NF-2015

INTERNATIONAL SCHOOL FOR STUDENTS AND YOUNG SCIENTISTS

“NON-EQUILIBRIUM AND HIGH-TEMPERATURE GAS FLOWS”

Khristianovich Institute of Theoretical and Applied Mechanics,

Siberian Branch of the Russian Academy of Sciences

Institutskaya st., 4/1, Novosibirsk, Russia

November 09-10, 2015.

Saint Petersburg State University, Russia

ITAM

Siberian Branch of Russian Academy of Sciences
Khristianovich Institute of Theoretical and Applied Mechanics

РНФ | Российский научный фонд

Russian Science Foundation

The school is organized by

- Saint Petersburg State University
- Khristianovich Institute of Theoretical and Applied Mechanics
- Russian Science Foundation

Organizing Committee

- Kustova E.V. (Co-chair, Saint Petersburg State University)
- Bondar Ye.A. (Co-chair, Khristianovich Institute of Theoretical and Applied Mechanics)
- Mekhonoshina M.A. (Scientific secretary, Saint Petersburg State University)
- Nagnibeda E. A. (Saint Petersburg State University)
- Molchanova A.N. (Khristianovich Institute of Theoretical and Applied Mechanics)

The school is organized as a course of invited lectures given by leading scientists working in non-equilibrium gas-dynamics, kinetic theory of gases, computational fluid dynamics.

Contact information

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Detailed Program

Monday, November 9, 2015		
8-00	**Registration**	
9-00	**School opening**	
	Chairperson: Kustova E.V.	
9-30	**Current models in relaxation aerodynamics. Problems and Results**	**Nagnibeda E.A., Saint Petersburg State University, Russia**
The kinetic theory method for derivation of models for strongly non-equilibrium reacting gas flows is briefly presented. Specific features of state-to-state, multi-temperature and one-temperature description for non-equilibrium kinetics and transport properties in multi-component mixtures are analyzed. Applications of different models for shock heated and expanding air flows are discussed as well as problems for further model refinement.		
10-20	**Plasma models consistent from kinetic to hydrodynamic scale**	**Thierry Magin, Von Karman Institute for Fluid Dynamics (VKI), Belgium**
An accurate modeling of dissipative effects in plasmas is crucial to many applications from black-out phenomena in atmospheric entry flows to magnetic reconnection in solar physics. First, we propose to calculate the crossed contributions to the mass and energy transport fluxes coupling the electrons and heavy particles, such as atoms and ions, in multicomponent plasmas. This coupling effect was first introduced by Kolesnikov. To derive asymptotic solutions for multicomponent plasmas based on kinetic theory, it is essential to solve the distribution functions in the Enskog expansion up to second-order for electrons and up to first-order for heavy particles. However, the second-order electron transport fluxes should not be confused with Burnett fluxes. The heavy-particle diffusion velocities and heat flux are proportional to an average electron force expressed in terms of the electron diffusion driving force and temperature gradient. Conversely, the electron diffusion velocity and heat flux are proportional to the heavy-particle diffusion driving forces and temperature gradient. The magnetic field induces anisotropic transport fluxes when the electron collision frequency is lower than the electron cyclotron frequency of gyration around the magnetic lines. The explicit expressions for the transport coefficients are obtained by means		

