



Austrian-Chinese Workshop on

**DISSIPATIVE SYSTEMS:
KINETIC THEORY AND
SEMICONDUCTOR APPLICATIONS**

**from 3 - 5 November 2010
at Vienna University of Technology, Austria**

Organizers:

A. Arnold, A. Jüngel, D. Matthes, W. Pötz, T. Yang, P. Zhang

co-financed by the Eurasia-Pacific UniNet and Vienna University
of Technology

Program:

Wednesday, November 03, 2010

15:20 - 16:00		Registration / <i>Coffee</i>
16:00		opening (Arnold, Vice-Rector Kaiser)
16:10 - 16:40	Tong YANG	Fluid Dynamic Limit to the Riemann Solutions of Euler Equations
16:45 - 17:15	Christian SCHMEISER	Measure solutions of a 2D Keller-Segel system as limit of a stochastic many particle model

Thursday, November 04, 2010

09:00 - 09:30	Hans KOSINA	Quantum Cascade Laser Modeling based on the Pauli Master Equation
09:35 - 10:05	Xiaoyan LIU	Simulation of Surrounding Strain Effects on the Performance of Nanowires Devices
10:10 - 10:40		<i>Coffee break</i>
10:40 - 11:10	Gang DU	3D Monte Carlo Simulation of Nano-scale MOSFETs: Physical accuracy and computational requirements
11:15 - 11:45	Tiao LU	A Finite Volume Method for the Multi Subband Boltzmann Equation with realistic 2D Scattering in DG MOSFETs
11:50 - 12:20	Karl RUPP	Deterministic numerical solution of the Boltzmann transport equation
12:20 - 14:20		<i>Lunch break</i>
14:20 - 14:50	Li CHEN	Semiclassical limit of quantum semiconductor models
14:55 - 15:25	Qiangchang JU	Quasi-neutral Limits of the Two-Fluid Euler-Poisson Systems
15:30 - 16:00		<i>Coffee break</i>
16:00 - 16:30	Stefan ROTTER	Probing decoherence through Fano resonances
16:35 - 17:05	Quansen JIU	Stability of Rarefaction Waves to the 1D Compressible Navier-Stokes Equations with Density-dependent Viscosity
17:10 - 17:40	Renjun DUAN	Regularity-loss property of some degenerately dissipative systems with the self-consistent electromagnetic field
19:00 - 22:00		Conference Dinner at a "Heurigen" (= Austrian wine restaurant)

Friday, November 05, 2010

09:00 - 09:30	Pingwen ZHANG	Mathematical Theory and Simulation of Liquid Crystal
09:35 - 10:05	Ulrich HOHENESTER	Phonon dephasing in semiconductor quantum dots
10:10 - 10:40		<i>Coffee break</i>
10:40 - 11:10	Walter PÖTZ	Open Boundary Conditions for Ballistic Transport Equations
11:15 - 11:45	Omar MORANDI	Numerical simulation of quantum transport of the electrons and holes in graphene devices
11:50 - 12:20	Markus WENIN	Computation of spin transport and magnetization dynamics in ferromagnetic/normal metal heterostructures using a drift-diffusion model
12:20 - 14:20		<i>Lunch break</i>
14:20 - 14:50	Othmar KOCH	High-order Structure-Preserving Discretization Methods for Nonlinear Evolution Equations
14:55- 15:25	Chunxiong ZHENG	Composite Gaussian beam approximation method for multi-phased wave functions
15:30 - 16:30		Closing / Discussion on individual cooperation projects

ABSTRACTS:

Semiclassical limit of quantum semiconductor models

Li CHEN

Department of Mathematics, Tsinghua University,
The Chinese University of Hong Kong, P.R. China

In this talk, we first briefly review some macroscopic quantum semiconductor models and then focus on the semiclassical limit problem of the quantum drift diffusion model and a simplified quantum energy transport model. In the second part, some of the known semiclassical limit result with positive boundary condition and the main technical tools will be reviewed. In the last section, we will introduce an interesting problem, i.e. the semiclassical limit problem with vanishing density on the boundary, which comes from the inversion layer in MOSFET devices.

