NEGF 26

5th European Conference on Non-Equilibrium Gas Flows

PROGRAM

MARCH 25TH–27TH 2026

Toulouse, Maison de la Formation Jacqueline Auriol (MFJA)
1 Rue Tarfaya, 31400 Toulouse

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Tuesday, March 24th 2026

PROGRAM

Meeting place :
Office de tourisme, Donjon du Capitole, Square Charles de Gaulle, 31000 Toulouse

16:30-18:30 - Guided tour of Toulouse
Free guided visit of Toulouse - registration is mandatory

You will discover the Place du Capitole; the Basilica of Saint-Sernin, a masterpiece of Romanesque art and a major stop on the pilgrimage routes to Santiago de Compostela; the Church of the Jacobins, the mother house of the Dominican Order with its remarkable architecture; and finally the banks of the Garonne River, offering splendid views of Toulouse's most iconic landmarks.

Donna Restaurant

19:00-22:00 - Welcome Party
Donna Restaurant, 8 rue Gabriel Péri, 31000 Toulouse

Wednesday, March 25th 2026

PROGRAM

Lecture Hall 001

08:30-09:15 - Onsite registration

09:15-09:30 – Welcoming word

09:30-10:15 - SESSION 1 - AEROTHERMODYNAMICS & SHOCKWAVES
Chair : Domenico BRUNO

09:30-09:45 (15min) - Simulation of the Entry of a Sphere into a Nitrogen Atmosphere with a Vibrational-Specific Model - Marie-Claude Druguet, Aix-Marseille Université

09:45-10:00 (15min) - Dynamics of MHD Flows in Low-Density Argon Plasmas at a Stagnation-Point Disk - Mattéo Comito, ONERA/ICARE

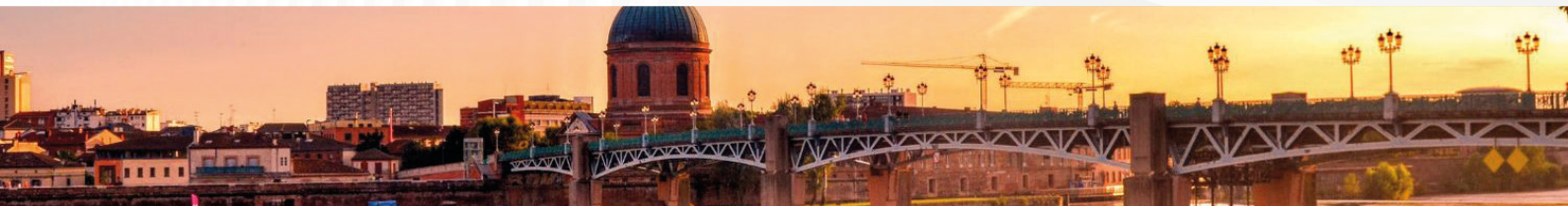
10:00-10:15 (15min) - Extension of UniGasFoam Solver to Multiscale Rarefied Polyatomic Gas Flows - Nikos Vasileiadis, Flow Matters Consultancy BV

Aeronautics Hall

10:15 - 10:45 - Coffee break

Lecture Hall 001

10:45-11:30 (45 min) Plenary Lecture 1: **Flying at Very Low Earth Orbit: An Application of Aerothermochemistry** - Thierry Magin, von Karman Institute for Fluid Dynamics.
Chair : Stéphane Colin



Wednesday, March 25th 2026

PROGRAM

Lecture Hall 001

11:30-12:45 – SESSION 2 - AEROTHERMODYNAMICS & SHOCKWAVES
Chair: Manuel TORRILHON

11:30-11:45 (15min)- A Novel Splitting Scheme and Its Application to Stochastic Particle Simulation of Diatomic Gas Flows - Ziqi Cui, Beihang University

11:45-12:00 (15min) - Hybrid Approach to Modeling Coupled Vibrational–Chemical Relaxation in Carbon Dioxide Mixtures - Denis Kravchenko, St Petersburg State University

12:00-12:15 (15min) - Kinetic Modelling of Chemically Reacting Mixtures: A BGK-Type Approach - Anna Macaluso, University of Parma

12:15-12:30 (15min) - Shock Thickness Analysis in Multi-Temperature Navier–Stokes Equations for Binary Inert Mixtures - Giorgio Martalo, University of Pavia

12:30-12:45 (15min) - Shock Wave Dynamics in Non-Equilibrium Gas Flow Regimes: Insights from Grad-Type Moment Systems - Satyvir Singh, RWTH Aachen University

Aeronautics Hall

12:45-14:00 – Lunch break

Lecture Hall 001

14:00-15:45 - SESSION 3 - MOMENTUM AND MASS TRANSPORT IN RAREFIED GAS FLOWS
Chair : Arjan FRIJNS

14:00-14:15 (15min) - Enhancing DSMC Simulations of Rarefied Gas Using a Fast-Converging and Asymptotic-Preserving Scheme - Lei Wu, Southern University of Science and Technology

14:15-14:30 (15min) - Efficient Adjoint Optimization of Rarefied Gas Flows - Lei Wu, Southern University of Science and Technology

14:30-14:45 (15min) - A Denoising Multiscale Particle Method for Simulating Nonequilibrium Gas Flows - Hao Yang, Beihang University

14:45 -15:00 (15min) - Experimental Measurements of Acetone Diffusion Coefficients in Gas Mixtures by Molecular Tagging - Andrea Luccon, University of Toulouse

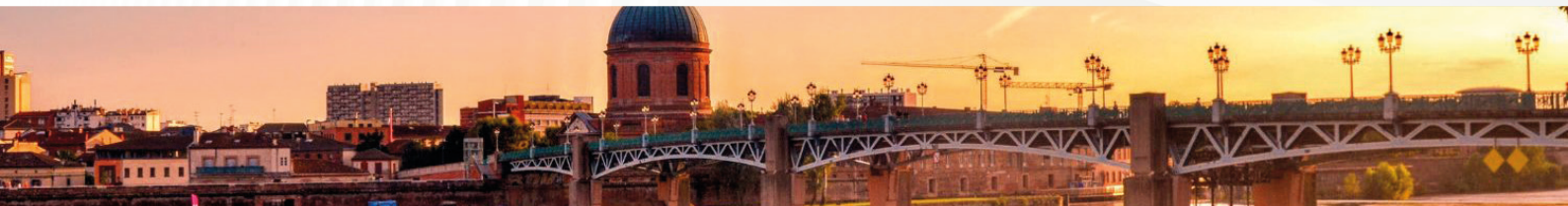
15:00-15:15 (15min) - Measurements of Helium Argon Mixture Using Constant Volume Technique - Irina Graur, Aix-Marseille Université

15:15-15:30 (15min) - Estimation of N_2 Volume Viscosity by Classical Trajectories Simulation - Domenico Bruno, Italian National Research Council

15:30-15:45 (15min) - On the Generation of Corner Flow Circulation at Highly Rarefied Conditions - Din Ben-Adva, Israel Institute of Technology

Aeronautics Hall

15:45-16:15 - Coffee break



Wednesday, March 25th 2026

PROGRAM

Lecture Hall 001

16:15-18:00 - SESSION 4 - MOMENTUM AND MASS TRANSPORT IN RAREFIED GAS FLOWS

Chair : Lei WU

16:15-16:30 (15min) - From 3D Tensors to 1D: A Reduction Strategy for Moment Closures in Multidimensional Systems - Eda Yilmaz, RWTH Aachen University

16:30-16:45 (15min) - High-Order Schemes for Stochastic Particle Solution of Fokker–Planck Kinetics - Montanaro Veronica, Swiss Federal Institute of Material Sciences

16:45-17:00 (15min) - Domain Decomposition for the Boltzmann Equation - Revanth Kollegala Sharma, Technische Universiteit Eindhoven

17:00-17:15 (15min) - Molecular Dynamics-Informed Collision Kernels for Polyatomic Gases - Bas Gieling, Technische Universiteit Eindhoven

17:15-17:30 (15min) - Non-Equilibrium Thermodynamics of Oriented Granular Gases Ben Nadler, University of Victoria

17:30-17:45 (15min) - Correcting Navier-Stokes-Fourier System for Rarefied Flows with Non-Linear Super-Stencil - Yijun Wang, ETH Zurich

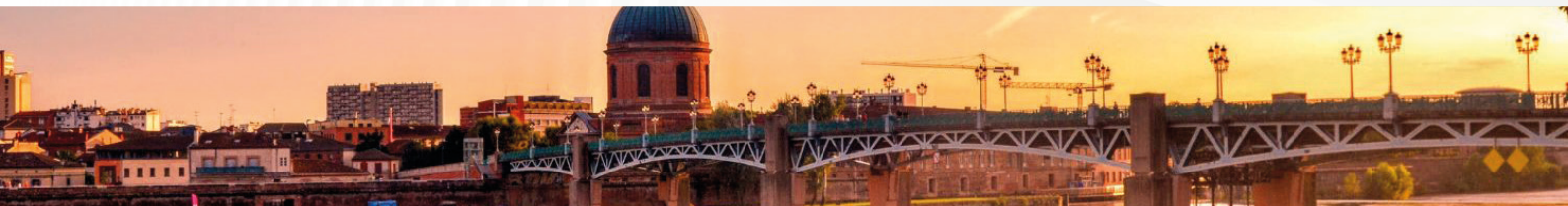
17:45-18:00 (15min) - Model-Adaptive Simulation of Moment Equations for Capturing Nonequilibrium Regions in Rarefied Gas Flows - Rik Verbiest, University of Groningen

J'Go Restaurant

20:00 - 22:30 - Scientific Committee Dinner

Le J'Go, Gascon Restaurant & Bodega

Free evening & scientific committee dinner for SC members



Thursday, March 26th 2026

PROGRAM

Lecture Hall 001

08:45-09:45 - SESSION 5 - GAS-SURFACE AND PLASMA-WALL INTERACTION
Chair : Stylianos VAROUTIS

08:45-09:00 (15min) - Thermal and Gas-Surface Interaction Effects in Rarefied Rayleigh-Bénard Convection - Sanjana Rao, IIT Madras

09:00-09:15 (15min) - Gas–Surface Interaction Models for Very Low Earth Orbit (VLEO) Systems - Ahilan Appar, Universidad Carlos III de Madrid

09:15-09:30 (15min) - Experimentally Determining the Effect of Gas–Surface Interactions on Particle Dynamics in Rarefied Flows - Rick Jansen, Eindhoven University of Technology

09:30-09:45 (15min) - Thermodynamically Consistent Incorporation of the Langmuir Adsorption Model into Compressible Fluctuating Hydrodynamics - Changho Kim, University of California

Aeronautics Hall

09:45 - 10:15 - Coffee break

10:15 - 11:00 (45min) - Plenary Lecture 2 - **Photophoretic Levitation: From Aerosols to Aircraft** - Ben Schafer, Rarefied Technologies Inc., Harvard University John A. Paulson School of Engineering and Applied Sciences - *Chair : Pierre Perrier*

Lecture Hall 001

11:00 - 12:30 - SESSION 6 - SENSORS, ACTUATORS, PUMPS, HEAT EXCHANGERS, AND OTHER DEVICES - *Chair : Martin WÜEST*

11:00-11:15 (15min) - Design and Modelling of Knudsen Micropumps Fabricated via Advanced Laser Manufacturing - Thanasis Basdanis, University of Toulouse

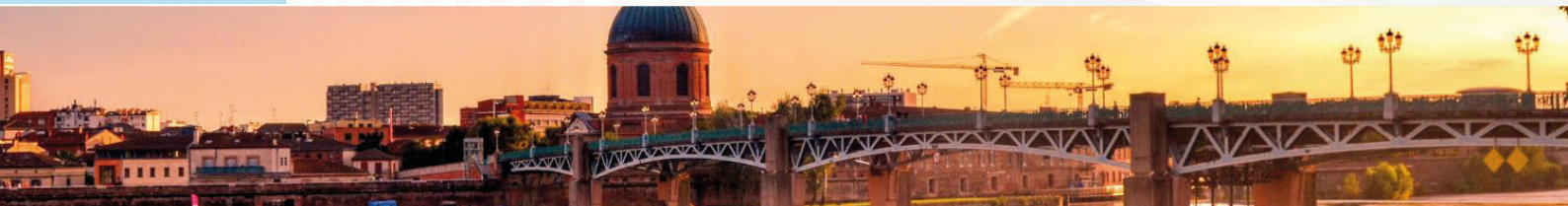
11:15-11:30 (15min) - Realization of Friction Reduction Acting on an Object Utilizing Knudsen Force - Hiroki Yamaguchi, Toyota Technological Institute, Nagoya University

