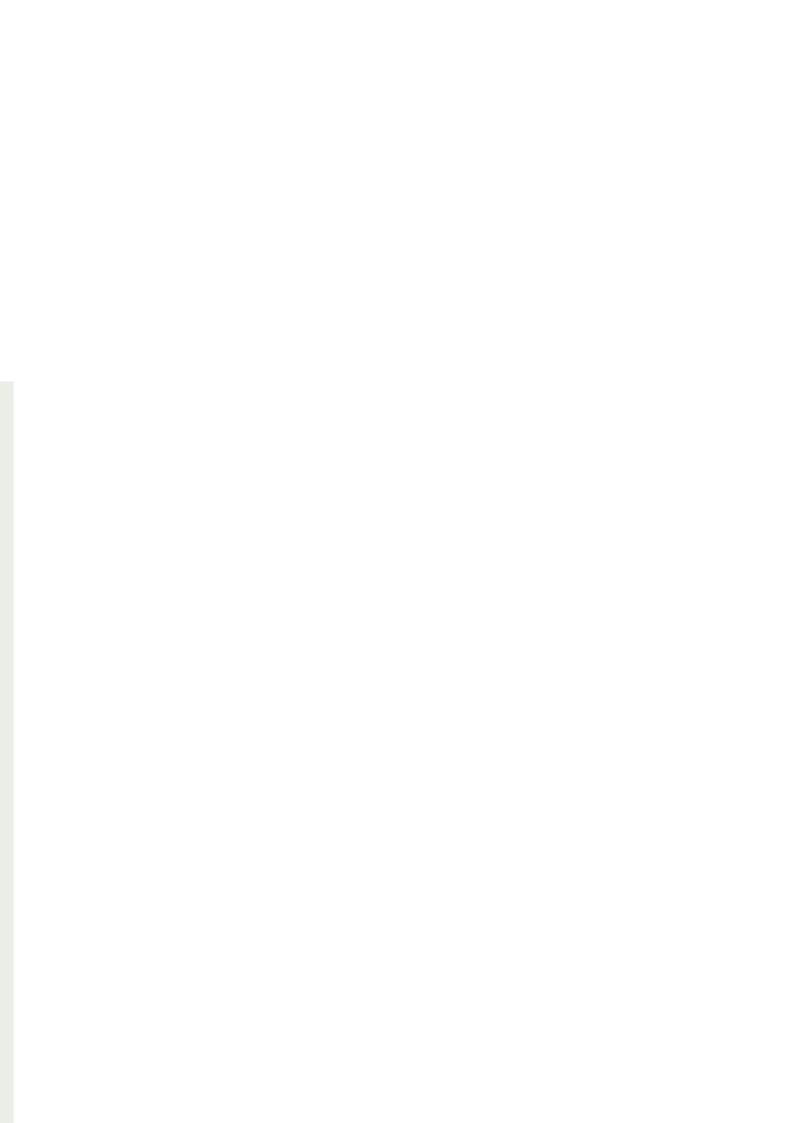
https://unserracingmuseum.com/

- American International Rattlesnake Museum https://www.rattlesnakes.com/
- New Mexico Steam Locomotive and Railroad Historical Museum https://www.visitalbuquerque.org/listing/new-mexico-steam-locomotive-and-railroad-historical-society/4673/
- Old Town Albuquerque