3D Monte Carlo Simulation of Nano-scale MOSFETs: Physical accuracy and computational requirements

Gang DU

Department of Microelectronics, Peking University, P.R.China

As the semiconductor industry scans down to nano-scale, both quantization and quasi ballistic transport become obvious. On the other hand short the channel effect becomes a critical issue. Multiple channel a MOSFET structure such as FINFET has good gate controllability toward the channel charge, and will be used in nano-scale CMOS technology.

Thus, 3D Monte Carlo Simulation with quantum effect correction is needed for the nano-scale MOSFET study. 3D simulation leads to huge computational resource requirements and the complexity of device structures may cause some difficulties with the quantum correction effect calculation.

Regularity-loss property of some degenerately dissipative systems with the self-consistent electromagnetic field

Renjun DUAN

The Chinese University of Hong Kong, P.R.China

In this talk, we present a study of the dissipative property of solutions to some degenerately dissipative kinetic and fluid dynamic equations when a self-consistent electromagnetic field is present through the Maxwell system. A common feature for this kind of coupled systems is that they all are of the regularity-loss type. Two typical examples are the Vlasov-Maxwell-Boltzmann system and the Euler-Maxwell system with relaxations both arising from plasma physics. In addition, we also discuss the time-decay property of solutions to these equations of the regularity-loss type.

Phonon dephasing in semiconductor quantum dots

Ulrich HOHENESTER

Department of Physics, University of Graz, Austria

The exciton-phonon coupling in semiconductor quantum dots (QDs) has a profound impact on the coherent optical properties. In this talk I will discuss such coupling within the framework of the independent Boson model, and will show that phonon-assisted dephasing strongly limits the performance of QD-based entangled photon sources. For a single QD embedded in a microcavity, the exciton-phonon coupling opens an efficient decay channel to the cavity. Our theoretical predictions are corroborated by experimental results.

Stability of Rarefaction Waves to the 1D Compressible Navier-Stokes Equations with Density-dependent Viscosity

Quansen JIU

School of Mathematical Sciences, Capital Normal University, Beijing, P.R. China

In this talk, we will present some recent results about the asymptotic stability of rarefaction waves for the compressible isentropic Navier-Stokes equations with density-dependent viscosity. A weak solution around a rarefaction wave to the Cauchy problem is constructed by approximating the system and regularizing the initial values. Furthermore, the stability of the rarefaction waves is proved. Both cases are discussed. One is that the rarefaction waves do not include vacuum. The other is that the rarefaction waves contact with vacuum. The theory holds for large-amplitudes rarefaction waves and arbitrary initial perturbations.

This is joint with Yi Wang and Zhouping Xin.

Quasi-neutral Limits of the Two-Fluid Euler-Poisson Systems

Qiangchang JU

Institute of Applied Physics and Computational Mathematics, Beijing, P.R.China

Quasi-neutral limits of the multi-dimensional two-fluid isentropic or non-isentropic Euler-Poisson systems are rigorously justified. For well-prepared initial data, convergence of the two-fluid Euler-Poisson systems to the compressible Euler equations (isentropic or non-isentropic) is proved as the Debye length goes to zero.

High-order Structure-Preserving Discretization Methods for Nonlinear Evolution Equations

Othmar KOCH

Faculty of Mathematics, University of Vienna, Austria

We investigate innovative higher-order adaptive integrators for high-dimensional nonlinear evolution equations. First we discuss high-order split-step time integrators in a general Banach space framework and apply the results to prove convergence for the equations of motion associated with the multi-configuration time-dependent Hartree-Fock equations for the time-dependent Schrödinger equation. To improve the efficiency, we put forward pairs of embedded splitting formulae for error estimation and adaptive step-size selection. In the second part we investigate the properties of dissipative full discretizations for the equations of motion associated with models of flow and radiative transport inside stars. We derive dissipative space discretizations and demonstrate that together with specially adapted total-variation-diminishing Runge-Kutta time integrators with adaptive step-size control this yields reliable and efficient integrators for the underlying high-dimensional nonlinear evolution equations.