11:30-11:45 (15min) - Microregenerators Designed for Oscillatory Gas Flows inside Cryocoolers - Samuel Bonnet, Université Grenoble Alpes

11:45-12:00 (15min) - Fabrication of a Knudsen Micropump For Operation Above Atmospheric Pressures - Phassawat Leelaburanathanakul, University of Toulouse

12:00-12:15 (15min) - Actuation of Artificial Micro-Muscles Using a Knudsen Micropump Marcos Rojas-Cárdenas, University of Toulouse

12:15-12:30 (15min) - Performance Study on a Knudsen Pump Prototype Fabricated via Two-Photon-Polymerization - Franz Schweizer, University of Toulouse



Thursday, March 26th 2026

PROGRAM

Lecture Hall 001 — **12:30 - 13:00 - Ceremony and Group Photo**

Aeronautics Hall — **13:00-14:15 – Lunch break**

Lecture Hall 001

14:15 - 16:00 - SESSION 7 - NON-EQUILIBRIUM PLASMA FLOWS

Chair : Dimitris VALOUGEORGIS

14:15-14:30 (15min) - Radiometric Forces on Structures Composed of Coaxial Rings
Benjamin Schafer, Rarefied Technologies Inc., Harvard University John A. Paulson School of Engineering and Applied Sciences

14:30-14:45 (15min) - H-Theorems for Dense Inert and Reactive Mixtures with Application to Global in Time Existence of Solutions - Jacek Polewczak, California State University

14:45-15:00 (15min) - Hyperbolicity of a Hermite-Laguerre Moment Model for the Plasma Edge in Slab Geometry - Julian Koellermeier, Ghent University

15:00-15:15 (15min) - Space Charge Compensation of Hydrogen Ion Beams: A Particle-in-Cell Study - Benzi John, STFC Daresbury Laboratory

15:15-15:30 (15min) - Ionic Wind Induced by a Dielectric Barrier Discharge between a Needle Tip and the Surface of a Liquid - Eric Moreau, University of Poitiers

15:30-15:45 (15min) - Cold Plasma-Induced Liquid Flow: What Is the Role of Electrohydrodynamic Phenomena? - Eric Moreau, University of Poitiers

15:45-16:00 (15min) - The Key Role of Non-Equilibrium Gas Flows on Edge Plasma Behavior and Exhaust Efficiency in Nuclear Fusion Reactors - Stylianos Varoutis, Max Planck Institute for Plasma Physics

Aeronautics Hall — **16:00-16:30 - Coffee break**

Lecture Hall 001

16:30 - 18:30 - SESSION 8 - HEAT TRANSFER IN RAREFIED GAS FLOWS

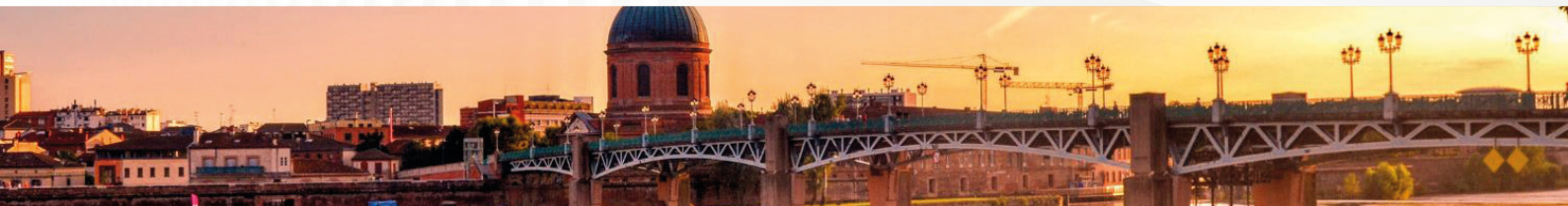
Chair : Lucien BALDAS

16:30-16:45 (15min) - Generalized Thermodynamically Admissible 13-Moment Equations
Luke Bell, University of Victoria

16:45-17:00 (15min) - Anomalous Nonequilibrium Effects in Supersonic Rarefied Flows
Vladimir Aristov, Russian Academy of Sciences

17:00-17:15 (15min) - A Semi-Lagrangian Method for the Polyatomic ESBGK Model and Its Comparison to DSMC - Erik Arlemark, ASML

17:15-17:30 (15min) - Particle Reduction Schemes for Binning-Based Merging Approaches in Variable-Weight DSMC - Georgii Oblapenko, RWTH Aachen University



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Lecture Hall 001

17:30-17:45 (15min) - DSMC Evaluation of the Thermophoretic Force on Micron-Sized Particles in Rarefied Gas Conditions with Hermite Boundary Domain Truncation - Ralf Reinartz, Eindhoven University of Technology

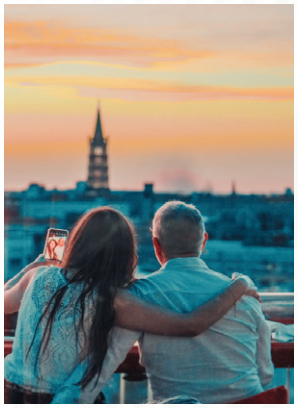
17:45-18:00 (15min) - Raman Thermometry of Confined Gas Microflows - José Maria Fernández, Instituto de Estructura de la Materia

18:00-18:15 (15min) - The Use of the Thermophoretic Force for Aerosol Particle Separation Irina Graur, Aix-Marseille University

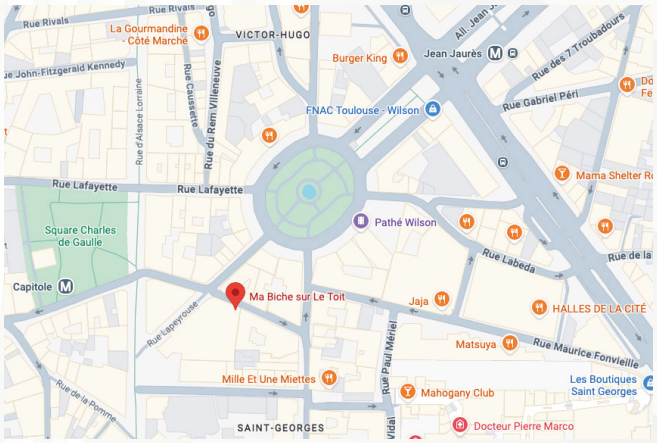
18:15-18:30 (15min) - Gas Transport through a Capillary Bundle Induced by a Temperature Gradient - Junhao Tu, Aix-Marseille University

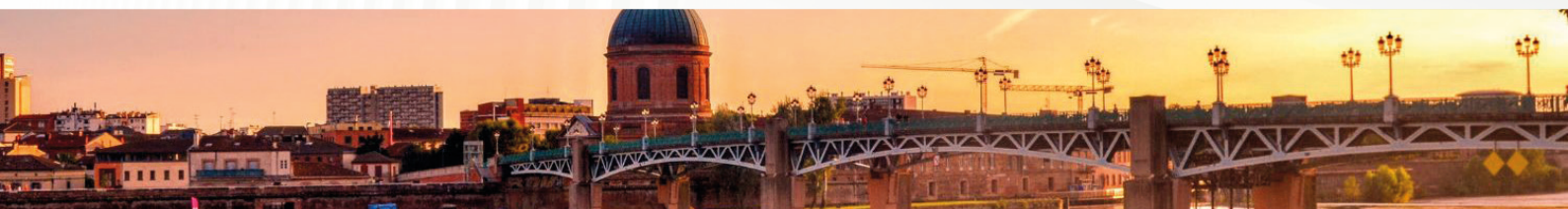
Ma Biche Sur Le Toit

20:00 - 23:30 - Conference Dinner
Ma biche sur le toit Rooftop Restaurant & Bar



How to get there :
Galeries Lafayette
(6th Floor)
4-8 rue du lieutenant colonel Pélissier,
31000 Toulouse

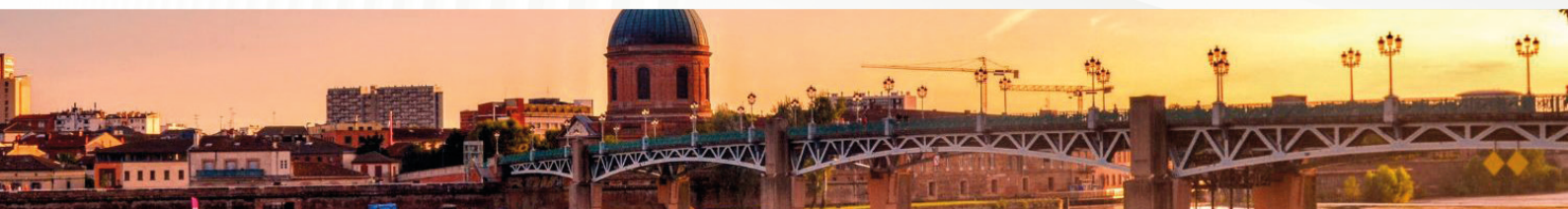




Friday, March 27th 2026

PROGRAM

Lecture Hall 001	**08:45 - 9:45 - SESSION 9 - MULTIPHASE MICROFLOWS AND INTERFACIAL PHENOMENA** *Chair : Irina GRAUR*
	08:45-09:00 (15min) - Mass and Heat Transfer at Liquid–Vapor Interfaces: Real Gas and Nonlinearity - Henning Struchtrup, University of Victoria
	09:00-09:15 (15min) - Molecular Kinetic Modelling of Surface-Confined Evaporative Flows - Yonghao Zhang, Chinese Academy of Sciences
	09:15-09:30 (15min) - Nonlocal Moment Equations for Liquid-Vapor Flows - Aldo Frezzotti, Politecnico di Milano
	09:30-09:45 (15min) - A Conforming Interface Approach for Phase Transitions in Rarefied Gas Dynamics Based on the R13 Equations - Manuel Torrilhon, RWTH Aachen University
Aeronautics Hall	**09:45 - 10:15 - Coffee break**
Lecture Hall 001	**10:15-11:00 (45min) - Plenary Lecture 3 - Thermally-Induced Flows in Microfluidic Systems: From Optothermal Fluidic Experiments to Non-Equilibrium Gaseous Modeling** Tetsuro Tsuji, Kyoto University - *Chair : Marcos Rojas-Cárdenas*
	11:00 - 11:45 - SESSION 10 - GAS FLOWS IN FLUIDIC MICROSYSTEMS *Chair : Erik ARLEMARK*
	11:00-11:15 (15min) - Interfacial Resistivities from a Shakhov-Enskog Kinetic Model Gaetan Brunetto, University of Toulouse
	11:15-11:30 (15min) - Evaporation & Condensation Coefficients under Non-Equilibrium Conditions - Arjan Frijns, Eindhoven University of Technology
	11:30-11:45 (15min) - Consistent Lattice Boltzmann Modeling of Low-Speed Isothermal Flows in the Slip Flow Regime: A Unified Slip Velocity Boundary Scheme - Goncalo Silva, Universidade de Évora
	11:45 - 12:00 (15min) - Closing Word - Lecture Hall 001
Aeronautics Hall	**12:00 - 13:00 - Lunch break**



Friday, March 27th 2026

PROGRAM

Airbus & Aeroscopia Museum

13:00 - 17:30 (4h30)
Industrial site and museum visit
Visit of Airbus Assemby Lines and of Aeroscopia Museum
Departure by bus from the conference venue

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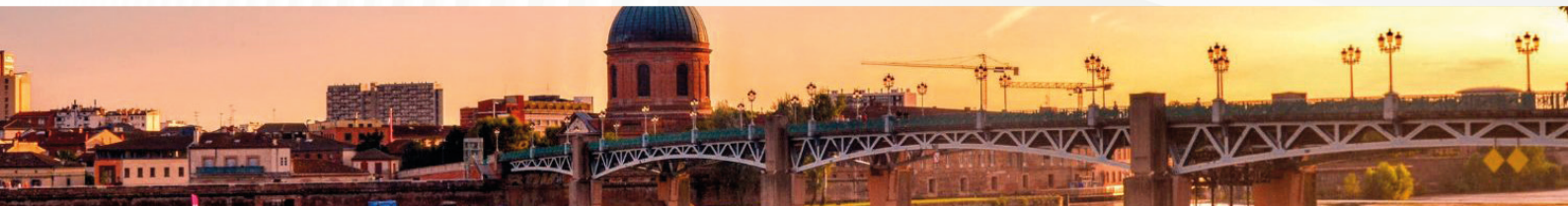

Author Index

NEGF26-686105

SIMULATION OF THE ENTRY OF A SPHERE INTO A NITROGEN ATMOSPHERE WITH A VIBRATIONAL-SPECIFIC MODEL

Marie-Claude Druguet[1], Arnaud Bultel[2]

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This paper is part of a progressive work to simulate with detailed chemical kinetics models the chemical composition and the thermodynamical state of a gas in the axi-symmeric shock layer surrounding a space body entering a planetary atmosphere, in reasonable computation times. A first step is to implement a state-specific vibrational model for Nitrogen into the PINENS code, that is a CFD code able to produce steady-state aero-thermodynamic flow-fields. Spatial distribution of the chemical species on their vibrational excited states, as well as Boltzmann distributions of the population densities on the vibrational levels, are presented and analysed.

