

Vacuum Science and Technology Division Fachverband Vakuumphysik und Vakuumtechnik (VA)

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Overview of Invited Talks and Sessions

(Lecture hall H2)

Invited Talks

VA 1.1	Mon	10:00–10:30	H2	Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics — ●STYLIANOS VAROUTIS, CHRISTOS TANTOS
VA 1.2	Mon	10:30–11:00	H2	Deterministic modeling of neutral gas flows of tokamak nuclear fusion devices — ●CHRISTOS TANTOS, STYLIANOS VAROUTIS
VA 1.3	Mon	11:00–11:30	H2	Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo — ●TIM TEICHMANN, CHRISTIAN DAY, THOMAS GIEGERICH
VA 2.1	Mon	11:45–12:15	H2	IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations — ●VOLKER HAUER
VA 2.2	Mon	12:15–12:45	H2	Current design status and outgassing considerations for the vacuum system of the Einstein Telescope — ●KATHARINA BATTES, CHRISTIAN DAY, STEFAN HANKE

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	Avoided quasiparticle decay from strong quantum interactions — ●RUBEN VERRESEN, RODERICH MOESSNER, FRANK POLLMANN
SYSD 1.2	Mon	10:25–10:50	Audimax 2	Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications — ●JULIANE BORCHERT
SYSD 1.3	Mon	10:55–11:20	Audimax 2	Attosecond-fast electron dynamics in graphene and graphene-based interfaces — ●CHRISTIAN HEIDE
SYSD 1.4	Mon	11:20–11:45	Audimax 2	The thermodynamics of stochastic systems with time delay — ●SARAH A.M. LOOS
SYSD 1.5	Mon	11:50–12:15	Audimax 2	First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM — ●BENJAMIN ZINGSEM

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	Organic semiconductors - materials for today and tomorrow — ●ANNA KÖHLER
SYAW 1.2	Wed	14:00–14:30	Audimax 1	PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors — ●GRZEGORZ KARCEWSKI
SYAW 1.3	Wed	14:40–15:10	Audimax 1	Fingerprints of correlation in electronic spectra of materials — ●LUCIA REINING
SYAW 1.4	Wed	15:10–15:40	Audimax 1	Artificial Spin Ice: From Correlations to Computation — ●NAËMI LEO
SYAW 1.5	Wed	15:40–16:10	Audimax 1	From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices — ●ANDREAS K. HÜTTEL

SYAW 1.6	Wed	16:20–16:50	Audimax 1	Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain — ●ZHE WANG
SYAW 1.7	Wed	16:50–17:20	Audimax 1	Imaging the effect of electron transfer at the atomic scale — ●LAERTE PATERA

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	DFMC-GEFES — ●JULIA HERRERO-ALBILLOS
SYES 1.2	Wed	13:40–14:10	Audimax 2	Towards Phononic Circuits based on Optomechanics — ●CLIVIA M. SOTOMAYOR TORRES
SYES 1.3	Wed	14:10–14:40	Audimax 2	Adding magnetic functionalities to epitaxial graphene — ●RODOLFO MIRANDA
SYES 1.4	Wed	14:45–15:15	Audimax 2	Bringing nanophotonics to the atomic scale — ●JAVIER AIZPURUA
SYES 1.5	Wed	15:15–15:45	Audimax 2	Hydrodynamics of collective cell migration in epithelial tissues — ●JAUME CASADEMUNT
SYES 1.6	Wed	15:45–16:15	Audimax 2	Understanding the physical variables driving mechanosensing — ●PERE ROCA-CUSACHS

Sessions

VA 1.1–1.3	Mon	10:00–11:45	H2	Rarefied gas flows and novel approaches for particle simulation
VA 2.1–2.2	Mon	11:45–12:45	H2	Vacuum technology: New developments and applications
VA 3	Mon	14:00–15:00	MVVA	Annual General Meeting

Annual General Meeting of the Vacuum Science and Technology Division

Monday 14:00–15:00 MVVA

- Bericht
- Wahl
- Verschiedenes

VA 1: Rarefied gas flows and novel approaches for particle simulation

Time: Monday 10:00–11:45

Location: H2

Invited Talk

VA 1.1 Mon 10:00 H2

Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics — ●STYLIANOS VAROUTIS and CHRISTOS TANTOS — Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

During the last decade research in the field of rarefied gas dynamics has attracted a lot of attention. This refreshed interest is due to applications in the emerging field of nano- and micro-fluidics, as well as to the more traditional fields of vacuum technology and high altitude aerodynamics. Some of these applications may include important phenomena such as those related to polyatomic gases, chemical reactions, evaporation and condensation. The gas rarefaction is specified by the Knudsen number (Kn), which is defined as the ratio of the mean free path over a characteristic length of the problem. In general, when the flow is considered as far from local equilibrium, then the well-known Navier-Stokes equations are not valid anymore. In this case, two main numerical approaches can be implemented. The first approach is based on the kinetic theory of gases as expressed by the Boltzmann equation or its associated kinetic models, in which a deterministic numerical solution is performed. The second approach is the Direct Simulation Monte Carlo (DSMC) method. Within the above framework, the first part of this talk will be devoted to the presentation of the aforementioned numerical approaches, while the second part will be devoted to the presentation of illustrative examples, as for instance, the modelling of the particle exhaust of a nuclear fusion reactor and the numerical modelling of a cryopump.