This is joint work with Friedrich Kupka, Christoph Neuhauser, and Mechthild Thalhammer.

Quantum Cascade Laser Modeling based on the Pauli Master Equation

Hans KOSINA

Department of Microelectronics, Vienna University of Technology, Austria

Quantum Cascade Lasers are practical sources of radiation in the mid-infrared and Terahertz regions. Cross-plane electronic transport through these semiconductor heterostructures can be described semi-classically using the Pauli master equation. This equation is derived from the Liouville-von Neumann equation by introducing the Markovian approximation. A Simulator solving the PME by means of a Monte Carlo method has been developed. All relevant electron-phonon scattering processes are included. As a prototypical example, a quantum cascade laser in the THz region has been investigated.

This is joint work with Oskar Baumgartner, and Goran Milovanovic.

Simulation of Surrounding Strain Effects on the Performance of Nanowires Devices

Xiaoyan LIU

Department of Microelectronics, Peking University, P.R.China

The simulation method of surrounding strain effects on the performance of nanowires devices is developed including strain distributions, band structures, effective mobility and the I-V curves. FEM is used to calculate the strain distributions and $k \cdot p$ method is used to calculate the band structure. The Schrödinger-Poisson system is solved self-consistently. The effective mobility is calculated via modified Kubo-Greenwood formula. The performance of Si and Ge nanowires FETs with different axial orientations, various surrounding material and surrounding stress induced during process can be simulated. The simulation can be served as a useful guide for future device optimization.

This is joint work with Honghua Xu, Gang Du, Chun Fan, Ruqi Han.

A Finite Volume Method for the Multi Subband Boltzmann Equation with realistic 2D Scattering in DG MOSFETs

Tiao LU

Department of Mathematics, Peking University, P.R.China

We propose a deterministic solver for the time-dependent multi-subband Boltzmann transport equation (MSBTE) for the two dimensional (2D) electron gas in double gate MOSFETs with flared out source/drain contacts. A realistic model with six-valleys of the conduction band of silicon and both intra-valley and inter-valley phonon-electron scattering is solved. We propose a second order finite volume method based on the positive and flux conservative (PFC) method to discretize the BTEs. In order to reduce the splitting error, the 2D transport problem in the wavevector space is solved directly by using the PFC method instead of splitting into two 1D problems. The solver is applied to a nanoscale DG MOSFET and the current-voltage characteristic is investigated. Comparison of the numerical results with ballistic solutions show that the scattering influence is not ignorable even when the size of a nanoscale semiconductor device goes to the scale of the electron mean free path.

This is joint work with Gang Du, Xiaoyan Liu, and Pingwen Zhang.

Numerical simulation of quantum transport of the electrons and holes in graphene devices

Omar MORANDI

Department of Physics, University of Graz, Austria

Graphene is an allotropic form of carbon where atoms are densely packed in a mono-layer in form of honeycomb-lattice. As a result of the conically shaped electronic band, the dynamics of electrons and holes in graphene is governed by the Dirac equation and they propagate as massless Fermions. In this contribution, quantum corrections to the electron-hole motion in graphene are investigated by applying the quantum phase-space approach. The Wigner-Weyl formalism is used to reduce the overall complexity of the system and a quasi-diagonalization procedure on the pseudo-spin degree of freedom is proposed. The resulting formulation of the equation of motion reveals to be particularly close to the classical description of the particle motion. The stationary state of graphene-based devices in the presence of strong electric fields and quantum barriers is numerically investigated. The connection of our formalism with the Berry-phases approach is also presented.