NEGF26-701282

DYNAMICS OF MHD FLOWS IN LOW-DENSITY ARGON PLASMAS AT A STAGNATION-POINT DISK

Matteo Comito[1,2], Viviana Lago[2], Benjamin Khiar[1]

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matteo.comito@onera.fr, benjamin.khiar@onera.fr
[2]FAST team, ICARE-CNRS, 45100, Orleans, France
viviana.lago@cnrs-orleans.fr

Atmospheric re-entry and hypersonic flight expose vehicles to extreme heat fluxes, aerodynamic loads, and communication blackouts, key issues for space missions and hypersonic systems. Magnetohydrodynamics (MHD) enables active control of ionized flows via Lorentz forces, with applications in heat-flux reduction, flow control, energy conversion, and blackout mitigation. This experimental and numerical study focuses on ionized argon flows to isolate fundamental plasma–magnetic interactions, aiming to characterize MHD-induced flow structures and compare experiments with PIC-DSMC/MHD simulations. Simulations provide access to quantities difficult to measure experimentally, enabling interpretation of the observed structures and validation of the models.

NEGF26-678798

EXTENSION OF UNIGASFOAM SOLVER TO MULTISCALE RAREFIED POLYATOMIC GAS FLOWS

Nikos Vasileiadis, Gianluca Di Staso

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nvasilei@flow-matters.com, gds@flow-matters.com

Rarefied gas flows arise in many applications ranging from microscale devices to hypersonic and atmospheric-entry problems, where flow regimes may span from continuum to free-molecular conditions. The classical Navier–Stokes–Fourier equations are efficient but fail in highly rarefied regimes, while DSMC is universally valid but computationally expensive in near-continuum flows. Hybrid continuum–particle approaches alleviate this cost but introduce coupling challenges and inefficiencies.

To address these limitations, hybrid particle-particle multiscale methods combining stochastic particle (SP/USP/CNSP) models with DSMC have been developed, offering improved efficiency in continuum regions while retaining accuracy in rarefied conditions. The open-source uniGasFoam solver provides such a unified particle-based framework within OpenFOAM but is limited to monoatomic gases.

In this work, uniGasFoam is extended to polyatomic gas flows by implementing a polyatomic ESBGK collision model. The solver employs a local-gradient Knudsen number criterion to dynamically decompose the domain into continuum and rarefied regions, applying SP-based relaxation or DSMC collisions accordingly. The extended uniGasFoam solver provides accurate and efficient simulation of multiscale polyatomic gas flows, significantly reducing computational cost compared to full DSMC while retaining fidelity in non-equilibrium regions. This development greatly extends the applicability of uniGasFoam to real-world industrial applications.

NEGF26-713744

FLYING AT VERY LOW EARTH ORBIT: AN APPLICATION OF AEROTHERMOCHEMISTRY

Thierry Magin[1,2], Pietro Parodi[2,3], Pedro Jorge[2,4], Damien Le Quang[2], Federico Bariselli[2]

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pedro.jorge@vki.ac.be, damien.lequang@vki.ac.be, federico.bariselli@vki.ac.be
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[4]Ann and H.J. Smead Department of Aerospace Engineering Sciences, University of Colorado, Boulder, Colorado, United States

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Aerothermochemistry is a multidisciplinary domain coined by von Karman, that integrates fluid mechanics, thermodynamics, and physical chemistry. An innovative application of aerothermochemistry is currently investigated at the von Karman Institute (VKI): satellites orbiting at lower altitudes than conventional satellites, between 120 and 300 km, in the region called Very Low Earth Orbit (VLEO). Benefits can be obtained in terms of resolution performance for optical and radio instruments, as well as a more favorable link budget for communication. However, atmospheric drag needs to be compensated to keep the satellite in orbit. The Air-Breathing Electric Propulsion (ABEP) concept proposes to collect the tenuous atmospheric gas and use it as the propellant. The DRAG-ON facility has been designed and built at VKI to test the performance of intakes for ABEP systems. A plasma source is used in the facility to generate the stream of particles at approximately 8 km/s that reproduces the atmospheric flow on a satellite. Here, we present the numerical reproduction of the experiments through Particle-in-Cell simulations. The simulations comprise the expansion of the plasma plume from the outlet of the plasma source and its interaction with the intake model. One of the objectives of this study is to assess the differences between the flow produced on ground and the one encountered in orbit. The effect of different gas-surface interaction models is analyzed. In particular, a physics-based “modified-washboard” model will be used and compared to the traditional diffuse and Cercignani-Lampis model. Understanding the experimental results and properly calibrating the models are essential steps to extrapolate intake performance from ground tests to VLEO conditions.

NEGF26-679350

A NOVEL SPLITTING SCHEME AND ITS APPLICATION TO STOCHASTIC PARTICLE SIMULATION OF DIATOMIC GAS FLOWS

Ziqi Cui, Jun Zhang

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Stochastic particle methods, exemplified by the Direct Simulation Monte Carlo (DSMC) approach, are widely used for nonequilibrium gas flows. However, they impose strict constraints on the time step (resolving the mean collision time) and cell size, which are fundamentally consequences of operator-splitting errors. Specifically, while standard Strang splitting is formally second-order accurate, its accuracy degrades to first order in the stiff regime. This "order reduction" implies that the scheme is not asymptotic-preserving with respect to the Navier-Stokes limit in under-resolved scenarios. In this work, we revisit this issue through a manifold-based analysis. We demonstrate that when the time step under-resolves the relaxation process, conventional splitting acting on the collision substep erroneously projects the distribution function directly onto the Euler limit (a perfect Maxwellian). This intermediate state of complete equilibrium directly leads to a final state after the subsequent half-step transport where the non-equilibrium components scale linearly with time step. Physically, this manifests as a spurious time-step dependent viscosity. To address this, we propose a structure-preserving splitting scheme that modifies the collision substep using an implicit midpoint method, thereby maintaining both symmetry and asymptotic consistency. The scheme is implemented within a Fokker-Planck model covering both monatomic and diatomic gases, where particle evolution is governed by Langevin equations coupled with implicit moment-level updates. The resulting Multiscale Stochastic Particle (MSP) method is validated against the SR3 low-density wind-tunnel condition. Results demonstrate that, compared to standard DSMC, the MSP method exhibits uniform second-order accuracy and significantly improved robustness in the coarse-resolution regime.

NEGF26-685871

HYBRID APPROACH TO MODELING COUPLED VIBRATIONAL–CHEMICAL RELAXATION IN CARBON DIOXIDE MIXTURES

Denis Kravchenko, Elena Kustova

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This work presents a hybrid multi-temperature approach for modeling coupled vibrational and chemical relaxation in carbon dioxide mixtures, a critical challenge in simulating high-enthalpy flows for aerospace applications such as planetary entry. The study implements and examines a generalization of the forced harmonic oscillator (FHO) model for the CO_2 molecule to calculate state-specific rate coefficients for vibrational energy exchange (VT/VV) and the generalized Marrone-Treanor model to describe state-specific dissociation-recombination. The detailed FHO model is rigorously compared against the semi-empirical Landau-Teller formula, which relies on pre-defined relaxation times, usually taken from experimental data. Validation via isothermal bath relaxation in pure CO_2 shows the FHO model agrees well with experimental relaxation times data, while the Landau-Teller approach overestimates the overall relaxation rate. Furthermore, simulations of an adiabatic, reacting CO_2 mixture reveal that the FHO model captures complex, non-monotonic temperature behavior due to competing vibrational energy exchange processes. The results demonstrate that the FHO-based hybrid method provides a more physically comprehensive description of nonequilibrium kinetics, essential for accurately predicting coupled vibrational and chemical relaxation in CO_2 flows.

NEGF26-679197

KINETIC MODELING OF CHEMICALLY REACTING MIXTURES: A BGK-TYPE APPROACH

Marzia Bisi, Maria Groppi, Anna Macaluso

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Parco Area delle Scienze 53/A, Parma, 43124, Italy
marzia.bisi@unipr.it, maria.groppi@unipr.it, anna.macaluso@unipr.it

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In classical kinetic theory the dynamics of gas mixtures is naturally described through integro-differential Boltzmann equations for species distribution functions. However, the analytical and numerical study of these equations is rather difficult due to the complexity of the nonlinear integral Boltzmann operator that describes the collision mechanisms in detail. For this reason, starting from the BGK model for a single gas proposed by Bhatnagar, Gross, and Krook in 1954, several simpler models have been introduced.

In this work, we present a new BGK-type model for a chemically reactive mixture of four monatomic rarefied gases whose collision operator is expressed as a sum of binary BGK operators to describe elastic mechanical collisions and a single BGK term for a bi-molecular reversible chemical reaction involving all the constituents.

The BGK relaxation operators involve appropriate Maxwellian attractors depending on auxiliary parameters that have to be properly computed in order to make the BGK model consistent. This goal is achieved by imposing that the exchange rates for momentum and total energy of BGK and Boltzmann operators coincide under the assumption of Maxwell molecule mechanical potential and slow chemical reaction.

We prove that such model correctly reproduces the conservation laws and admits the correct Maxwellian equilibrium solutions. To conclude, numerical simulations of the kinetic BGK system in space homogeneous conditions are performed to investigate the asymptotic trend of the reacting mixture to the equilibrium.

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SHOCK THICKNESS ANALYSIS IN MULTI-TEMPERATURE NAVIER-STOKES EQUATIONS FOR BINARY INERT MIXTURES

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The shock wave structure has been extensively studied, particularly in hyperbolic systems of conservation and balance laws, where discontinuities can arise and violate the physical meaning of solutions. In contrast, we discuss here the shock wave structure in Navier–Stokes equations, which yields smooth solutions for any Mach number. Our analysis focuses on shock thickness, which quantifies the transition region between equilibrium states. While one might expect shock thickness to decrease monotonically for increasing Mach number, the single gas case reveals a non-monotonic trend: thickness decreases to a minimum, then rises unexpectedly; partial similar results have been observed in inert binary mixtures whose evolution is modelled by single-velocity and single-temperature formulations.

We investigate shock thickness in various inert mixtures of noble gases, considering different component concentrations at equilibrium. Our results extend single-gas findings, confirming the non-monotonic behaviour in single-velocity and multi-velocity multi-temperature models. The Mach number at which shock thickness reaches its minimum is not unique but depends on the mass ratio and equilibrium concentrations of the components.

Differences arise between single- and multi-velocity formulations, particularly for mixtures with large mass disparities. When all species fields are considered, transitions are more gradual and less steep, and temperature overshoot effects diminish or vanish entirely. In multi-velocity models, the minimum shock thickness occurs at slightly higher Mach numbers, especially for small mass ratios.