of a Galerkin spectral method. Then, we study the influence of ionization and excitation reactions for homogenous plasmas. Expressions for the symmetric multi-temperature reactive rate constants are obtained rigorously, as well as the zero-order chemical production rates compatible with the law of mass action. The set of differential equations derived is proved to be compatible with the second principle of thermodynamics; the entropy production rate for each type of chemical reaction is shown to be non-negative and involves a new definition of the Gibbs free energy in thermal non-equilibrium conditions.		
11-10	**Coffee break**	
	Chairperson: Domenico Bruno	
11-30	**State-to-state collision-radiative models and their applications**	**Gianpiero Colonna, Institute of Nanotechnology, Bari, Italy**
A collisional-radiative model for H2-He mixture, coupled self-consistently with the Boltzmann equation for free electrons, has been applied to model a shock tube and nozzle flows. The kinetic model has been completed considering atom–atom collisions and the vibrational kinetics of the ground state of hydrogen molecules. The He levels have been separated in the Ortho and Para system, optically uncoupled. The atomic level kinetics has been also coupled with a radiative transport equation to determine the effective adsorption and emission coefficients and non-local energy transfer only for the shock wave. In nozzle flow radiative properties are calculated a-posteriori, uncoupled from the level kinetics.		
12-20	**Kinetics and transport processes in mixtures containing CO_2.**	**Kustova E.V., Saint Petersburg State University, Russia**
Structure and various mechanisms of vibrational relaxation in CO_2 molecules are discussed as well as available data on the rate coefficients of vibrational transitions. State-to-state and several multi-temperature models of carbon dioxide flows are considered. Application of proposed models for simulation of vibrational kinetics and transport processes in different non-equilibrium flows is presented.		
13-10	**Lunch**	
	Chairperson: Nagnibeda E.A.	
14-40	**Elementary processes for state-to-state kinetic modeling of plasmas**	**Annarita Laricchiuta, Institute of Nanotechnology, Bari, Italy**

The extended knowledge on elementary processes, constructed exploiting the modern accurate approaches in quantum molecular dynamics, has significantly enhanced the predictive capability of kinetic models, allowing to conduct numerical experiments that not only give a reliable estimation of macroscopic plasma parameters, but also shed light on the collisional mechanisms at microscopic level. Different web-access databases are nowadays available to the modeling community and, due to the present asserting of the state-to-state kinetics, the challenging goal is the construction of a reliable, complete and consistent database of cross sections and rate coefficients for collision processes involving ground and excited chemical species, with resolution on the electronic, vibrational and rotational degrees of freedom. In this scenario the Phys4EntryDB, collecting and validating state-specific dynamical information relevant to the modeling of planetary-atmosphere entry conditions, can be considered as a valuable tool with expected impact on different fields from the aerothermodynamics to fusion and environment, making practicable the state-to-state approach.		
15-30	**Experimental investigations of aerospace plasma flows**	**Yacine Babou, University Carlos III, Madrid, Spain**
The talk proposes an outline of experimental methods currently adopted to investigate non-equilibrium plasmas flows of interest in the field of aerospace. As a rule, different ground facilities are used to generate such dissociating, ionizing and radiating flows: shock tubes, plasma wind tunnels, and so on. The measurement techniques implemented to produce empirical data regarding the collisional and radiative processes occurring in non-equilibrium plasma flows will be presented and their advantages and drawbacks will discussed.		
16-20	**Coffee break**	
	Chairperson: Gianpiero Colonna	
16-40	**Transport phenomena in nonequilibrium molecular flows**	**Domenico Bruno, Institute of Nanotechnology, Bari, Italy**
The lecture will discuss the transport processes that play a role in nonequilibrium molecular flows. In particular, it will focus on the role of inelastic collisions: - Chapman-Enskog treatment of bulk viscosity for a gas with a single internal degree of freedom. Slow relaxation vs fast relaxation - Chapman-Enskog treatment of bulk viscosity for a gas with a multiple internal degrees of freedom. - Green-Kubo formulas for transport coefficients - Thermal conductivity in the nonequilibrium gas - Role of inelastic collisions on the thermal conductivity - Chapman-Enskog/Green-Kubo treatment of scalar source terms - Results from toy models and H-H2, He-H2, O2-O2 systems		

17-30	**Numerical simulation of nonequilibrium high-enthalpy rarefied gas flows**	**Bondar Ye.A., Khristianovich Institute of Theoretical and Applied Mechanics, Russia**
The fundamentals of the Direct Simulation Monte Carlo method as applied to problems of high-altitude aerothermodynamics of space vehicles and other problems of rarefied gas dynamics are presented. The emphasis is made on issues associated with the development and models for the description of nonequilibrium physical and chemical processes in the gas phase and on the space vehicle surface, as well as validation of these models through comparisons with results of in-flight and ground-based experiments in different flow regimes.		