Open Boundary Conditions for Ballistic Transport Equations

Walter PÖTZ

Department of Physics, University of Graz, Austria

We discuss a physically motivated approach to realize open boundary conditions based on scattering theory. It assumes flat potential regions outside of the simulated region and is based on slow variation of S-matrix elements. It is equally suited to treat pure state (wave packet) and mixed state (density matrix) dynamics. In fact it has first been applied to the quasi-one-dimensional nonlinear Schrödinger equation and mixed states[1]. Here we discuss application to multi-component wave equations, specifically the Bogoliubov-deGennes and 1+1 Dirac equation, each of which represent two-component wave equations. The case of time-independent external potentials offers a special case which, within this method, allows for a very simple and stable solution. We discuss pitfalls arising from discretization schemes which lead to non-trivial modifications of the energy spectrum, such as fermion doubling for the Dirac equation or the non-Hermiticity (complex eigenvalues), and eigenfunctions.

[1] M. A. Talebian and W. Pötz, Superlattices and Microstructures, Volume 20, Number 3, October 1996, pp. 267-272(6); M. A. Talebian and W. Pötz, „Open boundary conditions for a time-dependent analysis of the resonant tunnelling structure“, Appl. Phys. Lett., Bd. 69, Nr. 8, S. 1148-1150, 1996.

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Probing decoherence through Fano resonances

Stefan ROTTER

Institute for Theoretical Physics, Vienna University of Technology, Austria

In this talk I will present results on a theoretical and experimental study of Fano resonances in transmission through resonant scattering structures. In particular, I will demonstrate that asymmetric Fano resonances contain detailed information on the underlying decoherence mechanisms present in a given system. Our theoretical investigations show, e.g., that dissipative and dephasing sources for decoherence leave distinct signatures in the Fano resonance lineshapes. These predictions are confirmed by microwave experiments using metal cavities with different

absorption coefficients and by measurements on electron transport through quantum dots. Our results open up new possibilities for studying the effect of decoherence in a wide array of physical systems where Fano resonances are present.

This work was carried out with A. Bärnthaler, F. Libisch, J. Burgdörfer, S. Gehler, U. Kuhl, and H.-J. Stöckmann.

Deterministic Numerical Solution of the Boltzmann Transport Equation

Karl RUPP

Institute for Microelectronics, Vienna University of Technology, Austria

Monte-Carlo methods are typically employed to solve the Boltzmann Transport Equation for semiconductors numerically. However, they suffer from high computational costs and resolve low-probability regions of the carrier distribution function inaccurately. These limitations can be overcome with deterministic methods at the cost of high memory consumptions. A memory reduction scheme for the most prominent deterministic solution approach, the Spherical Harmonics Expansion method, is presented. It allows to save up to two orders of magnitude in memory by storing the resulting system matrix in a factorized form. Implications on the choice of the iterative solver and efficient implementations are discussed.

Measure solutions of a 2D Keller-Segel system as limit of a stochastic many particle model

Christian SCHMEISER

Faculty of Mathematics, University of Vienna, Austria

The two-dimensional parabolic-elliptic Keller-Segel system is a model for the aggregation of particles under the influence of diffusion and of an attractive binary interaction. Depending on the value of a dimensionless parameter proportional to the total mass, either diffusion wins and the particles are dispersed, or attraction wins and concentration of particles occurs in finite time. In the latter case, solutions of the Keller-Segel system can be extended as time dependent measures globally in time.

A stochastic many particle model will be presented, which can be used as the basis of numerical simulations of measure solutions. It can also be shown that in the limit of infinitely many particles, the (Boltzmann) hierarchy for the sequence of marginals possesses a solution preserving molecular chaos, where the one-particle marginal is a measure solution of the Keller-Segel system.

This is joint work with Jan Haskovec.