NEGF26-686098

SHOCK WAVE DYNAMICS IN NON-EQUILIBRIUM GAS FLOW REGIMES: INSIGHTS FROM GRAD-TYPE MOMENT SYSTEMS

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Shock waves in rarefied and non-equilibrium gas flows exhibit multiscale structures that cannot be accurately described by classical continuum models such as the Navier–Stokes–Fourier equations. In the transition regime, moderate to high Knudsen numbers produce strong thermodynamic non-equilibrium characterized by anisotropic stresses, non-Fourier heat flux, and higher-order transport effects within the shock layer. These phenomena require modeling approaches derived from kinetic theory.

In this work, shock wave dynamics are investigated using Grad-type moment systems to improve the physical representation of non-equilibrium transport processes. Extended moment equations, including Grad's 13-moment system and higher-order variants, are employed to resolve rarefied shock structures by retaining higher-order tensorial moments associated with stress, heat flux, and energy transport. A high-order Discontinuous Galerkin (DG) method is developed to solve the resulting hyperbolic moment equations, enabling accurate resolution of steep gradients and nonlinear wave interactions.

Numerical experiments are conducted for one- and multi-dimensional shock problems over a range of Mach and Knudsen numbers. The Grad-based framework demonstrates improved prediction of shock thickness, temperature overshoot, stress relaxation, and nonlinear heat-flux behavior compared with classical continuum descriptions. The simulations also capture non-monotonic temperature profiles and higher-order moment oscillations characteristic of non-equilibrium shock layers. In summary, Grad-type moment systems combined with high-order DG discretization provide an efficient and physically consistent framework for modeling transitional and rarefied shock flows relevant to hypersonic aerothermodynamics and microscale gas-flow applications.

NEGF26-679102

ENHANCING DSMC SIMULATIONS OF RAREFIED GAS MIXTURES USING A FAST-CONVERGING AND ASYMPTOTIC-PRESERVING SCHEME

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The numerical simulation of rarefied gas mixture dynamics with disparate masses using the direct simulation Monte Carlo (DSMC) method is slow, primarily because the time step is constrained by that of the lighter species, necessitating an enormous number of evolution steps to reach a steady state. Here, we address this issue by developing a general synthetic iterative scheme (GSIS), in which the traditional DSMC simulation is intermittently enhanced using a macroscopic synthetic equation. Specifically, after running the DSMC for a certain number of time steps, the high-order constitutive relations for stress and heat flux, as well as the momentum and energy exchange terms from inter-species collisions, are extracted from the DSMC and incorporated into the macroscopic synthetic equations. These equations are solved to obtain the steady state, and the solution is then used to update the particle distribution in DSMC, thereby skipping unnecessary intermediate evolutions. This two-way coupling not only accelerates convergence to the steady state but also asymptotically preserves the Navier-Stokes limit in the continuum flow regime, allowing the spatial cell size to be much larger than the molecular mean free path. The accuracy of our method is validated for one-dimensional force-driven Poiseuille flow and two-dimensional hypersonic flow past cylinders, considering Maxwell and hard-sphere gases with mass ratios of 10 and 100. Moreover, the one-dimensional shock wave structure and thermal driven low-speed flow have been investigated using a more realistic intermolecular potential. Although our in-house DSMC method is approximately an order of magnitude slower than the open-source DSMC code SPARTA, intermittently augmenting it with the synthetic equation makes it roughly 30 times faster at a Knudsen number of 0.01, with even greater computational gains anticipated at smaller Knudsen numbers. This work represents a critical step toward developing fast-converging and asymptotic-preserving schemes for hypersonic chemical reactions.

NEGF26-677857

EFFICIENT ADJOINT OPTIMIZATION OF RAREFIED GAS FLOWS

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Traditional aerodynamic optimization methods have primarily focused on continuum flows, with limited attention to rarefied flows—despite their significance in applications such as ultra-low Earth orbit vehicles, EUV lithography systems, and vacuum pumping equipment. To address this gap, we have developed two sets of adjoint-based optimization methods emphasizing efficiency and innovation, respectively: a shape optimization method using body-fitted grids, and a topology optimization method based on material density. The first method targets extreme efficiency, seeking to achieve most optimization effects within approximately ten iterations, thereby alleviating the high computational cost of rarefied flow simulations. The second method broadens the design space, allowing the independent evolution of shape, size, and topology to explore more innovative configurations without relying on prior knowledge or experience. Both methods are built upon the General Synthetic Iterative Scheme (GSIS), which deterministically and efficiently solves the Boltzmann model equation. This report will present the core concepts of these methods and their preliminary applications to airfoils, pipelines, jets, and other systems.

NEGF26-678700

A DENOISING MULTISCALE PARTICLE METHOD FOR SIMULATING NONEQUILIBRIUM GAS FLOWS

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The direct simulation Monte Carlo (DSMC) method is promising for simulating rarefied nonequilibrium flows, but its inherent statistical noise and spatiotemporal resolution limitation hinder its applications for low-signal and near-continuum regimes.

This work presents a denoising multiscale particle (DMP) method for efficient particle simulation of non-equilibrium gas flows. By extending particle attributes, each simulated particle in the DMP method carries both microscopic velocity and macroscopic flow information. Its low-noise property, where the signal-to-noise ratio is independent of signal magnitude, is achieved by statistically averaging the macroscopic information carried by particles. Additionally, anti-dissipation terms and spatial interpolation of macroscopic quantities are introduced to effectively compensate for numerical dissipation under large spatiotemporal steps, enabling multiscale computational capability. The method maintains high accuracy at coarse resolutions and significantly reduces the number of sampling particles required.

NEGF26-679548

EXPERIMENTAL MEASUREMENTS OF ACETONE DIFFUSION COEFFICIENTS IN GAS MIXTURES BY MOLECULAR TAGGING

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Understanding gas microflows through experimental characterization remains essential for validating rarefied gas dynamics models and refining the performance of microfluidic systems. Among the available diagnostic methods, molecular tagging (MT) techniques have proven particularly powerful for probing local flow properties. These methods rely on the photoluminescent response of tracer molecules introduced into a carrier gas, allowing the extraction of velocity and temperature fields from the temporal evolution of the emitted signal.

In Molecular Tagging Velocimetry (MTV), flow velocity is typically determined by dividing the mean molecular displacement by the observation time interval. However, under low-pressure conditions, diffusion becomes comparable to advection and must be accounted for through the advection–diffusion equation. Accurate reconstruction of velocity profiles therefore requires a precise knowledge of tracer diffusion coefficients.

This work aims to provide the experimental diffusion data necessary to improve the quantitative reliability of MTV-based measurements. Acetone vapor is employed as the tracer, and its self-diffusion and binary diffusion in helium and argon mixtures are investigated using a phosphorescence-based molecular tagging approach. The temporal broadening of the tagged region is analyzed through Gaussian fitting to extract the diffusion coefficient from the Einstein relation. Experimental results are compared with theoretical predictions derived from Blanc's law and the Chapman–Enskog kinetic theory, incorporating Lennard–Jones and Stockmayer intermolecular potentials. The molecular parameters for acetone, helium, and argon are taken from literature data derived from viscosity measurements.

NEGF26-679608

MEASUREMENTS OF HELIUM ARGON MIXTURE USING CONSTANT VOLUME TECHNIQUE

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A methodology for measuring the flow of a gas mixture through a channel is proposed based on the constant-volume technique. The behavior of the He–Ar mixture is analyzed for different helium concentrations ranging from 10 to 90 %. The analytical expression for the pressure variation over time in the inlet tanks, previously derived in the slip-flow regime, is used here to extract the velocity slip coefficients of the mixture. These coefficients exhibit a non-monotonic dependence on the helium concentration in the mixture. The experimental results for the pressure variation over time in the inlet tank and the normalized mass flow rate are compared with previous results obtained from gas kinetic theory, showing good agreement.

NEGF26-686009

ESTIMATION OF N_2 VOLUME VISCOSITY BY CLASSICAL TRAJECTORIES SIMULATIONS

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The knowledge of nitrogen transport coefficients is of fundamental importance. However, not all of them have been determined with the same accuracy. In particular, volume viscosity experimental measurements and theoretical estimations exhibit considerable uncertainties. In this work, a well known technique which combines Classical Trajectories (CT) calculations with nonequilibrium Direct Simulation Monte Carlo (DSMC), is used to estimate molecular nitrogen bulk viscosity. CT binary collisions are computed from a potential enegy surface (PES) proposed by Hellmann in 2013. The PES describes the interaction of two N_2 molecules in the rigid rotator approximation and it has been derived from accurate *ab initio* methods. The PES provided very accurate prodictions of N_2 shear viscosity and thermal conductivity. Unfortunately, no estimations of volume viscosity seem to have been obtained, yet. In the present work, N_2 volume viscosity is obtained by two different CT-DSMC configurations. In the first one, isochoric and adiabatic space homogeneous rotational-translational relaxation simulation are used to obtain volume viscosity from the relaxation time to equilibrium. In the second configuration, a gas flow characteriized by uniform and constant velocity divergence is reduced to a space homogeneous problem and the bulk viscosity is obtained from the difference between the equilibrium pressure and the pressure computed from translational temperature.

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ON THE GENERATION OF CORNER FLOW CIRCULATION AT HIGHLY RAREFIED CONDITIONS

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We investigate the occurrence of flow circulation in an open triangular cavity filled with a gas at highly rarefied conditions. The cavity is subject to an external shear flow that is either in the circular or lin- ear direction at its inlet. The problem is studied analytically in the free-molecular limit and numerically based on the direct simulation Monte Carlo (DSMC) method. The corner walls are modelled based on the Maxwell boundary condition, as either specular or diffuse. The results are obtained for arbitrary values of the outer flow speed and corner angle. Remarkably, it is found that multiple recirculation zones occupy the corner domain in the absence of molecular interactions. In the specular-corner setup, such topolo- gies occur at non-large outer-flow speeds and distinct corner-angle intervals. In the diffuse-wall case, the cavity flow field contains two recirculation zones at sufficiently low corner angles for both circular and straight outer flows. The results are rationalized based on the ballistic particle kinematics, suggesting insight into the relation between the microscopic description and the hydrodynamic (observed) genera- tion of circulation. The effects of molecular collisions on the corner flow pattern is inspected via DSMC calculations.

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FROM 3D TENSORS TO 1D: A REDUCTION STRATEGY FOR MOMENT CLOSURES IN MULTIDIMENSIONAL SYSTEMS

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Modeling rarefied gases requires frameworks beyond classical fluid descriptions, as the Navier-Stokes and Fourier equations fail in non-equilibrium regimes. Kinetic theory provides a fundamental formulation via the Boltzmann equation, describing the time evolution of the particle distribution function in phase space. Direct solution of the Boltzmann equation is computationally challenging due to the high dimensionality of the velocity space and the nonlinear nature of the collision operator.

Moment methods provide a systematic reduction by projecting the kinetic equation onto a finite set of velocity moments. Each moment corresponds to an integral of the distribution function against monomials of velocity, and represents macroscopic quantities such as density, momentum, and higher-order fluxes. The resulting system is an open hierarchy, since the evolution of the n^{th} moment depends on the $(n+1)^{\text{th}}$ moment, necessitating a closure relation. Classical approaches, such as Grad's Hermite expansion and maximum entropy closures, perform well in one-dimensional problems but face difficulties in higher dimensions or far-from-equilibrium regimes. While Grad's closure fails to preserve key structural properties like hyperbolicity in these regimes, maximum entropy closures maintain many such properties at the cost of significant computational effort.

The Gramian closure, recently proposed for 1D moment systems, constructs orthogonal polynomials using the Gram matrix, whose entries are inner products of velocity monomials weighted by the distribution. This allows for an explicit expression of the next higher-order moment in terms of known lower-order moments, avoiding the reconstruction of the underlying distribution function. Even and odd moment orders can be treated with extended Gramian formulations, allowing control over hyperbolicity and equilibrium preservation. Numerical studies in 1D show that Gramian closures are competitive with classical closures.