### **UNM Campus Map**

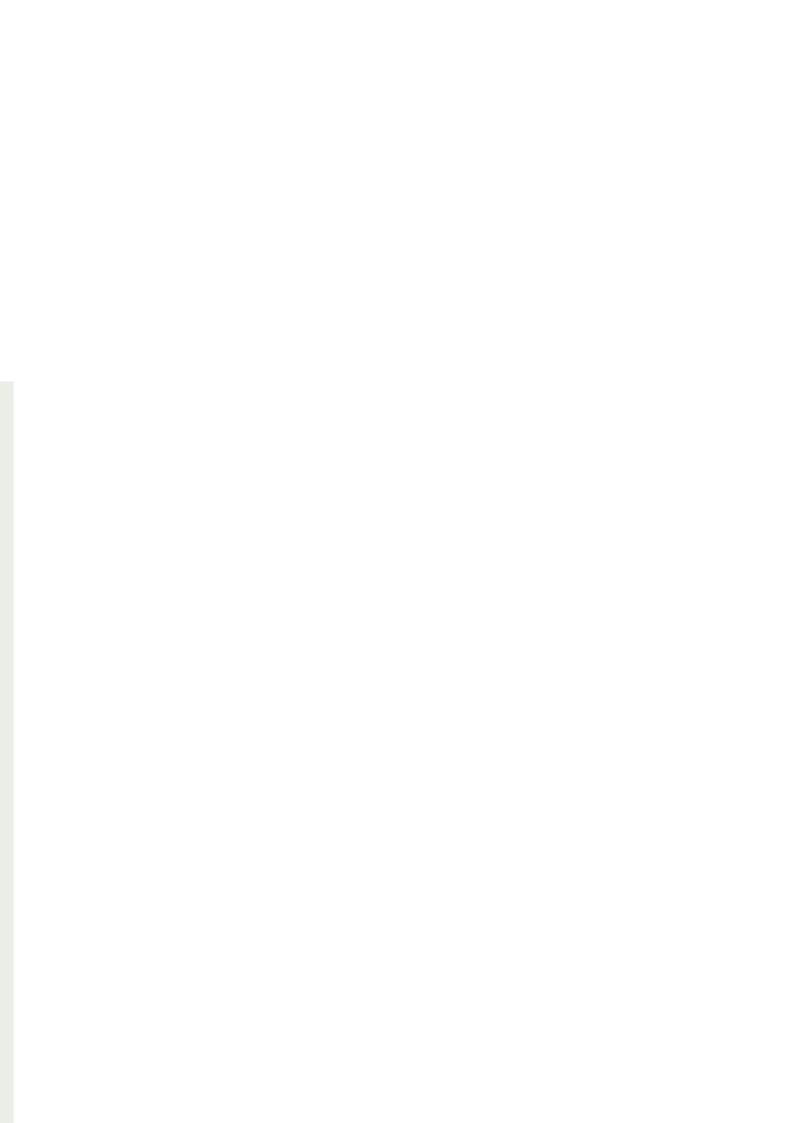




The DSFD conference venue is located at

Student Union Building (Level 3) The University of New Mexico 1 87106 US Albuquerque, NM 87131

If you need a **parking permit** during the DSFD conference, please, contact **Aleksandra Pachalieva** (apachalieva@lanl.gov).



### Social Program - Sandia Peak Aerial Tramway\*

Start: 17:00 (5:00 pm) Bus ride from the UNM Student Union Building End: 21:00 (9:00 pm) Bus ride back to the UNM Student Union Building

\*The bus ride and the Sandia Peak Aerial Tramway ticket are covered by the registration fee.



The Sandia Peak Tramway is an aerial tramway located adjacent to Albuquerque, New Mexico. It stretches from the northeast edge of the city to Sandia Peak on the ridge line of the Sandia Mountains and has the world's third-longest single span. It is the longest aerial tram in the Americas and was the longest in the world from 1966 until being surpassed in 2010 by the Wings of Tatev in Armenia.

At the top of Sandia Peak, there are many year-round recreational options. The restaurant, TEN 3 (stylized as 10|3), is directly adjacent to the top tram terminal and offers scenic views to the west. Many Forest Service trails offer recreational hiking, backpacking, and nature hikes to visitors. Additionally, the tram terminal is located at the top of Sandia Peak Ski Area, which is on the opposite side of the mountain from the tramway and the city. Skiing is available in the wintertime, and during the summer, more than 26 miles (42 km) of mountain biking trails are available. Bikes cannot be taken onto tram cars. There is no public transportation in this area of Albuquerque; the tram is accessible only by car, bicycle, or foot.

