REQUIREMENTS FOR STATE EXAM
MATHEMATICAL AND COMPUTATIONAL MODELLING IN PHYSICS [PHYSICS]

1. Introduction

This document is an informal guide to state exam at the study programme "Mathematical and computational modelling in physics". Let us first clarify one thing. Study programme "Mathematical and computational modelling in physics" is a study programme for students of *physics*. If you are studying *mathematics*, you are studying in a different study programme called "Mathematical modelling in physics and technology". The organisation of the state exam at this programme is *slightly different*, please check the corresponding document at our webpages.

The state exam consists of two parts

- thesis defense,
- oral exam.

The exam takes place in one day, while the thesis defense usually precedes the oral exam. Detailed description of both parts is available below.

The student presents[1], usually in twenty minutes, the results of his/her thesis. After that he/she must discuss the issues pointed out in the referee reports. (The referee reports are available in the Study Information System beforehand. It is absolutely crucial to be ready to discuss referee's comments in a highly qualified manner.) At the end the student answers questions by the committee members and the audience.

2. Oral exam

2.1. Organisation of oral exam.
The oral part of state exam consists of answering several questions concerning the topics specific for the given study programme. In principle the student will be answering questions regarding the topics studied in the compulsory courses. More precisely, the student answers, after a preparation, in total six questions regarding

- theory of partial differential equations (one question),
- functional analysis (one question),
- finite element method (one question),
- theory of solution of systems of algebraic equations (one question).

The remaining two questions are focused on specialized topics by student choice. The student chooses, according to his/her specialisation *one* of the following topics:

- continuum mechanics (two questions),
- molecular dynamics (two questions),
- quantum systems (two questions),
- relativistic physics(two questions),
- particle physics (two questions).

Answering one question is expected to take ten minutes. The student is expected to demonstrate deeper insight into the discussed topics and the ability to see the subject matter in a broad context. (The student is not expected to give *extreme technical details* of each proof. He/she should be able to describe the basic ideas behind the proofs and explain why the definitions/notions/theorems are stated as they are.) Detailed list of topics for the state exam is listed below.

2.2. Topics.

(1) **Partial differential equations**

The topics are covered in courses Partial differential equations 1 and Partial differential equations 2. It is expected that the student is also familiar with the classical theory of partial differential equations at the level of the course Introduction to partial differential equations.

(a) Sobolev spaces

Weak derivative, definition and basic properties of Sobolev spaces $W^{k,p}$ – reflexivity, separability, density of smooth function, extension operator for $W^{1,p}$ functions and domain with Lipschitz boundary. Theorems concerning the continuous and compact embedding of Sobolev spaces into Lebesgue and Hölder spaces. Definition of the trace operator for functions in Sobolev spaces, trace theorem, inverse trace theorem.

(b) Weak solution of linear elliptic partial differential equations in bounded domain

Definition of the weak solution to linear elliptic partial differential equation with various boundary conditions. Existence of a solution via Riesz representation theorem (symmetric operator), via Lax–Milgram lemma and via Galerkin method. Compactness of the solution operator, eigenvalues and eigenvectors. Fredholm alternative

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[1]We expect a presentation using a projector. A computer with Adobe Acrobat Reader and Windows operating system will be available at the defense. If you have some non-standard requirements on available software such as codecs for your videos, please make sure beforehand that everything will work seamlessly. You can also use your own computer, the projector is typically equipped with a VGA/HDMI connector, if you want to use DisplayPort/USB-C connector, you will probably need an adaptor. Again please check it beforehand!

and its applications. Maximum principle for the weak solution. $W^{2,2}$ regularity via finite differences technique. Selfadjoint operator, equivalence with the minimization problem for a quadratic functional.

(c) Weak solution of nonlinear elliptic partial differential equations in bounded domain

Fundamentals of calculus of variations, fundamental theorem of calculus of variations, dual formulation, relation to convexity. Existence and uniqueness of the solution to nonlinear problems via fixed point theorems (nonlinear Lax–Milgram). Existence via Galerkin method and Minty trick – monotone operator and semilinear term.