This talk will present the method of moments for kinetic equations and introduce the Gramian closure, a novel approach based on orthogonal polynomials that provides explicit formulas for higher-order moments from given lower-order moments. We then show how this closure, originally developed for one-dimensional systems, can be extended to multidimensional moment tensors using a rotation-based reduction strategy, allowing the 1D closure to be applied along multiple axes and reconstructing the full 3D higher-order moments efficiently while preserving key tensorial properties such as symmetry and trace invariance.

NEGF26-684269

HIGH-ORDER SCHEMES FOR STOCHASTIC PARTICLE SOLUTION OF FOKKER-PLANCK KINETICS

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In recent years, stochastic approximations of the Boltzmann equation based on simplified collision operators have gained popularity for being a computationally affordable alternative to common approaches such as Direct Simulation Monte Carlo (DSMC). Within these methods, collision operators constructed from the Fokker-Planck equation have been widely studied given their promising potentials.

In fact, the Fokker-Planck equation gives rise to a drift-diffusion process, which leads to a system of Stochastic Differential Equations (SDEs) of Langevin type for the velocity and position of the particles. This, in principle, allows for algorithms whose runtime is independent of the collision frequency. Despite this potential, there still exist open problems on constructing high-order solution algorithms based on the Fokker-Planck equation. Currently, time integration schemes for the position and velocity SDEs may not exceed first-order accuracy.

In this study, we focus on devising high-order time integration scheme for particles following SDEs resulting from Fokker-Planck kinetic models. This is a relevant issue as it will be crucial for applying Fokker-Planck methods in settings where the time-step is much larger than the mean-collision-time.

However improving the order of convergence is a challenging task given the statistical coupling between velocity and position updates.

Following ideas of operator-splitting in Hamiltonian systems, we propose here a solution algorithm based on splitting methods that allows second-order time integration of coupled SDE systems arising in the Fokker-Planck kinetic description. We further show that this approximation is potentially grid-free, making the integration amenable to coarser grids.

NEGF26–678653

DOMAIN DECOMPOSITION FOR THE BOLTZMANN EQUATION

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The Boltzmann equation (BE) for rarefied gas dynamics presents significant computational challenges due to its high dimensionality in phase space, requiring substantially more memory and computational resources than equivalent Navier-Stokes simulations. A domain decomposition approach is presented to address these challenges by distributing the computational load across high-performance computing infrastructure.

A finite element formulation with discontinuous Galerkin (dG) spatial discretization and the method of moments for velocity space is employed. The spatial domain is partitioned into subdomains that exchange flux information at interfaces during each timestep, with inflow to one subdomain corresponding to outflow from its neighbor. This framework enables several key advantages: reduced system matrix sizes and improved memory efficiency.

Entropy-based closure relations are incorporated within the method of moments approach to ensure physically consistent entropy dissipation. Anderson acceleration is employed to minimize subiteration overhead within each timestep. The closure also necessitates assigning a prior distribution, which, along with the velocity discretization, can be varied between different subdomains based on the local degree of rarefaction. Therefore, finer discretizations can be chosen (with better prior guesses) only where highly rarefied flows are expected, which results in further reduction of computational overhead. As an example, fluid dynamics within a channel connected to reservoirs with different pressures is analysed, with the decomposed domain solutions demonstrating excellent agreement with monolithic solutions across a range of Knudsen numbers.

This domain decomposition strategy naturally extends to multiscale coupling, enabling hybrid simulations where the BE is solved in rarefied regions while continuum models (Euler or Navier-Stokes equations) are applied elsewhere, with appropriate flux exchange at interfaces. This provides a more accurate treatment of rarefaction effects compared to slip boundary condition approaches.

NEGF26-677749

MOLECULAR DYNAMICS-INFORMED COLLISION KERNELS FOR POLYATOMIC GASES

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Non-equilibrium gas dynamics play a crucial role in various industrial applications, such as spacecraft reentry, microporous systems, and semiconductor lithography. In these regimes, the molecular mean free path becomes comparable to the system's characteristic length, and the Knudsen number approaches unity, causing continuum models like the Navier-Stokes equations to break down.

The Boltzmann equation offers a kinetic model valid across all Knudsen numbers, describing gas behavior through a particle distribution function. While particle-based simulations can also capture these dynamics, they become computationally expensive for large systems over long timescales. Moment methods provide a more efficient numerical framework, enabling simulations where continuum models fail and particle methods are infeasible.

A central challenge lies in the collision operator of the Boltzmann equation. For monatomic hard sphere molecules, an explicit formulation for this operator is available, but for polyatomic or complex interactions, approximations like the BGK operator often lack physical accuracy.

This work introduces a data-driven approach using high-fidelity Molecular Dynamics data to fit a parametrized collision kernel. This ensures compliance with conservation laws and entropy dissipation. To simulate polyatomic gases, the phase space is extended to include internal energy, with collisions modeled via the Larsen-Borgnakke framework. The resulting Boltzmann equation is solved using the Discontinuous Galerkin Method of Moments (DGMoM), combining spatial and moment-based discretization. Simulations of heat flux and micro-channel flow show strong agreement with experimental data, recovering known results in both continuum and free molecular limits.

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NON-EQUILIBRIUM THERMODYNAMICS OF ORIENTED GRANULAR GASES

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In this work, we develop a continuum model for the thermodynamics of granular systems consisting of rigid oriented particles by extending the state variables to account for the additional granular state variables.

The state variables to describe oriented granular gas are the granular temperature and the granular orientation in addition to the standard state variables which are density, velocity and thermodynamic temperature. The granular temperature is a nonnegative scalar value that represents the energy of the agitated particles (energy of the translation and rotation velocities fluctuations). The orientation is a symmetric, trace-free and bounded second order tensor representing the particles orientation distribution. The orientation tensor measures the deviation from isotropic orientation distribution.

The two additional granular state variables are governed by associated balance laws that are the granular energy and orientation which are in addition to the conservation of mass, balances of linear momentum, thermal energy and entropy.

Defining the orientation entropy contribution in terms of the orientation tensor, the Gibbs equation is used to identify entropy thermodynamic fluxes (driving to equilibrium) in terms of the thermodynamic forces (deviation from equilibrium) and the state variables. Using the non-negative entropy production requirement, the constitutive laws are constructed for all the fluxes. The constitutive laws for the fluxes, as first order approximation, are constructed by taking the fluxes to be linear combinations of the forces. The phenomenological coefficients matrix is obtained using the Onsager-Casimir reciprocity principles, which is required to be positive semi-definite. The general representation of the phenomenological coefficients matrix includes all the possible coupling, and the phenomenological coefficients are tensor of up to sixth order.

This formulation is too general and can only serve as a reference to generalize the constitutive laws if needed. To obtain a meaningful model we must make substantial simplifications by neglecting, what we consider, secondary effects. The developed constitutive laws are compared with models available in the literature for spherical particles as a special case. It is shown that the developed constitutive laws can describe spherical particles, and more importantly, to provide a systematic framework to generalize these laws to oriented particles.

NEGF26-679624

CORRECTING NAVIER-STOKES-FOURIER SYSTEM FOR RAREFIED FLOWS WITH NON-LINEAR SUPER-STENCIL

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Conventional particle-based methods for simulating rarefied gas flows, such as Direct Simulation Monte Carlo (DSMC), become prohibitively expensive in the near-continuum regime. While considerable efforts have been made to replace kinetic descriptions with generalized hydrodynamic models, such as the Burnett and Grads 13-moment equations, these approaches have achieved limited practical success. We propose a Non-Linear Super-Stencil (NLSS) model correction to augment the Navier-Stokes-Fourier (NSF) system for rarefied flow simulations. NLSS employs a compact stencil that samples local macroscopic flow features and maps them to corrective source terms in the original NSF system via a neural network, effectively capturing non-equilibrium effects beyond the continuum regime. We demonstrate the NLSS framework on planar channel flow. For the wall boundary conditions, a second map is applied to predict velocity and temperature slips. After training on a limited dataset spanning a range of only Mach and Knudsen numbers, the corrected NSF system accurately predicts macroscopic flow behavior and wall slips in unseen conditions, including cases with different wall temperatures and velocities. This highlights the potential of NLSS as a generalizable surrogate for rarefied flow simulation.

NEGF26-679212

MODEL-ADAPTIVE SIMULATION OF MOMENT EQUATIONS FOR CAPTURING NONEQUILIBRIUM REGIONS IN RAREFIED GAS FLOWS

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The need for space- and time-adaptivity in simulations of rarefied gases arises because different time-variable subdomains within a rarefied gas domain often require varying levels of modelling complexity. Different-order moment models are effective at describing rarefied flows with respective levels of complexity in each subdomain. In this work, an adaptive numerical method for simulating the non-linear Hyperbolic Moment Equations (HME) model is proposed to simulate a rarefied gas flow using a HME model with time- and space-dependent model order. The first step of the adaptive procedure is a domain decomposition into subdomains each modelled by an HME model of an appropriate order, using a combination of a distribution-based nonequilibrium criterion and a gradient-based nonequilibrium criterion. In the second step of the adaptive procedure, a non-linear adaptation of a recently developed padded buffer cell approach is proposed to couple these varying-order HME models. The proposed adaptive numerical method yields accurate results compared to a high-order HME model while obtaining a computational speedup.

NEGF26-684971

THERMAL AND GAS-SURFACE INTERACTION EFFECTS IN RAREFIED RAYLEIGH-BENARD CONVECTION

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Rayleigh–Bénard convection (RBC) in the rarefied regime is investigated using the Direct Simulation Monte Carlo (DSMC) method. In the non-continuum regime, non-equilibrium effects at walls arising from the exchange of momentum and energy between gas molecules and solid walls play a crucial role in determining flow dynamics and heat transfer. Molecular reflections at surfaces are modeled using various gas–surface interaction (GSI) kernels, including specular, fully diffuse, partially diffuse, and Cercignani–Lampis–Lord (CLL) models, which characterize the degree of momentum and thermal accommodation during molecule–wall collisions.

This study examines the influence of various GSI models and wall thermal boundary conditions, specifically isothermal and constant heat-flux walls, on the onset of convection and the overall heat transfer behavior in rarefied RBC. The neutral curve, which delineates the transition from conductive to convective heat transfer, is established in the Knudsen–Froude (*Kn*–*Fr*) number plane. The impact of these boundary conditions on the neutral curve is analyzed for cases with $Kn \geq 0.01$.

NEGF26-678891

GAS-SURFACE INTERACTION MODELS FOR VERY LOW EARTH ORBIT (VLEO) SYSTEMS

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Accurate estimation of the drag force is essential for spacecraft in very low Earth orbit (VLEO), as it significantly impacts orbit prediction, control, and collision avoidance. Accurate gas–surface interaction (GSI) models are crucial for predicting drag, particularly in collisions involving hyperthermal atomic oxygen with spacecraft surfaces operating in VLEO environments. This work examines the scattering of atomic oxygen on amorphous silica, a common satellite material, using reactive molecular dynamics. A comparison of angular scattering distributions and energy transfer between molecular dynamics calculations and experiments reveals excellent agreement. Based on the physical insights from molecular dynamics calculations, a new hybrid GSI model has been developed. The new model, termed the diffuse–Cercignani–Lampis–Lord (DCLL) model, combines velocity contributions from non-drifting diffuse Maxwellian and impulsively scattering drifting distributions. The new model reproduces angular flux distributions observed in molecular dynamics and beam experiments, while maintaining a structure suitable for implementation into particle solvers. The DCLL model is both simple and accurate, effectively bridging molecular-level fidelity with practical usability and providing a reliable tool for drag prediction and orbital analysis of VLEO spacecraft.