Tuesday, November 10, 2015		
	Chairperson: Bondar Ye.A.	
9-00	**Deterministic numerical methods for solving the Boltzmann equation and their software implementation for graphic processor units**	**Malkov Ye.A., Siberian State University of Telecommunications and Information Sciences, Russia**
An approach to the description of transport of interacting particles in a medium based on the nonlinear Boltzmann transport equation is presented. The physical meaning of the equation, the area of its applicability, and its mathematical properties are discussed. The main content of the lectures is the description of deterministic numerical schemes for solving the Boltzmann kinetic equation. Results of numerical calculations for some of the classic problems of rarefied gas dynamics are presented. Significant attention is paid to software implementation of numerical algorithms of these schemes on graphics processor units. In this regard, the architecture requirements to software for hybrid cluster computations are discussed.		
9-50	**Transport processes in nanofluids: mythology, dreams and reality**	**Rudyak V.Ya., The Novosibirsk State University of Architecture and Civil Engineering, Russia**
A talk on the current myths in the theory of nano-liquids will be given as an introduction. Then a systematic discussion of various aspects of		

<table>
<tr><td colspan="3">transport processes and thermophysical characteristic of nano-liquids will take place, including (i) Molecular Dynamics (MD) modeling data of equations of state of nano-liquids; (ii) MD data on nano-particle thermodiffusion; (iii) MD and experimental data on viscosity and heat conductivity of nano-liquids; (iv) experimental data on heat transfer coefficients of nano-liquids in cylindrical pipes (in both laminar and turbulent flow regimes); (v) experimental data on the critical heat flux during boiling of nano-liquids on a cylindrical heater.</td></tr>
<tr><td>10-40</td><td colspan="2">Coffee break</td></tr>
<tr><td></td><td colspan="2">Chairperson: Kudrayvtsev A.N.</td></tr>
<tr><td>11-00</td><td>Spatial structure of laminar supersonic separated flow at neighborhood of a compression corner</td><td>Zapryagaev V.I., Khristianovich Institute of Theoretical and Applied Mechanics, Novosibirsk, Akademgorodok, Russia</td></tr>
<tr><td colspan="3">Experimental results and CFD data of spatial structure of laminar supersonic separated flow at neighborhood of a compression corner is presented. Such features of flow structure as dynamic flow which was observed downstream after reattachment line, streamwise vortices generated after flow reattachment are discussed. Analysis of vorticity equation with goal of a clarification of streamwise vortices generation mechanism was performed.</td></tr>
<tr><td>11-50</td><td>Two-phase gas-particle flows over bodies: modeling of random effects</td><td>Tsirkunov Yu.M., Baltic State Technical University «VOENMEH» named after D.F. Ustinov, Saint Petersburg, Russia</td></tr>
<tr><td colspan="3">Two-phase gas–particle flows as a subject of study are much more complex than particle-free flows. The presence of particles induces a wide variety of particle-phase flow patterns in flows over bodies. Such phenomena as particle velocity lag, particle–wall and particle–particle collisions, aerodynamic focusing and accumulation of particles can result in substantial redistribution of particles in the flow field and therefore modify flow properties. Many elementary processes in gas–particle flows are random in nature that can be caused by fluctuation of the carrier gas flow parameters if the flow is turbulent, particle–particle collisions resulting in chaotic particle motion, particle scattering in particle–wall collisions due to the wall roughness and non-spherical shape of particles, particle size distribution (polydispersity), etc. The Brownian motion of extremely small particles may also play an important role. With accounting for random effects, mathematical models of particle-phase flows become much more complicated. In the past ten years, random effects in gas–particle flows have attracted the great interest. The lecture describes the state-of-the-art in modeling of random effects, as applied to dusty gas flow over</td></tr>
</table>