Computation of spin transport and magnetization dynamics in ferromagnetic/normal metal heterostructures using a drift-diffusion model

Markus WENIN

Department of Physics, University of Graz, Austria

We present a self-consistent simulation of the magnetization dynamics and the spin dynamics in ferromagnetic/normal metal/ferromagnetic (FNF) heterostructures. We use the stationary solution of a drift-diffusion equation (SDDE) to compute the spin dynamics and the Landau-Lifshitz-Gilbert equation to compute the magnetization dynamics. Both equations couple via the spin-transfer torque and the magnetic field in the SDDE.

Fluid Dynamic Limit to the Riemann Solutions of Euler Equations

Tong YANG

Department of Mathematics, City University of Hong Kong, P.R.China

Fluid dynamic limit to the compressible Euler equations from the compressible Navier-Stokes and Boltzmann equation has been an active topic. Even though intensive studies have been made when the solution to the Euler equations has noninteracting single waves, the problem on the genuine Riemann problem is still open. In this talk, we present some recent results on this problem when the Riemann solution contains a superposition of either shock-rarefaction wave or rarefaction wave contact discontinuity. In addition, uniform convergence rates in terms of the physical parameters will also be given.

This is joint work with Feimin Huang and Yi Wang.

Mathematical Theory and Simulation of Liquid Crystal

Pingwen ZHANG

School of Mathematical Sciences, Peking University, P.R.China

This talk provides a brief review of our basic understanding of liquid crystal phases from both macroscopic and microscopic points of view. From the macroscopic perspective, phases can be identified utilizing a series of thermodynamic properties based on classical thermodynamics; from the microscopic perspective, a phase needs to be defined on the basis of its structural symmetry and the types of order found in the phase. These two different perspectives can be reconciled by using statistical mechanics to bridge the length scale differences.

The Ericksen-Leslie model, Tensor model, Onsager model will be introduced to study the phase and phase transition, the kinetic-hydrodynamic liquid crystalline model will be used to classify the pattern formation of microstructures and the dynamics of defects. The relation of liquid crystalline models and their limited regions, will be pointed out. The simulation methods and mathematical theory for different models will also be introduced.

Composite Gaussian beam approximation method for multi-phased wave functions

Chunxiong ZHENG

Tsinghua University, Peking, P.R.China

The Gaussian beam approximation for multi-phased wave functions is considered in this talk. The wave functions are assumed to oscillate with the characteristic wave length $O(\epsilon)$. A parameter recovery algorithm for the single-phased data function is developed based on the moment asymptotic expressions. This algorithm is then extended to multi-phased wave functions. If cross-points or caustics appear in the phase space, the beam approximation algorithm based on the parameter recovery will fail. In these cases, we resort to the windowed Fourier transform technique, and propose the composite Gaussian beam approximation method. Numerical experiments show that the beam number derived by the proposed method is much less than that by the direct windowed Fourier transform technique.

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PRACTICAL INFORMATION

Accommodation

HOTEL PENSION SHERMIN

Rilkeplatz 7, 1040 Wien

phone: +43 1 586 618 30

fax: +43 1 586 618 310

There are three ways to go from the airport to your hotel:

- Take the City Airport Train (16 EURO return ticket, every 30 min., travel time: 16 min.), leave the train at Wien Mitte (Landstraße), and take the subway U4 in the direction of Hütteldorf (half-fare ticket, one journey, 0.90 EURO), exit two stops later at Karlsplatz and walk Wiedner Hauptstrasse past the buildings of the Vienna University of Technology on the right hand to a small square - Rilkeplatz - where your hotel is located.
- Take the bus (Vienna Airport Line, 11 EURO return ticket, every 30 min., travel time: 20 min.), leave at Schwedenplatz, take the subway U1 in the direction of Reumannplatz (half-fare ticket, one journey, 0.90 EURO) and leave 1 stop later at Karlsplatz. From there continue as above.
- Take the local train (Schnellbahn, 3.40 EURO one way, every 30 min., travel time: 24 min.), leave the train at Wien Mitte (Landstraße), and take the subway U4 in the direction of Hütteldorf, exit two stops later at Karlsplatz. From there continue as above.