NEGF26-679128

EXPERIMENTALLY DETERMINING THE EFFECT OF GAS-SURFACE INTERACTIONS ON PARTICLE DYNAMICS IN RAREFIED FLOWS

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Particle dynamics in equilibrium and non-equilibrium rarefied flows must be understood to reduce the impact of contaminants in equipment of the semiconductor industry. The particle dynamics in rarefied flows is described by the Knudsen number, which is the ratio of the mean free path of gas molecules over a characteristic length scale of the system, which in this case is the volume-equivalent radius. Gas-surface interactions are shown to be important in describing the net effect of the particle dynamics for the drag and thermophoretic forces; especially in the free-molecular limit. We conduct experiments where the momentum and energy accommodation coefficients of nitrogen, helium and argon can be measured indirectly and where we can see the effect of the accommodation coefficients on the dynamics of microparticles. This has been done by measuring settling velocities of these microparticles in low-pressure systems with and without a thermal gradient. Our measurements cover the entire transition regime and far into the free-molecular limit. Our results will contribute to an active contamination control in the semiconductor industry.

NEGF26-686014

THERMODYNAMICALLY CONSISTENT INCORPORATION OF THE LANGMUIR ADSORPTION MODEL INTO COMPRESSIBLE FLUCTUATING HYDRODYNAMICS

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For a gas-solid interfacial system where chemical species undergo reversible adsorption, we develop a mesoscopic stochastic modeling method that simulates both gas-phase hydrodynamics and surface coverage dynamics by coupling the Langmuir adsorption model with compressible fluctuating hydrodynamics. To this end, we derive a thermodynamically consistent mass-energy update scheme that accounts for how the mass and energy variables in the gas and surface subsystems should be updated according to the changes in the number of molecules of each species in each subsystem due to adsorption and desorption events. By performing a stochastic analysis for the ideal Langmuir model and the full hydrodynamic system, we analytically confirm that our mass-energy update scheme captures thermodynamic equilibrium predicted by equilibrium statistical mechanics. We find that an internal energy correction term is needed, which is attributed to the difference in the mean kinetic energy of gas molecules colliding with the surface from that computed from the Maxwell-Boltzmann distribution. By performing an equilibrium simulation study for an ideal gas mixture of CO and Ar with CO undergoing reversible adsorption, we validate our overall simulation method and implementation.

NEGF26-694028

PHOTOPHORETIC LEVITATION: FROM AEROSOLS TO AIRCRAFT

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Photophoresis, or light-driven motion, of aerosols in Earth's upper atmosphere has been studied since the 1960s. When sunlight warms an aerosol particle surrounded by rarefied gas, an asymmetry in the temperature or accommodation coefficient on the aerosol's surface creates a photophoretic force on the aerosol, allowing it to levitate. With recent advancements in nanofabrication, could we build engineered devices that are bigger than aerosols, yet lightweight enough to fly on their own? Using aerosols as a starting point, I will discuss advancements in the field of photophoretic levitation, focusing on macroscopic platforms for near-space flight. I will touch on practical concepts for photophoretic flight in near-space including payload capacity, structure lifetimes, and deployment methods. The promise of photophoretic aircraft for atmospheric sensing, telecommunications, and Martian exploration has spurred new research into ultra-lightweight 2D materials that generate photophoretic gas flows.

NEGF26-679627

DESIGN AND MODELLING OF KNUDSEN MICROPUMPS FABRICATED VIA ADVANCED LASER MANUFACTURING

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Knudsen pumps use thermal transpiration flow to provide vibration-free gas pumping without moving parts, finding applications in various scientific and industrial fields. Achieving optimal rarefied conditions at atmospheric pressure requires submicron channels, which are technically challenging. This work presents two Knudsen pumps for over- and sub-atmospheric applications, fabricated using advanced laser techniques, namely Bessel beams and Selective Laser-Induced Etching (SLE), which are applied for the first time in Knudsen pump fabrication. Bessel beams create nanochannels with diameters of a few nanometers and length-to-radius ratios >100, while SLE produces channels down to 3 µm with ratios >50. Numerical simulations of gas flow and heat transfer were performed to design and optimize a single-stage, parallel-channel architecture with approximately 300,000 channels on a 1×1 cm² glass substrate with thickness up to 500µm. Under atmospheric conditions, temperature differences of around 47 ℃ for the Bessel beams and 20 ℃ for the SLE pump yielded pressure differences of 1575 Pa and 72 Pa, and maximum mass flow rates of 3.5×10^{-10} kg/s and 2.46×10^{-8} kg/s, respectively. The Bessel beams pump achieves higher pressures, while the SLE pump provides higher mass flows, enabling selection based on the intended application. By using advanced laser manufacturing, this work represents a significant step toward the development of high-performance Knudsen pumps across a wide range of operating pressures.

NEGF26-679329

REALIZATION OF FRICTION REDUCTION ACTING ON AN OBJECT UTILIZING KNUDSEN FORCE

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In high Knudsen number environments, such as rarefied gas flows or micro / nano gaseous flows, the existence of temperature difference / gradient induces a flow called a thermal transpiration flow. This thermally driven flow has been extensively studied for a long time, and it has been utilized in Knudsen pumps / compressors. As a reaction of this flow, the Knudsen force acts on the surface. In this study, we followed the numerical study by the DSMC in which an object placed above a heated flat plate was subjected to a lift force. We observed an object on a inclined heated flat plate to evaluate the friction reduction. The observations suggested that heating the flat plate induced a thermal transpiration flow and a Knudsen lift force, reducing the friction acting on the object.

NEGF26-685635

MICROREGENERATORS DESIGNED FOR OSCILLATORY GAS FLOWS INSIDE CRYOCOOLERS

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A simple model has been established in order to determine the cut-off frequency of periodical gaseous flows inside micromachined silicon-Pyrex regenerators, as used in miniaturized cryocoolers. Increasing the cut-off frequency of such microdevices is crucial to keep constant the heat power extracted from the cold source. The model has been experimentally validated with different networks of well-shaped structures. This model makes possible to foresee microdevices with cut off frequencies of around 600 Hz.

NEGF26-678830

FABRICATION OF A KNUDSEN MICROPUMP FOR OPERATION ABOVE ATMOSPHERIC PRESSURES

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Knudsen pumps driven by thermal transpiration are effective for micro-gas flow delivery, but achieving operation at or above atmospheric pressure requires fabricating channels with sub-micron diameters (≈ 600 nm) to maintain the transitional rarefied regime. Conventional fabrication methods like DRIE, nanoporous membranes (AAO), and two-photon polymerization (TPP) are ill-suited for this, limited by insufficient aspect ratios, high flow impedance, or impractically slow processing speeds for the large-area channel arrays required.

To overcome these limitations, this work presents the design and fabrication of a Knudsen pump utilizing ultrafast femtosecond laser processing with nondiffracting Bessel beams. This technique enables the rapid, single-shot fabrication of ≈ 300,000, high-aspect-ratio nanochannels with 600 nm diameters directly into a 500 µm-thick Borofloat 33 glass wafer. A thermal gradient is established by 20-nm Titanium resistive heaters on the "hot side" and silicon micro-pillar heatsinks on the "cold side."

The device is realized via a multi-step MEMS process: RIE/DRIE of the silicon heatsinks and inlets, anodic bonding of the Si to the glass wafer, Bessel beam drilling of the nanochannels, and a sequential Ti/TiW/Au metal deposition and wet-etching process to define the heaters and electrodes. The device is assembled in a custom test fixture with a polymer gasket and PCB, ready for experimental characterization using the constant volume technique with capacitance diaphragm gauges (CDGs).

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ACTUATION OF ARTIFICIAL MICRO-MUSCLES USING A KNUDSEN MICROPUMP

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Pneumatic artificial micro-muscles (PAμMs) offer large strain, low weight, and compliant actuation, making them attractive for microscale soft robotic applications. Recent developments in negative-pressure actuation enable efficient operation at small pressure differences, motivating the integration of compact pressure-generation mechanisms directly within microsystems. In this context, Knudsen micropumps (KμPs), which generate gas flow by thermal transpiration in rarefied regimes without moving parts, represent a promising solution compatible with microfabrication.

This work presents a theoretical investigation of a coupled microsystem in which a single-stage Knudsen micropump actuates an artificial micro-muscle. The pump consists of *n* parallel microchannels connected to a macrochannel, allowing scalable mass flow rates while maintaining a fixed maximum pressure difference. A simplified analytical model based on mass conservation and ideal gas behavior is developed and solved numerically to describe the coupled evolution of pressure and muscle deformation.

Simulation results show that increasing the number of parallel microchannels significantly reduces the actuation response time, while the final contraction amplitude remains unchanged and is determined solely by the maximum achievable pressure difference. These trends are explained by the linear characteristic curves of the Knudsen pump and the near-linear relationship between contraction ratio and pressure difference of the micro-muscle.

The results highlight channel parallelization as an effective design strategy to tune actuation dynamics without increasing system complexity or power consumption, paving the way toward compact, thermally driven soft microsystems.

NEGF26-678812

PERFORMANCE STUDY ON A KNUDSEN PUMP PROTOTYPE FABRICATED VIA TWO-PHOTON-POLYMERIZATION

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This work presents a performance study on an additively fabricated Knudsen pump prototype. The prototype is manufactured via two-photon-polymerization using a low thermal conductivity polymer and includes an array of 203 parallel pumping channels. A thin film heater, which is directly deposited on the polymer structure, generates a temperature gradient that activates the thermal transpiration phenomenon. The temperature distributions are obtained as a function of the heater power via finite element modeling (Comsol Multiphysics ©). The extracted temperature distributions along the channels are utilized as an input for simplified flow modeling based on the infinite capillary theory.

NEGF26-678339

RADIOMETRIC FORCES ON STRUCTURES COMPOSED OF COAXIAL RINGS

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Recent work suggests that photophoretic forces could levitate thin, 10 centimeter-scale membranes in near-space. Such devices could be useful for atmospheric science or telecommunications on Earth and Mars. Generally, the photophoretic force reaches its maximum value when the molecular mean-free-path (MFP) of the surrounding gas is about the same as the size of a solid, non-porous structure. This restricts photophoretic levitation to mm-scale or smaller structures at high altitudes. However, numerical calculations of the radiometric force exerted on perforated membranes suggest that the perforations increase the force when the membrane radius is significantly larger than the MFP. A main assumption throughout these calculations and experiments is that the perforation size should be much smaller than the MFP. However, the costs and difficulty of fabricating membranes increases as the perforations are made smaller. In other words, it is easier to drill or cut fewer holes with larger sizes. To study the trade-off between perforation size and photophoretic force, we study a circular membrane composed of coaxial rings, with varying ring sizes, numbers of rings, and distances between the rings. The aim of the present work is to model gas flows near a circular membrane composed of coaxial rings.

NEGF26-678358

H-THEOREMS FOR DENSE INERT AND REACTIVE MIXTURES WITH APPLICATION TO GLOBAL IN TIME EXISTENCE OF SOLUTIONS

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I consider simple reacting spheres (SRS) model of chemically reacting fluids for moderately dense regime. In the SRS model, the molecules behave as if they were single mass points with two internal states of excitation. Collisions may alter the internal states. In contrast to the dilute gas regime, in this work the two-particle distribution function of the chemically reacting mixtures is approximated by the products of one-particle distribution functions and the pair correlation fucntion of hard spheres at non-uniform equilibrium (modified Enskog Theory of H.van Beijeren and M.H.Ernst). First, I show existence of an H-functional for system. This is the first result for dense reacting systems. The H-functional is the sum of the kinetic and the correlational part. The structure of the correlational part is similar to the algebraic structure of the equilibrium non-uniform entropy for the mixture of infinity system of hard--spheres. With the help of this H-functional I prove global in time existence theorem for the SRS model of chemcally reacting fluids. This is the first such existence result for dense reactive mixture. Also, in the case when no reactions are consdered, the system becomes an inert dense mixture of hard spheres and this work also provides the first global in time existence of a solution for such system.

NEGF26-678583

HYPERBOLICITY OF A HERMITE-LAGUERRE MOMENT MODEL FOR THE PLASMA EDGE IN SLAB GEOMETRY

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Simulating the plasma edge of magnetic confinement fusion devices requires a stable and efficient numerical approach. Particle dynamics can be modeled by a kinetic equation, which is difficult to solve due to the high dimensionality of the phase space. In this paper we derive a moment model for a reduced kinetic equation to elucidate the question of hyperbolicity of the system, which is necessary to create a stable numerical model. The system matrix of an infinite set of moment equations is derived, after which the hyperbolicity of the model is investigated through the characteristic polynomial of said matrix. Hyperbolicity regions of the models are calculated and loss of hyperbolicity is investigated in scenarios relevant to magnetic confinement fusion. Regularization procedures that make the system globally hyperbolic are used to overcome that loss of hyperbolicity leading to a stable moment model hierarchy for plasma edge simulations.