bodies, and presents the most impressive numerical results obtained by the author's research team.		
12-40	**Lunch**	
	Chairperson: Tsirkunov Yu.M.	
14-00	**Laminarisation and turbulent suppression by thermochemical relaxation.**	**Grigoryev Yu.N., Institute of Computational Technologies of SB RAS, Russia**
The lecture is devoted to possibilities of laminarization and LT- transition delay in supersonic boundary flows by means active and passive methods based on vibrational relaxation and dissociation-recombination of molecular gases. Some mechanisms of suppression of instability acoustic disturbances are discussed in frameworks of multitemperature aerodynamics. Corresponding processes are illustrated by experimental and computational results of H.Hornung's group. Analytical estimations and numerical calculations of growth of the critical Reynolds numbers with increasing vibrational nonequilibrium in the Couette plane flow of diatomic gas are presented obtained on the base of linear and nonlinear energetic stability theories.		
14-50	**Numerical simulation of nonequilibrium rarefied gas flows on the basis of model kinetic equations**	**Kudrayvtsev A.N., Khristianovich Institute of Theoretical and Applied Mechanics, Russia**
An approach to simulating nonequilibrium flows in the transitional regime is considered. This approach is based on the numerical solution of equations for the distribution function, where the Boltzmann collision integral is replaced by a simple relaxation term. Though the most popular model kinetic equations (Bhatnagar-Gross-Krook model, ellipsoidal statistical model, and Shakhov model) were proposed long ago, the interest to such models has drastically increased in the last two decades. The reason is that the development of powerful supercomputers made it possible to solve these equations for fairly complex flows with high efficiency and accuracy; as a result, this approach can be considered as a promising tool for numerical simulation of rarefied gas flows, in particular, flows in microscopic devices. We discuss the main properties of solutions of model kinetic equations and their relationship with solutions of the Boltzmann equations and continuum equations. Direct deterministic methods of solving such equations are considered in detail: discretization in the physical space and in the velocity space, approximation of convective and relaxation terms, and integration of equations in time. Examples of using the model kinetic equations for calculating nonequilibrium flows in the transitional regime are given; the results obtained are analyzed and compared with data obtained by other		

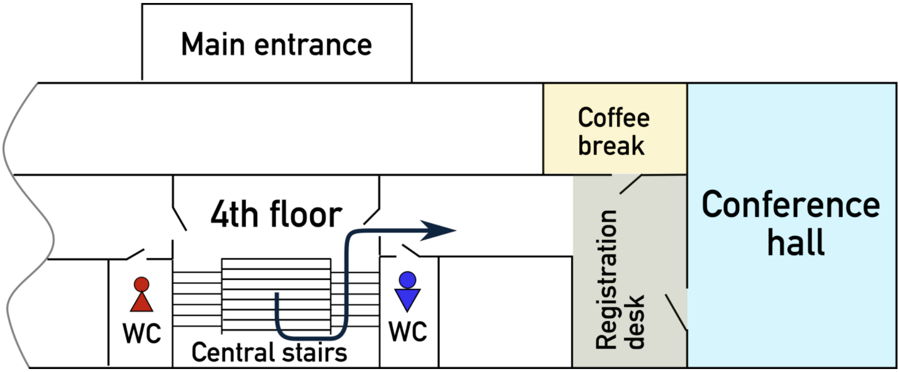
approaches.		
15-40	**Coffee break**	
	Chairperson: Zapryagaev V.I.	
16-00	**Direct Monte Carlo Simulations of Rarefied Gas Flows on GPU's**	**Kashkovsky A.V., Khristianovich Institute of Theoretical and Applied Mechanics, Russia**
The Direct Simulation Monte Carlo (DSMC) method is the principal numerical technique for studying non-equilibrium rarefied flows such as flows typical of high-altitude aerothermodynamics of reentry space vehicles. The major issue associated with the application of the method to real aerospace problems is tremendous computational cost of 3D numerical studies for moderate flight altitudes (about 80 km), where more than a billion simulation particles are normally required. Rarefactions effects can be still significant for such conditions, which makes it hard to use continuum CFD methods. The use of the Graphics Processing Units (GPUs) ensures computation speedup by a factor of 30-40 compared to usual CPUs, and, therefore, development of the parallel DSMC codes for heterogeneous GPU/CPU supercomputers could make such computations feasible. Particular attention should be paid to techniques of reducing the amount of information to be stored, minimizing data exchange, and applying the dynamic load balancing algorithm, which takes into account the real time of computations on each GPU. A parallel DSMC code SMILE GPU for 3D simulations of non-equilibrium chemically reacting ionized flows on GPU/CPU supercomputers developed at ITAM will be presented in the lecture.		
16-50	**Simulations of single- and two-phase flows in long pipelines and channels**	**Matveev S.K., Saint Petersburg State University, Russia**
A method of quasi-stationary quasi-one-dimensional approach to computational of non-stationary flows in pipes and channels of varying cross-sections is presented. Equations of two-phase flows in pipes, along with problems complicating their solutions are given. Examples of deriving additional equations to obtain a closed set of equations in stratified gas and liquid flows are presented.		