## **Timetable**

CT: Contributed Talk

IT : Invited Talk Tu : Tutorial

# Monday, July 17

8:00-9:00	Breakfast / Registration		
9:00-9:45	Welcome remarks		
9:45-10:00	Coffee Break		
		Chair: Timm Krüger	
10:00-11:00	Tu	Alexander Wagner	Deriving lattice Boltzmann from
	i d	_	Molecular Dynamics
11:00-11:30			offee Break
		C	hair: Luiz Hegele
11:30-11:50	СТ	Xiaowen Shan	Grad's eigen-function collision model
11.00 11.50	C1	Aldowell Shall	and the Spectral MRT LBM model
11:50-12:10	СТ	Paul Dellar	Vector lattice Boltzmann formulation
11.50-12.10	CI	raui Deliai	for hydrodynamics
			Sedimentation Modelling using Lattice
12:10-12:30	CT	Abhijeet Chodankar	Boltzmann Method in Newtonian and
			Non-Newtonian Fluids
12:30-14:00			Lunch
		Chaiı	r: Alexander Wagner
			Modeling magnetically responsive
14.00 14.45	ıT	LIIED Cabillan	particle-stabilized emulsion gels using
14:00-14:45	IT	Ulf D. Schiller	multicomponent lattice Boltzmann
			methods
14:45-15:00	Coffee Break		
		CI	nair: Qinjun Kang
			Generalized Multi-Component Lattice
15:00-15:20	CT	Adam Quintana	Boltzmann Method for Phase
			Separating Liquid Systems
45.00 45.40	СТ	Olivan Baalakaa	Lattice Boltzmann for linear elastic
15:20-15:40	CT	Oliver Boolakee	solids
			Lattice Boltzmann-based applications
15:40-16:00	СТ	Hongkyu Yoon	for pore-scale reactive transport
			processes
16:00-16:30		Co	offee Break
	Chair: Ulf Schiller		
16:30-16:50	СТ	Victor E. Ambruș	Multiphase flows on curved geometries
47.50.47.40	СТ	Flina Dallandani	Lattice Boltzmann Method for Fluid
16:50-17:10	CT	Elisa Bellantoni	Flows on Spherical Surfaces
	10-17:30 CT Satish Muthu		CFD Investigation of Transonic Axial
47.40.47.00			Compressor Rotor at Off-Design Speeds
17:10-17:30		Satish Muthu	Using Very Large Eddy Simulation
			(VLES) Lattice-Boltzmann Method
			, .,

# Tuesday, July 18

8:00-9:00	Breakfast		
	Chair: Paul Dellar		
			Facing Challenges in Computational
9:00-9:45	IT	Mathias J. Krause	Fluid Mechanics with Lattice
			Boltzmann Methods
9:45-10:00	Coffee Break		
		Cha	air: Victor Ambrus
10:00-11:00	Tu	Ilya Karlin	Asymptotic freedom in the lattice
10.00-11.00	Tu	·	kinetic theory
11:00-11:30			ffee Break
		Chair:	Alessandro Gabbana
11:30-11:50	СТ	Alexander Wagner	Analytical solutions for lattice
11.00 11.50	01	Alexander VVagner	Boltzmann methods
11:50-12:10	СТ	Aleksandra Pachalieva	Coarse-graining of molecular dynamics
11.50 12.10	0.	7 Hensariara i dellaneva	to derive the lattice Boltzmann method
12:10-12:30	СТ	Noah Seekins	Integer lattice gas method for the
	0.	rtouri ocennis	fluctuating Navier-Stokes equation
12:30-14:00	Lunch		
		Cha	ir: Mathias Krause
14:00-14:45	IT	Timm Krüger	Particle pairs in inertial microfluidics -
			insights from simulations
14:45-15:00	Coffee Break		
		Chair:	: Andrea Montessori
15:00-15:20	СТ	Vivek Krishna	Flow over tandemly placed square
			cylinders inside a channel
15:20-15:40	СТ	Sergiu Busuioc	Flows of dense gases confined
		-	between two parallel plates
15:40-16:00	СТ	Luiz Hegele	Dirichlet boundary condition for
15:40-16:00	CI		curved geometries within the lattice  Boltzmann framework
16:00-16:30	Coffee Break		
16:30-18:00			Posters

# Wednesday, July 19

8:00-9:00	Breakfast		
	Chair: Mateo Lulli		
9:00-9:45	IT	Andrea Montessori	Lightweight lattice Boltzmann models
9:45-10:00	Coffee Break		
		Chair: Ilya Karlin	
			The magic two-relaxation-time lattice
10.00.11.00	т	5 15 "	Boltzmann MHD scheme as a mimetic
10:00-11:00	Tu	Paul Dellar	finite difference scheme for extended
			Maxwell equations
11:00-11:30		(	Coffee Break
		Cha	ir: Timofey Kozhukhov
			Physics-constrained neural networks
11:30-11:50	CT	Alessandro Gabbana	for learning a lattice Boltzmann
			collisional operator
			Quantification of methane emission
11:50-12:10	CT	Ismot Jahan	from 2D images using large eddy
			simulation data and deep learning
12:10-12:30	СТ	Michael Woodward	Physics-informed machine learning
12:10-12:30	CI	Michael Woodward	with smoothed particle hydrodynamics
12:30-14:00	Lunch		
		Chair: Galen Craven	
			Exascale Ready Molecular Dynamics
14:00-14:45	IT	Mitchell Wood	Simulations With LAMMPS; Application
14.00 14.43	11	Witterien Wood	to Fluid Instabilities at Liquid-Vapor
			Coexistence
14:45-15:00	Coffee Break		
		Chair: Michael Woodward	
15:00-15:20	СТ	Dimiter N. Petsev	Molecular Dynamics of Binary Fuid
13.00 13.20	C1	Diffiller N. Petsev	Droplets Impacting Surfaces
15:20-15:40	СТ	Galen Craven	Molecular heat transport across an
.5.25 15.16	<u> </u>		oscillating temperature gradient
15:40-16:00	СТ	Timofey Kozhukhov	Active Flows using Multi-Particle
		-	Collision Dynamics
16:00-20:00	Social Program (Outing)		