Invited Talk

VA 1.2 Mon 10:30 H2

Deterministic modeling of neutral gas flows of tokamak nuclear fusion devices — ●CHRISTOS TANTOS and STYLIANOS VAROUTIS — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Over the last few years much effort has been invested in modeling transport phenomena appearing in the complex geometry of the divertor region in tokamak fusion devices. Depending on the upstream plasma conditions, the flow reference Knudsen number, defined as the ratio of the mean free path over a characteristic length, may vary over a wide range. The rarefied flow behavior in these systems cannot be properly captured by the typical Navier-Stokes-Fourier approach and must be described by the integro-differential Boltzmann equation or re-

liable kinetic model equations. The Discrete Velocity Method (DVM) has developed into one of the most common techniques for solving the Boltzmann equation and the kinetic models. As it is well known simulating multidimensional rarefied gas problems based on the Boltzmann equation is computationally time consuming. Therefore, successful implementation of reliable kinetic models in such problems is important. In the present work, the Boltzmann equation is approximated by the well-known Bhatnagar Gross Krook (BGK) and Shakhov kinetic models supplemented with the deterministic discrete velocity method. Results are presented for He and D2 covering a wide range of the involved parameters. Extended comparisons between the deterministic approach and the stochastic Direct Simulation Monte Carlo (DSMC) method are presented.

Invited Talk

VA 1.3 Mon 11:00 H2

Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo — ●TIM TEICHMANN, CHRISTIAN DAY, and THOMAS GIEGERICH — Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Currently, a continuously working pump train for DEMO (the European demonstration fusion power plant) is under active development. Mercury driven diffusion pumps have been chosen as possible candidates for the high vacuum pumping of the exhaust gases. In order to design and optimize diffusion pumps for DEMO, a reliable numerical simulation method is required.

The numerical simulation of the DEMO diffusion pumps is a complex challenge as the gas flow in the pump spans a wide Knudsen number range. Typical inlet pressures of the diffusion pumps for DEMO are expected to be in the order of 10^{-3} Pa during dwell and up to 1 Pa during burn respectively. This is equivalent to estimated Knudsen numbers in the range of 10 to 0.01. As the Navier-Stokes equations lose their validity at $Kn > 0.1$, classic continuum solvers cannot be applied to the problem at hand. Therefore, the Boltzmann equation has to be solved to describe this flow regime. In this case the Direct Simulation Monte Carlo (DSMC) method was chosen to solve the Boltzmann equation. This presentation focuses on the application of DSMC on the simulation of diffusion pumps.

15 min. break

VA 2: Vacuum technology: New developments and applications

Time: Monday 11:45–12:45

Location: H2

Invited Talk

VA 2.1 Mon 11:45 H2

IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations — ●VOLKER HAUER — Karlsruhe Institute of Technology, Institute for Technical Physics, Karlsruhe, Germany

IFMIF, the International Fusion Materials Irradiation Facility, is a test facility for materials foreseen in fusion reactors. High neutron fluxes are generated with an energy spectrum and intensity similar to the conditions at the burn phase inside a fusion reactor. The high energy neutrons result from accelerating deuterons onto a lithium target. Simulations of the gas flow inside the IFMIF-DONES vacuum system were performed with the Test Particle Monte-Carlo code Molflow+. The IFMIF-DONES model is based on the latest design and of the LIPAc accelerator, which is being built for testing IFMIF accelerator components. Both, LIPAc and IFMIF-DONES share the same type of accelerator subsystems. The model was prepared for simulation by adding different sets of boundary conditions for the pumping of deuterium and hydrogen originating from beam losses and outgassing, respectively. The simulations of the gas pumping show pressure profiles which are mainly determined by the beam losses in this subsystem except for the Linac modules where the beam losses are very low. As LIPAc and IFMIF-DONES share most sections the pressure profiles are very similar.

Invited Talk

VA 2.2 Mon 12:15 H2

Current design status and outgassing considerations for the

vacuum system of the Einstein Telescope — ●KATHARINA BATTES, CHRISTIAN DAY, and STEFAN HANKE — Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen, Deutschland

As third-generation, underground gravitational-wave observatory the Einstein Telescope is currently being planned in Europe. In order to enhance sensitivity compared to the current detectors as well as to expand the frequency band to lower frequencies, the length of the vacuum pipe arms will be increased to 10 km and the main optics will partly be cooled to cryogenic temperatures below 20 K.

Designed as an equilateral triangle, the Einstein Telescope will consist of six laser interferometers, which require high to ultra-high vacuum conditions. As especially residual gases like water can cryosorb as frost on the cryogenic mirror surfaces and thus degrade its optical performance, this frost formation has to be mitigated by properly designing the cryostat and additional pumping as well as considering the outgassing characteristics of the room temperature parts.

Therefore, potentially relevant materials are investigated at the Outgassing Measurement Apparatus, which uses a modified throughput method. As a result, besides total outgassing rates, information on the outgassing species are determined by a mass spectrometer.

This paper describes the current design of the Einstein Telescope vacuum system and evaluates materials and possible pre-treatments with respect to their potential application based on optimized outgassing characteristics.

Lunch break

VA 3: Annual General Meeting

Time: Monday 14:00–15:00

Location: MVVA

Annual General Meeting