KOLPINGHAUS MEIDLING

Bendlgasse 10-12, 1120 Wien

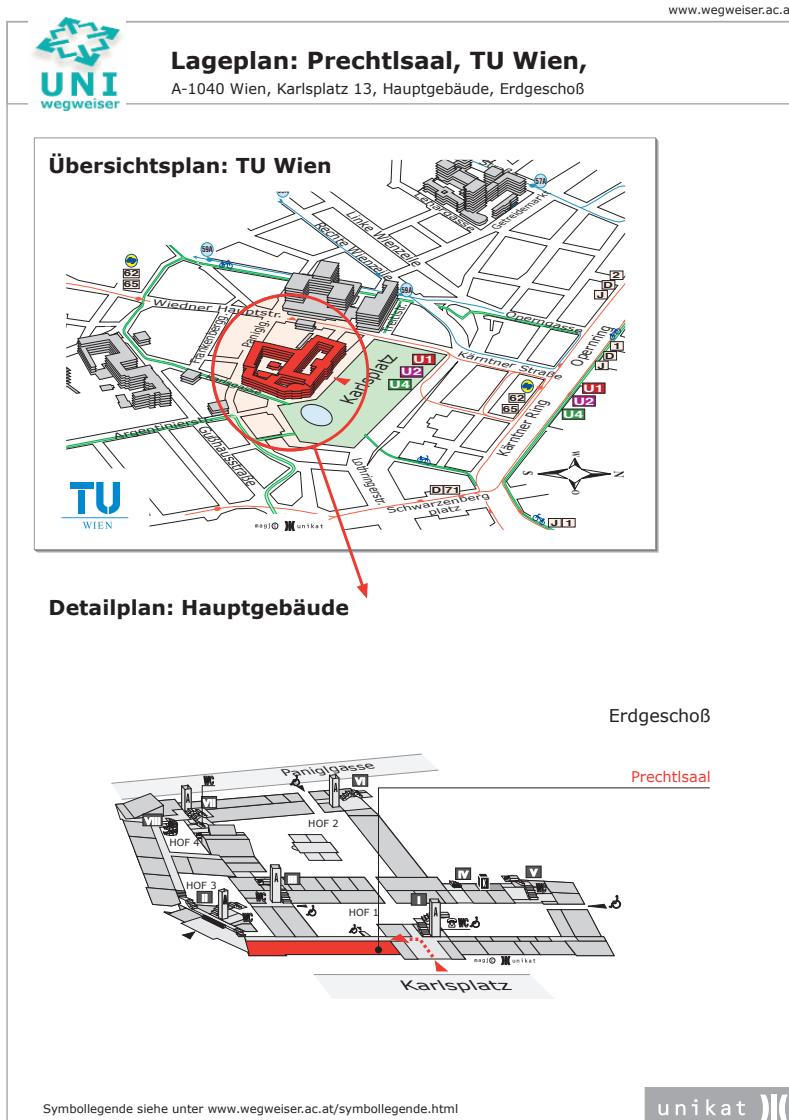
phone: +43 1 813 54 87

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There are three ways to go from the airport to your hotel:

- Take the bus (Vienna Airport Line, 11 EURO return ticket, every 30 min., travel time: 20 min.), leave at Wien Meidling and take the subway U6 in the direction Floridsdorf (half-fare ticket, one journey, 0.90 EURO) and leave after one stop at Niederhofgasse. From there to take the exit Niederhofgasse, turn right and walk and you find Bendlgasse as the fourth lane on the right hand. The hotel is situated opposite a church.
- Take the local train (Schnellbahn, 3.40 EURO one way, every 30 min., travel time: 24 min.), leave the train at Wien Mitte (Landstraße), change to subway U4 in the direction Hütteldorf, leave at Längenfeldgasse, change to subway U6 in the direction Floridsdorf and leave after one stop at Niederhofgasse. From there proceed as above.
- Take the City Airport Train (16 EURO return ticket, every 30 min., travel time: 16 min.), leave the train at Wien Mitte (Landstraße), and take the subway U4 in the direction of Hütteldorf (Einzelfahrschein, 1.80 EURO), leave at Längenfeldgasse, change to subway U6 in the direction Floridsdorf and leave after one stop at Niederhofgasse. From there proceed as above.