School venue

Lectures will take place in the Conference hall of the Institute of Theoretical and Applied Mechanics (ITAM). The address of the institute is Institutskaya str. 4/1 (see the map of Akademgorodok below). If you are using online map services and navigation software, please note that some of them identify the ITAM address as Akademika Rzhanova str. 4/1.

After entering the building, take the central stairs to the 4th floor (the top floor) and go all the way to the right to the lobby of the Conference hall (registration desk on the scheme). Registration of attendees will begin at 8:00 on November 9. Please do not forget to wear your name badge which will be given to you on the registration. It will be used as a pass to the institute.

Open access WiFi network will be available at the Workshop venue (connection name: BKZ).



Coffee breaks between sessions will take place in the room next to the Conference hall. Lunch will take place in Canteen of ITAM (number 

on the map of Akademgorodok below).

Presentation requirements

English and Russian are official languages of the School.

The Conference hall is equipped with a laptop, running Windows 7 with MS Office 2010 (*.ppt and *.pptx) and Adobe Reader 11 (*.pdf), connected to a data projector. The Organizing Committee cannot guarantee correct work of the projector with attendees' laptops, so using the School laptop is highly encouraged.

Please check who your chairperson is, upload your presentation to the laptop in advance and do not forget to check that all your slides are displayed correctly. Invited talks will be 45 minutes long, including a 5 minute question-answer session.

How to get from the Novosibirsk airport (Tolmachevo) to the Zolotaya Dolina hotel

The Tolmachevo airport is located 45 km away from Akademgorodok. There are main two ways you can get from there to Zolotaya Dolina:

1. **Taxi** (travel time is 1-1.5 hours, travel cost is 600-800 □, cash only).

   Taxi is the most convenient way to get from airport to any part of the city. You can book a taxi by calling one of the phone numbers listed below right after landing. If you need a receipt, you have to ask for it when booking. Phone numbers of the recommended taxi companies: +7 (383) 2 383 383, +7 (383) 233 1111, +7 (383) 223 23 23. The Organizing Committee *highly recommends* using this transfer option.

   We do not suggest that the Workshop participants book a taxi at the counter at the airport or use the service of unlicensed taxi drivers.

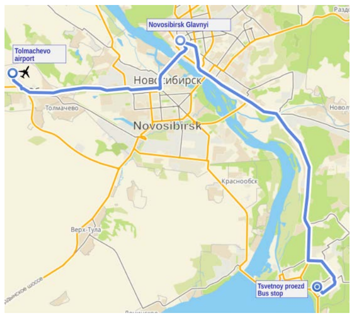
2. **Public transportation** (travel time is 2.5-3.5 hours, travel cost is 70-80 cash only).

   There is no direct transfer from the Tolmachevo airport to Akademgorodok. Two shortest routes are given below.

   - Tolmachevo airport – Novosibirsk Glavnyi: Bus **111**
     Novosibirsk Glavnyi – Tsvetnoy proezd: Bus **8**

     Bus **111** stops directly in front of Terminal A (terminal for domestic flights) of the Tolmachevo airport. Operating hours of the Bus **111**: from 4:00 to 22:30. The bus departs every 30 minutes.