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SPACE CHARGE COMPENSATION OF HYDROGEN ION BEAMS: A PARTICLE-IN-CELL STUDY

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Hydrogen ion sources are extensively used in particle accelerators worldwide for a range of applications. A typical problem encountered in the low energy beam transport (LEBT) region of such particle accelerators is beam divergence and transport losses due to space charge effects. Space Charge Compensation (SCC) is a process that helps to minimise transport losses by lowering the space charge of the ion beam. The focus of the present study is to investigate the SCC process of hydrogen ion beams using the Particle-in-Cell (PIC) method.

NEGF26-679178

IONIC WIND INDUCED BY A DIELECTRIC BARRIER DISCHARGE BETWEEN A NEEDLE TIP AND THE SURFACE OF A LIQUID

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Over the past decade, the interaction between non-equilibrium plasmas and liquids has gained increasing significance due to various applications, such as water treatment for instance. In this context, we developed a simple design consisting of a high-voltage needle placed a few millimetres above the surface of the liquid to be treated, whereas the grounded electrode is located below the glass tank containing the liquid (Figure 1). Therefore, between the two conductive electrodes, there is an air gap of a few millimetres, three centimetres of water and a 2-mm thick dielectric barrier of glass (Figure 1). Depending on the values of the applied voltage and its frequency, three different types of dielectric barrier discharges (DBD) may be observed between the needle tip and the water surface: a corona discharge, a transient regime and a filamentary discharge. Moreover, due to different physical phenomena, several mechanical effects can occur: a gas flow induced by the discharge, a deformation of the liquid surface and a flow inside the liquid, all these electrohydrodynamic phenomena being investigated by our team. The present experimental study focuses on the ionic wind produced between the needle tip and the water surface when a corona-type DBD is ignited. The velocity of this gas flow is measured with a 400-Hz PIV system (particle image velocimetry), that allows us to obtain 2D velocity fields with a spatial resolution smaller than 100 µm (see the field of view, FOV, in Figure 1). The input parameters that have been investigated are the distance between the needle tip and the water surface (from 11 mm down to 4 mm), the values of the applied voltage and its frequency (from 20 Hz up to 2 kHz), and the water conductivity (from 2 µS/m to 400 µS/m). The results highlight that the characteristics of the produced ionic wind jet depend strongly on all these parameters. Moreover, time-resolved measurements show that the positive corona discharge (occurring during the positive half-cycle) results in a fast and stable ionic wind jet when the ionic wind produced during the negative discharge is strongly unstable.

NEGF26-679210

COLD PLASMA-INDUCED LIQUID FLOW: WHAT IS THE ROLE OF ELECTROHYDRODYNAMIC PHENOMENA?

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The goal of this experimental study is to characterize the water flow induced by a DC discharge ignited between the water surface and a needle located a few millimeters above it. Firstly, we highlighted that two discharge regimes can be observed: a corona-like discharge with current from a few µA to a few dozen of µA, and a glow discharge with current of several mA. Secondly, particle image velocimetry (PIV) measurements allowed us to precisely characterize the liquid flow, that results in the formation of two symmetric and counter-rotating vortices. In the case of a normal-glow discharge, we highlighted that the velocity reaches about 14 cm/s at the interface and the topology of the flow depends on the voltage polarity, the water conductivity and on its surface tension. Several phenomena can explain the origin of the liquid flow, such as a thermal effect or a Marangoni effect. However, we think that the water flow is mainly due to two electrohydrodynamic (EHD) forces: a surface force due to the repulsion of charges at the surface, and an upward force in the liquid due to the migration of opposite charges from the bulk of the liquid. In the case of a corona-like discharge, there is still a significant water flow, even for current of a few µA. In this case, a third phenomenon can be at the origin of the liquid flow: the shear stress due to the ionic wind induced in the air, between the needle tip and the water surface, resulting in a gas flow above the liquid surface.

NEGF26-684533

THE KEY ROLE OF NON-EQUILIBRIUM GAS FLOWS ON EDGE PLASMA BEHAVIOR AND EXHAUST EFFICIENCY IN NUCLEAR FUSION REACTORS

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The control of neutral particle dynamics in the plasma edge and divertor regions is a fundamental challenge for the operation of magnetic confinement fusion devices such as tokamaks and stellarators. In these boundary regions, the plasma interacts with material surfaces, leading to steep density gradients and conditions where the mean free path of neutral particles becomes comparable to key geometric dimensions. This transition to the rarefied gas regime critically affects particle recycling, impurity transport, and exhaust efficiency, thus influencing overall plasma confinement and reactor performance.

In fusion devices such as ITER and Wendelstein 7-X, rarefied flow phenomena become especially prominent due to narrow divertor geometries and high vacuum requirements. These conditions produce Knudsen numbers spanning transitional to free-molecular regimes, which cannot be accurately described by conventional fluid models. Instead, kinetic approaches based on the Boltzmann equation, are required to resolve the local variations in neutral density, temperature, and velocity distributions. Integrated plasma–neutral modeling frameworks have therefore become essential tools in fusion research. Codes such as SOLPS-ITER and EMC3-EIRENE couple multi-fluid plasma solvers with Monte Carlo neutral transport solvers to provide a self-consistent description of plasma–neutral interactions across both continuum and rarefied regimes. An advanced alternative, the DIVertor GAs Simulator (DIVGAS), enables accurate modeling across all collisionalities. Validated against experiments on JET and W7-X, DIVGAS has been applied to the design and optimization of exhaust systems for next-generation devices including JT-60SA, ITER and DEMO. Within this context, as highlight of this paper the numerical study on the neutral transport of fuel gas (H_2) along with seeding impurities Ar, Ne and He in the W7-X sub-divertor is presented.

Beyond exhaust optimization, rarefied gas behavior influences tritium retention, surface erosion, and redeposition processes that govern plasma-facing component lifetimes and reactor safety. Future reactor-scale devices such as ITER and DEMO will demand enhanced modeling fidelity and diagnostic capabilities to control these effects. Continued advances in hybrid plasma–neutral simulations, adaptive numerical algorithms, and experimental validation will be crucial to achieving efficient exhaust, stable detachment, and safe tritium management.

NEGF26-679276

GENERALIZED THERMODYNAMICALLY ADMISSIBLE 13-MOMENT EQUATIONS

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The study of rarefied gas dynamics aims to describe phenomena in flows where the mean free path of molecules is comparable to the characteristic system length. In such nonequilibrium regimes, the standard Navier–Stokes–Fourier equations fail to accurately represent observed transport behavior. Although the Boltzmann equation provides a complete microscopic description, it is computationally expensive and impractical for large-scale applications. As an alternative, this work develops a generalized, thermodynamically admissible 13-moment model derived phenomenologically for arbitrary molecular potentials. The formulation explicitly enforces the second law of thermodynamics by constructing a nonequilibrium entropy and its balance equation, guaranteeing non-negative entropy generation and thermodynamic consistency. The resulting transport equations extend beyond the Grad-13 and regularized R13 models, introducing additional coupling terms between stress and heat flux that capture higher-order nonequilibrium and boundary-layer effects. Coefficient restrictions arise naturally from the entropy inequality, while remaining parameters can be tuned to kinetic or experimental data. Generalized boundary conditions are also derived to maintain enforcement of the second law at fluid–wall interfaces. Reductions to Couette and Poiseuille flow geometries are underway and will be compared to NSF, R13, and DSMC results for validation and optimization of coefficients. The framework provides a systematic foundation for developing higher-order transport equations that remain thermodynamically consistent while improving macroscopic accuracy to molecular behavior.

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ANOMALOUS NONEQUILIBRIUM EFFECTS IN SUPERSONIC RAREFIED FLOWS

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The study of nonequilibrium flows with new and various nonclassical effects is a continuation of our previous research conducted for a monatomic gas. Currently, a series of direct Monte Carlo simulations with the SMILE++ software system have been performed for a diatomic gas. Nonequilibrium distributions behind high-permeability (0.9 or more) grids should, according to the previous monatomic gas calculations, provide anomalous heat transfer: the heat flux and the downstream temperature gradient have the same signs. In the problem under consideration a supersonic equilibrium flow with Mach number $M = 4$ enter the grid at Knudsen number $Kn = 2$ (this parameter is determined by the wire diameter in the grid). A nonequilibrium flow is formed behind this high-permeability grid. The calculations for a diatomic gas confirm anomalous heat transfer in this supersonic nonequilibrium flow behind the grid. Its positive value indicates the deviation from the Fourier law. Theoretical and numerical research is currently being suplemented by experimental exploratory studies of anomalous transfer effects conducted in Novosibirsk State University.

NEGF26-677751

A SEMI-LAGRANGIAN METHOD FOR THE POLYATOMIC ESBGK MODEL AND ITS COMPARISON TO DSMC

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We present a new semi-Lagrangian scheme for the polyatomic Ellipsoidal Statistical BGK (ESBGK) model of the Boltzmann equation. The polyatomic ESBGK model describes molecular collisions as a relaxation towards a generalized Gaussian distribution with an anisotropic covariance matrix and an exponentially decaying internal energy distribution. The semi-Lagrangian framework, being deterministic and grid-based, removes the time-step restriction associated with the linear transport term by following the method of characteristics. The potentially stiff relaxation term is treated using an implicit A-stable linear multistep method which, owing to the structure of the BGK operator, can be reformulated into a fully explicit time-stepping scheme. This yields a highly efficient and numerically stable method. In addition, we propose inflow and outflow boundary conditions suitable for BGK-type kinetic equations. Several numerical experiments are presented to verify the accuracy and efficiency of the scheme, and to compare its performance with results obtained from the Direct Simulation Monte Carlo (DSMC) method.

NEGF26-678764

PARTICLE REDUCTION SCHEMES FOR BINNING-BASED MERGING APPROACHES IN VARIABLE-WEIGHT DSMC

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Particle merging schemes are investigated in terms of simulation accuracy and computational efficiency in the context of Direct Simulation Monte Carlo simulations of non-equilibrium rarefied flows. Both grouping and particle reduction schemes for particle merging within the groups are consiered.

The grouping approaches investigated in the present work are the octree binning method of Martin & Cambier, 2016, and a grid-based grouping method of Vranic et al., 2015. The particle reduction schemes investigated include the conservative N:2 merging scheme, a N:3 extension thereof which ensures conservation of the stress tensor components, and a modified N:1 scheme that ensures conservation via an additional particle post-processing step.

The combinations of the grouping and reduction approaches are applied to the simulation of microchannel flows in the transitional regime and are compared in terms of accuracy of bulk flow and surface properties, as well as their computational performance.

NEGF26-685492

DSMC EVALUATION OF THE THERMOPHORETIC FORCE ON MICRON-SIZED PARTICLES IN RAREFIED GAS CONDITIONS WITH HERMITE BOUNDARY DOMAIN TRUNCATION

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We present results on the evaluation of the thermophoretic force on a finite-size spherical particle at moderate to high particle Knudsen numbers by using the Direct Simulation Monte Carlo (DSMC) method. The influence of the accommodation coefficient (representing fully diffuse, specular or adiabatic properties) is investigated over a range of particle Knudsen numbers and the simulation predictions are compared to both approximate theoretical relations and numerical results.

We ultimately aim to investigate the influence of particle properties, like the shape and the particle thermal conductivity, in combination with different accommodation coefficients. Feasibility of large parameter sweeps requires a strongly reduced computational load. Therefore, advanced surrogate boundary conditions based on Grad's Hermite polynomial expansion of the molecular velocity distribution function are developed and implemented into the in-house DSMC code. We will show that the application of such boundary conditions drastically reduces the computational load while still obtaining accurate results on the thermophoretic force.