# Thursday, July 20

8:00-9:00	Breakfast			
	Chair: Jens Harting			
			On the transformation of flow	
0.00 0.45	ıT	Shayath Civimali	instabilities and vortex structures with	
9:00-9:45	IT	Sharath Girimaji	rarefaction - Results from gas kinetics	
			based simulations	
9:45-10:00		Coffee Break		
		Chair:	Christoph Junghans	
			Lattice Boltzmann Modeling of Flow	
10:00-11:00	Tu	Qinjun Kang	and Transport Processes in Porous	
			Media	
11:00-11:30			ffee Break	
			r: Adam Quintana	
11:30-11:50	СТ	Victor E. Ambruș	Shakhov model for relativistic flows	
			Effect of fracture attributes and flow	
11:50-12:10	CT	Prakash Purswani	properties on multiphase flow through	
			fractures	
12:10-12:30	СТ	Alessandro Gabbana	Fast kinetic simulator for relativistic	
			matter	
12:30-14:00			Lunch	
14.00.14.45			ir: Daniel Livescu	
14:00-14:45	IT	Federico Toschi	Turbulent dense emulsions	
14:45-15:00		Coffee Break Chair: Prakash Purswani		
15:00-15:20	СТ	Jens Harting	Inertial focusing of dilute suspensions	
13.00-13.20	CI	Jens Harting	Redistribution of Residual CO <sub>2</sub> due to	
			Interfacial Pressure Driven Mass	
15:20-15:40	СТ	Richard Larson	Transport in Heterogeneous Pore	
			Structures	
			Validation of a high-fidelity	
15:40-16:00	СТ	Chenghai Sun	phase-field-based lattice Boltzmann	
			model for multiphase flows	
16:00-16:15		Co	ffee Break	
	Chair: Federico Toschi			
			Hydrodynamic Metastability:	
16.15 17.00	IT	Mattee Lulli	Fluctuations and Pressure Tensor in	
16:15-17:00		Matteo Lulli	Shan-Chen multi-phase lattice	
			Boltzmann	
17:00-17:30	Round Table (Scientific Committee Meeting)			
17:30-20:00	Banquet			

# Friday, July 21

8:00-9:00	Breakfast		
	Chair: Xiaowen Shan		
9:00-9:45	IT	Jens Harting	From droplets to capsules: rheology,
7.00-7.43	11	Jens Harting	capillary interactions and wetting
9:45-10:00	Coffee Break		ee Break
			r: Hongkyu Yoon
10:00-11:00	Tu	Tyler John Edward Reddy	Version Control with git for Scientists
11:00-11:30			ee Break
		Chair	: Richard Larson
			Simplifying Fluid Flow Simulations with
11:30-11:50	CT	Dennis Teutscher	paint2sim: A Just-in-Time Visualization
			Tool Using Lattice Boltzmann Method
			Load Balancing of Lattice Boltzmann
11:50-12:10	CT	Adrian Kummerländer	Methods for Heterogeneous High
			Performance Computers
			Mixed convection over square
12:10-12:30	CT	Shivakumar Kandre	cylinders placed inside a
			two-dimensional horizontal channel
12:30-14:00	Lunch		
		Chair: Ale	eksandra Pachalieva
			Lattice Boltzmann method for topology
14:00-14:45	IT	Li Chen	optimization of heat and mass transfer
			problems (virtual)
14:45-15:00	Coffee Break		
		Chair: Aleksandra Pachalieva	
			Interfacial Dynamics and
			Thermocapillary Convection in
15:00-15:20	СТ	Bashir Elbousefi	Self-Rewetting Fluids in Drop
.5.55			Impingement Processes and in
			Enclosed Layers of Fluids Using Lattice
			Boltzmann Method
		William Schupbach	A Robust Lattice Boltzmann Scheme for
15:20-15:40	СТ		Interface-Bound Transport of a Passive
			Scalar: Application to Surfactant-Laden
15 12 11 21			Multiphase Flows
15:40-16:00	Coffee Break		
16:00-16:30	Closing Remarks		