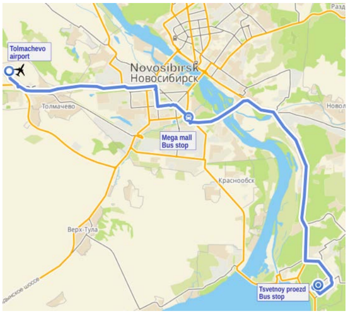
     On the Novosibirsk Glavnyi bus stop, get off Bus **111**, walk 50 meters in the travel direction, and get on Bus **8**. Operating hours of Bus **8**: from 06:33 to 22:17. The period between bus departures is 15-20 minutes on weekdays and 20-30 minutes on weekends.



- Tolmachevo airport – Mega mall: Bus **112**
  Mega mall – Tsvetnoy proezd bus stop: Minibus **15**

  Bus **112** stops directly in front of Terminal A (terminal for domestic flights) of the Tolmachevo airport. Operating hours of Bus **112**: from 5:40 to 20:90. The bus departs every 20 minutes.

  On the Mega mall stop, get off Bus **112**, walk 50 meters in the travel direction, and take Minibus **15** to Tsvetnoy proezd.



Get off the bus/minibus and walk 300 m along the Vesennyi proezd to the Zolotaya Dolina hotel.

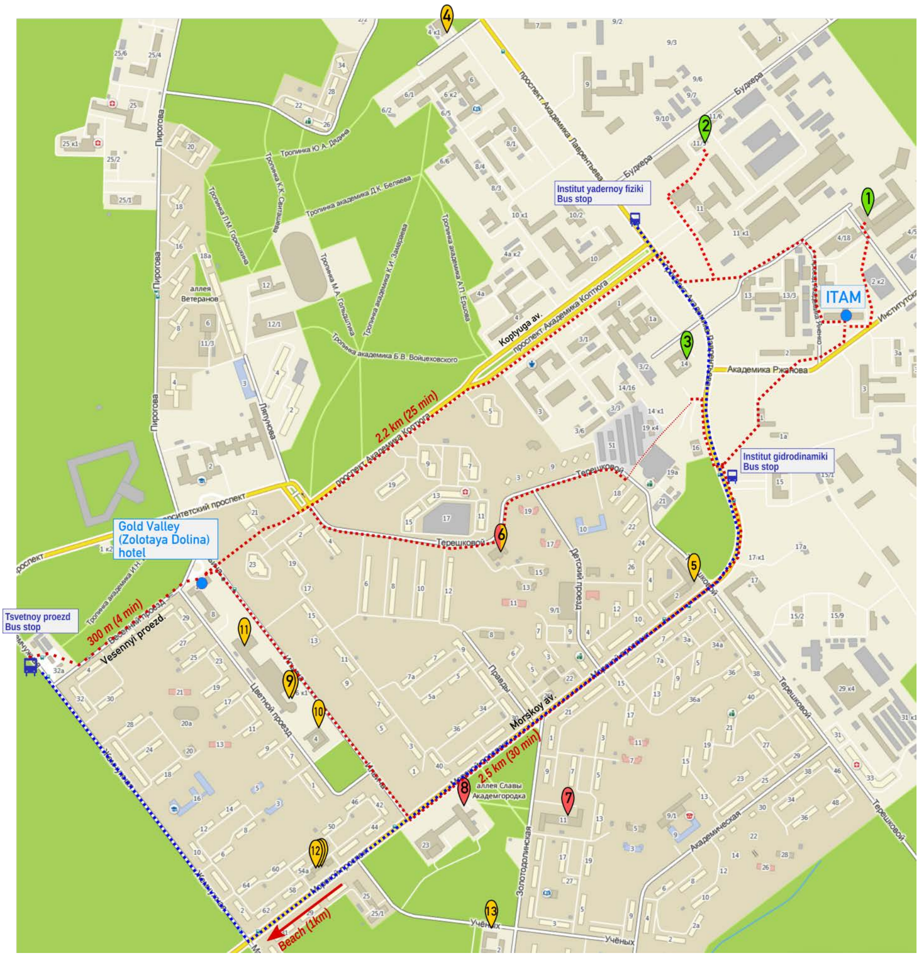
The Organizing Committee *does not recommend* the public transportation because of overly long travel time, probable traffic jams and difficulties of traveling with baggage.