Lecture room



Prechtlsaal in the main building, ground floor (turn to left side after entering the building), Karlsplatz, 1040 Wien Beamer is available. Please notice that there is no blackboard! If you need an overhead projector, please tell us in advance.

Internet connection

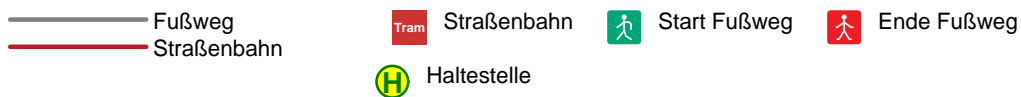
You will be able to use wireless internet connections at TU Wien. The networks **tunet** and **eduroam** are available. To use **tunet**, please use an open authentication, deactivate data encryption, and automatic IP address and DNS server. You can login by opening any homepage; you will be directed to the page **Captive Portal** at which you can login using your personal user name and password written on the separate leaflet. There, you will find more detailed instructions how to use WLAN for Windows and Mac. To use **eduroam**, you need to have an account from your home institution. Then you can simply login with your home data.

Conference Dinner

The Conference Dinner takes place on November 4, 7:00 p.m. at the Heuriger called **Steinschaden** at Kahlenbergerstrasse 18, 1190 Wien. The tram with the number D takes you in about 40 minutes from the station **Kärntner Ring, Oper** to Nussdorf where you get off at **Beethovengang**. From there you walk the short Schätzgasse to Kahlenbergerstrasse 18.



Stadtplan der Umstiegshaltestelle Nußdorf, Beethovengang



- | | | | |
|---|--|----------------------------------|---|
| 1 | | Straßenbahn D Kärntner Ring/Oper | Nußdorf, Beethovengang |
| 2 | | Fußweg | Nußdorf, Beethovengang Wien, Kahlenberger Straße 18 |

Food

Three cafeterias (Mensa Markt, Marktcafé and Cafe Schrödinger) are located in the Freihaus building where the workshop is held. On the 1st floor in the yellow aisle you find *Mensa Markt* and *Marktcafé*. The latter is open from 9.00 a.m. to 4.00 p.m. Breakfast, cold and warm beverages, pastry and snacks are served.

Mensa Markt is open from 11.00 a.m. to 14.30 p.m. You have a choice of 2 menus. A non-alcoholic beverage is included in the menu. Or you can have a choice of soups, pizzas, grilled meats, a salad buffet and a pastry buffet.

Café Schrödinger: Opening hours from 8.00-19.00. You find it on the ground floor in the green aisle. In the vicinity of the University of Technology there are quite a few bistros and small restaurants ranging from the typical Viennese to the exotic. Most of them are situated on the Naschmarkt, a few minutes walk to the west of the Freihaus building down Faulmannngasse. 3

- *Gastwirtschaft am Rilkeplatz* at Rilkeplatz 9 (next to Pension Shermin): simple dishes
- *Café für Sie* at Faulmannngasse 2: simple dishes
- *Centimeter* at Schleifmühlgasse 7: famous for its beer and spicy snacks
- *Red Apple* at Operngasse 20: Thai food
- *Yamo-Yamo* at Favoritenstrasse 2: Japanese and Thai food
- *Aqua* at Favoritenstrasse 4-6: Thai, Cantonese and Japanese food
- *Kebabhaus* at Faulmannngasse 1: a variety of Turkish food.