NEGF26-686060

RAMAN THERMOMETRY OF CONFINED GAS MICROFLOWS

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Microfluidics devices with internal gas flows are nowadays subject of a rapid development. These devices often operate in rarefied gas flow regimes, since the ratio (Knudsen number, Kn) of the molecular mean free path over the channel dimensions becomes non-negligible. In those rarefied flows, non-equilibrium effects are expected to occur, like temperature-jumps near the wall. However, there is a lack of experimental techniques capable of measuring the internal properties, such as temperature, in gas flows confined in small channels.

Raman spectroscopy is an optical tool based on the inelastic light scattering process, and has become a powerful non-intrusive technique to probe gas flows at the molecular level with spatial resolution of a few microns. These capabilities have been widely demonstrated in gas free microjets of small molecules at the Laboratory of Molecular Fluid Dynamics of the IEM-CSIC.

Raman spectroscopy relies on the structure of the Quantum-Mechanical energy levels of the gas molecules, like other molecular spectroscopies based on the absorption or emission of microwave or infrared radiation. Therefore, it can access the population of the energy levels of their internal motions (rotation and vibration), even when those populations deviate from the equilibrium Boltzmann distribution.

In order to extend the diagnostics capabilities of Raman spectroscopy to confined gas flows, we present here several examples of the application of Raman thermometry to gas flows within millimeter-sized channels. For this work, we have designed several channels with different geometries, and forced thermal gradients between some of their surfaces while flowing gases through the channels. The pressures ranged from atmospheric down to 20 mbar, and the flow velocities ranged from 10 to 300 cm/s. The most rarefied flows lie in the slip regime ($Kn \geq 10^{-3}$).

The experiments carried out so far have demonstrated that the gas temperature in the flow can be mapped with high spatial resolution, from the rotational and vibrational Raman spectra of molecules like N_2, CO_2 and H_2. The recorded temperature maps of the confined flows under thermal gradients show a different thermal behavior for gases like CO_2, that absorbs IR radiation, versus those like N_2 or H_2 which are transparent to it.

NEGF26-686055

THE USE OF THE THERMOPHORETIC FORCE FOR AEROSOL PARTICLE SEPARATION

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The design of a micro-separator for aerosol particles based on the thermophoretic effect is proposed. The first step in designing of such a micro-device is the development of a mathematical model. A three-dimensional model of a mini-channel (millimetric size) is proposed, and several key parameters are tested, including the length and width of the mini-channel, the intensity of the temperature gradient, and the velocity of the carrier gas. The next steps will be the fabrication of a mini-prototype followed by experimental testing of its efficiency. Ultimately, the final micro-device will be manufactured and tested.

NEGF26-686068

GAS TRANSPORT THROUGH A CAPILLARY BUNDLE INDUCED BY A TEMPERATURE GRADIENT

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The gas flow rate generated by a temperature difference across a bundle of optical fibers is studied experimentally. The measured data are compared with the mathematical model developed previously.

NEGF26-677682

MASS AND HEAT TRANSFER AT LIQUID-VAPOR INTERFACES: REAL GAS AND NON-LINEARITY

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This contribution concerns evaporation and heat transfer processes at liquid vapor interfaces in thermodynamic nonequilibrium. In the case of small scales, i.e., large resolution, and/or large heat and mass fluxes, these processes are accompanied by marked temperature jumps between vapor and liquid, and deviation of pressure from saturation.

Thermodynamic modelling of these jumps introduces interfacial resistivities, while kinetic theory models rely on condensation and accommodation coefficients. The jumps are microscale effects and thus difficult to measure, with experimental uncertainties making it almost impossible to verify models or extract reliable data. Molecular dynamics (MD) simulations provide high resolution on the molecular scale but unavoidable stochastic noise affects determination of resistivities.

Kinetic theory models are typically restricted to ideal gases, while MD simulations are often run in denser gases, where real gas effects affect the results, and, in order to reduce noise, in strong non-equilibrium with large fluxes. In this presentation, I combine elements of the Hertz-Knudsen-Schrage model of kinetic theory with the Tsuruta condensation coefficient and the Enskog-Vlasov model for real gases to the non-linear Tsuruta–EV–HKS model, which is valid up to the critical point. The resulting interfacial resistivities markedly decrease with temperature towards the critical point, and depend non-linearly on mass and heat flux.

NEGF26-679318

MOLECULAR KINETIC MODELLING OF SURFACE-CONFINED EVAPORATIVE FLOWS

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Surface-confined non-equilibrium evaporative flows play a central role in new technologies that exploit nanoscale confined flows, ranging from nanoporous membranes for distillation, hydrogen/carbon dioxide storage, to evaporative cooling in electronics. Understanding of non-equilibrium liquid-vapour phase changes and fluid-solid molecular interactions that are critical to these and other such technologies is still at an early stage. In this work, we propose a molecular kinetic model that consistently resolves the coupled interactions among vapour, liquid and solid surface in such flows. This ‘bottom up' approach can describe the formation of the liquid-vapour, liquid-solid and vapour-solid interfaces and the effects of non-equilibrium and real fluids, which does not need empirical models depending on *ad hoc* parameters such as evaporation/condensation coefficients and contact angle. In addition, fluid-solid molecular interactions are explicitly considered in the transport equations, eliminating the reliance on pre-defined boundary conditions. This mesoscopic framework bridges the gap between molecular-scale dynamics and macroscopic hydrodynamics, striking a balance of computational accuracy and efficiency.

NEGF26-677758

NONLOCAL MOMENT EQUATIONS FOR LIQUID-VAPOR FLOWS

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Recently, a system of moment equations has been derived from Enskog-Vlasov equation and applied to various types of nonequilibrium flows in which liquid and vapor regions coexist, being separated by a fully resolved interface.

The EV equation has an intrinsic nonlocal structure, inherited from Enskog's kinetic theory of the dense hard sphere fluid. Grad-26 moment equations are based on a local (differential) expansion of the hard sphere collision integral and self-consistent field term, generated by the potential attractive tail. Expanding nonlocal terms is fully justified in regions where flow variations are small across a distance on the order of the range of molecular forces. However, expansions accuracy must be confirmed in the liquid-vapor interface region, whose thickness is on the order of ten molecular diameters. Here, higher order moments, crucial for the description of kinetic layers in the vapor, are produced in an extremely narrow region, corresponding to the vapor-side half of the interface.

The present work aims at obtaining a set of moment equations, based on the linearized EV equation, in which fluxes and sources keep their exact, nonlocal form. Then, the accuracy of the moment approximation depends only on the number of moments, not on the order of the expansion turning nonlocal into local terms.

Local and nonlocal form of the moment equations are compared on the description of a two-phase Couette flow.

NEGF26-684788

A CONFORMING INTERFACE APPROACH FOR PHASE TRANSITIONS IN RAREFIED GAS DYNAMICS BASED ON THE R13 EQUATIONS

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The regularized 13-moment (R13) equations extend Grad's classical moment system to provide stable and accurate closures for stress and heat flux in rarefied gas dynamics. They overcome deficiencies of traditional continuum models, enabling reliable simulations of non-equilibrium flows across a wide range of Knudsen numbers. The software fenicsR13 is a tensorial mixed finite element solver for the linearized R13 equations, built on the FEniCS computing platform. It enables a near one-to-one translation of the mathematical formulation into source code, ensuring accurate, validated simulations of rarefied gas dynamics. This talk presents a conforming interface simulation tool for phase transitions in nonequilibrium gas flow using the R13 system build on top of FEM code fenicsR13.

NEGF26-691080

THERMALLY-INDUCED FLOWS IN MICROFLUIDIC SYSTEMS: FROM OPTOTHERMAL FLUIDIC EXPERIMENTS TO NON-EQUILIBRIUM GASEOUS MODELING

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In this talk, some recent experimental and theoretical studies on thermally-induced microflows will be introduced. In the experimental part, we focus on thermophoresis, namely, a microparticle motion along a temperature gradient in fluids. Using an optothermal microfluidic system in liquids combined with optical trapping, thermally-induced flows around microparticles are detected, and the connection between the thermally-induced flows and the thermophoresis is clarified. To measure such slow microflows, optically-trapped particle tracking velocimetry is also proposed. Optothermal microfluidic systems are found to be effective, feasible, and convenient experimental setup to investigate thermal microflows. As an instant computational tool for optothermal microfluidic systems, a semianalytical model has been developed. In the modeling part, a kinetic model on thermally-induced non-equilibrium gas flows will be introduced. The model incorporates the fluid–solid molecular interaction potential, and a thermal-slip boundary condition is derived using the generalized slip-flow theory. Although the model is extremely simple, we have shown that the model reproduces qualitatively the sign reversal of the thermal-slip coefficients depending on the strength of the fluid-solid interaction. These outcomes on thermally-induced microflows are expected to contribute to the development of novel microfluidic functions such as separation and concentration.

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INTERFACIAL RESISTIVITIES FROM A SHAKHOV-ENSKOG KINETIC MODEL

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The modelling of strong density gradient regions in fluids is a challenging task. It becomes even more complex when the fluid is fairly dense and out of equilibrium. It is however a central question in order to address the exchanges of heat and mass across a liquid vapor interface, which is fundamental to meet the design requirements of modern technological needs. For small departure from equilibrium, one could expect close equilibrium approaches, i.e., hydrodynamic regime, to be an appropriate description of the system, giving access to the interfacial resistivities and their dependence to the state of the fluid. In this work, using a BGK-Shakhov model, we show that we can obtain the same hydrodynamic equations as Enskog for dense fluids. The close equilibrium limit of the resulting set of equations is then shown to be reducible to linear relations between fluxes and thermodynamical forces. The link between those quantities is associated with resistivities.

NEGF26-682197

EVAPORATION & CONDENSATION COEFFICIENTS UNDER NON-EQUILIBRIUM CONDITIONS

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Evaporation and condensation at the liquid–vapor interface are critical phase-change phenomena. As devices become increasingly miniaturized and energy-efficient, a deeper understanding of interfacial heat and mass transfer becomes essential. Molecular Dynamics (MD) simulations offer detailed insights, but are computationally intensive. The S-model kinetic equation presents a more efficient alternative but requires accurate input parameters, including the liquid temperature and evaporation/condensation coefficients. This study investigates the behavior of these parameters under varying vapor flow conditions, characterized by different Mach numbers, using the S-model. By positioning the so-called liquid boundary near the liquid/vapor interface, good agreement is obtained between the S-model and MD results. Evaporation coefficients are similar for different far-field liquid temperature (90 K and 120 K). While the condensation coefficients deviate more than 0.2 for these far-field temperatures. These findings help improve the alignment between S-model and MD results under non-equilibrium conditions.

NEGF26-701929

CONSISTENT LATTICE BOLTZMANN MODELING OF LOW-SPEED ISOTHERMAL FLOWS IN THE SLIP FLOW REGIME: A UNIFIED SLIP VELOCITY BOUNDARY SCHEME

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Accurate simulation of rarefied gas flows in microfluidic geometries requires a consistent numerical treatment of slip velocity boundary conditions, particularly in the presence of curved or non–mesh–aligned solid walls and of boundary constraints with different mathematical character in the normal and tangential directions. Within the lattice Boltzmann method, the construction of such direction–dependent boundary schemes remains a central difficulty and is frequently addressed through problem–dependent formulations with limited geometric robustness.

In this work, a unified boundary strategy is proposed for the lattice Boltzmann modeling of low–speed isothermal flows in the slip–flow regime. The approach is based on a consistent closure relation obtained from a second–order Taylor expansion of the physical slip condition and exploits its Robin–type structure to separate Dirichlet and Neumann contributions associated with impermeability and tangential slip. This formulation enables the combined use of link–wise and wet–node operation principles within a single boundary closure, allowing an independent and accurate enforcement of normal and tangential boundary constraints with parabolic accuracy on arbitrarily discretized walls.

The scheme is implemented within a two–relaxation–time lattice Boltzmann formulation and assessed in several channel–like configurations. In both inclined planar and curved annular geometries, the proposed boundary treatment yields accurate solutions across mesh refinements and parameter variations, including coarse discretizations and strong geometric non–alignment.

These results confirm that the proposed unified boundary formulation provides a consistent, accurate, and geometrically flexible framework for the lattice Boltzmann simulation of slip flows, offering a robust alternative to existing boundary treatments for rarefied microfluidic applications.

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