To get from the hotel to the Tolmachevo airport, you can use the same options. We recommend booking a taxi at the hotel reception or by phone numbers: +7 (383) 333 7777, +7 (383) 33 00000, +7 (383) 330 4646, or +7 (383) 330 3040. Please be aware that traffic is intense during the daytime and you should leave for the airport at least 3.5 hours before the flight.

Useful information about Novosibirsk for guests

- Emergency phone number: 112.
- The time zone of Novosibirsk is UTC+6:00, MSK+3:00.
- Public transport operating hours: from 6:00 to 22:00.
- Credit/debit Visa and Mastercard cards are accepted in most of the shops and restaurants. If you need cash, you can exchange Euro and USD in banks or use ATM.
- Electricity in Russia: power supply 220V, 50 Hz.
- Most grocery stores are open from 8:00 till 23:00. The nearest one to the Zolotaya Dolina hotel is located in the Torgovyi Tsentr building marked by number 11 on the map of Akademgorodok and is open 24/7.
- Selling of alcoholic beverages in Novosibirsk is prohibited from 22:00 till 9:00. During night hours, you can buy beverages in restaurants and bars only.

Map of Akademgorodok



Walking route, paved	Low-priced
Walking path	Medium-priced
Bus route (Buses: 8, 23, 139, minibuses 1235, 7, 52, 225, 15, 1062)	High-priced

Addresses

Zolotaya Dolina hotel:	Ilicha str. 10
Institute of Theoretical and Applied Mechanics:	Institutskaya str. 4/1

Meal and drink in Akademgorodok

	Place	Average check (□) Business lunch / dinner
1	Canteen of ITAM*	180 / - (cash only)
2	Canteen of Institute of Nuclear Physics*	180 / - (cash only)
3	Canteen of the local administration*	200 / - (cash only)
4	Vkusnyi Tsentr cafe/restaurant	180 / 500
5	Traveler's Coffee cafe	250 / 700
6	Peoples cafe/bar	- / 900
	Campus time cafe**/restaurant	150/250
7	TBK Lounge restaurant	- / 2000
8	Dom Uchenykh restaurant	- / 800
9	Vilka-Lozhka cafe	180 / 250
	Pechki-Lavochki cafe/restaurant	300 / 800
10	Traveler's Coffee cafe	250 / 700
11	Vostok-Zapad cafe	200 / 500
12	Yanczy chinese cafe/restaurant	500
	Chashka Kofe cafe	300 / 1000
	Clever bar	300 / 800
	Pelmenissimo cafe	300
13	Köln bar	400 / 1000

* Working hours: 12:00 – 15:00
** In the time cafe you pay for the time spent in it. For the Campus cafe, the price is 50-70 □/hour (max – 150 □).

How to get from the Zolotaya Dolina hotel to the Workshop venue

ITAM is located at a walking distance (about 2.2–2.5 km) from the Zolotaya Dolina hotel. The main walking routes are shown on the map of Akademgorodok with red lines.

An alternative option is to take a bus from the Tsvetnoy Proezd bus stop, which is 300 meters from Zolotaya Dolina. ITAM is located between the bus stops Institut Gidrodinamiki (Institute of Hydrodynamics) and Institut Yadernoy Fiziki (Institute of Nuclear Physics). Almost all bus routes include these bus stops. For any bus route, the travel time to the Institut Gidrodinamiki bus stop will be 7-10 minutes. The bus route is marked with a blue line on the map of Akademgorodok. Please note that as a rule public transportation staff does not speak English. The following bus routes can be used:

- Buses **8**, **139**, **23**, cost 20 □.
- Minibuses **7**, **52**, **225**, cost 30 □.
- Minibus **15**, costs 45 □.

You can also book a taxi from the hotel reception. A typical cost of the one-way ride is about 100