(d) Second order linear parabolic partial differential equations

Bochner spaces and their basic properties, Gelfand triple, Aubin–Lions lemma. Definition of the weak solution. Initial conditions. Existence of a solution via Galerkin method, uniqueness and regularity of the solution (spatial and temporal), smoothing property, maximum principle.

(e) Second order linear hyperbolic partial differential equations

Definition of the weak solution. Initial conditions. Existence of a solution via Galerkin method, uniqueness, regularity (spatial and temporal), finite propagation speed.

(2) **Numerical mathematics**

The topics are covered in courses Finite element method and Matrix iterative methods 1. It is expected that the student is also familiar with fundamentals of numerical mathematics at the level of the course Analysis of matrix calculations 1 and Fundamentals of numerical mathematics.

(a) Finite element method for solution of linear elliptic partial differential equations

Galerkin and Ritz methods for solution of abstract linear elliptic equations. Estimate on the discretization error, Céa lemma. Defintion of the abstract finite element, simple examples of finite elements of Lagrange and Hermite type. Approximation theory in Sobolev spaces, approximation properties of polynomial preserving operators. Application of these results to Lagrange and Hermite type finite elements. Rate of convergence of approximate solutions to linear elliptic partial differential equations. Estimate of the rate of convergence in L^2 norm, Nitsche lemma.

Fundamentals of numerical integration in finite element method.

(b) Solution of systems of algebraic equations and eigenvalues computation

Methods for solution of systems of linear algebraic equations and eigenvalues computation. Spectral decomposition of operators and matrices. Invariant subspaces and spectral information, normality. Comparison of direct and iterative methods for solution of systems of linear algebraic equations. Projection process. Description of the convergence of the iterative methods. Relation between iterative methods for linear equations and methods for eigenvalues computation. Comparison of methods for solution of linear and nonlinear systems of algebraic equations. Numerical stability and algebraic error.

(3) **Functional analysis**

The topics are partially covered in course Functional analysis I. Theory of function spaces is also partially discussed in courses Partial differential equations 1 and Partial differential equations 2. It is expected that the student is also familiar with fundamental of functional analysis at the level of the course Inroduction to functional analysis.

(a) Hilbert and Banach spaces

Definition, norm, scalar product, examples. Linear functionals. Hahn-Banach theorem. Dual space, representations of some dual spaces (Hilbert spaces, Lebesgue spaces). Riesz representation theorem. Weak and weak-* topology. Banach-Alaoglu theorem. Weak compactness. Reflexivity.

(b) Continuous linear operators

Definition, basic properties, norm, space of linear operators, adjoint operator. Spectrum and its basic properties, spectral radius. Compact operators, symmetric operator, selfadjoint operator, closure, closed operator, definition and properties of adjoint operator. Eigenvalues and eigenvectors of symmetric elliptic operators.

(c) Fixed point theorems

Banach theorem, Brouwer theorem, Schauder theorem, Schaefer theorem.

(d) Integral transformations and fundamentals of the theory of distributions

Definition of Fourier transform in L^1 and its basic properties, Fourier inversion theorem, Fourier transform of convolution and derivative, Plancherel theorem. Space of test functions, definition of a distribution, basic examples of distributions, characterization of a distribution, order of a distribution, operations with distributions (derivative, multiplication), Schwarz space and tempered distributions. Fourier transformation for functions in Schwarz space $\mathcal{S}$ and in the space of tempered distributions $\mathcal{S}'$, its basic properties. Fourier transform in L^2.

(4) **Continuum mechanics**

The topics are covered in courses Continuum mechanics, Thermodynamics and mechanics of non-newtonian fluids and Thermodynamics and mechanics of solids.

(a) Kinematics

Description of the motion of continuous media. Deformation of line, surface and volume elements, deformation, deformation gradient, polar decomposition of deformation gradient and its interpretation, right and left Cauchy–Green tensor, Green–Saint-Venant tensor. Rate of deformation of line, surface and volume elements. Velocity, velocity gradient, symmetric velocity gradient, material time derivative. Isochoric deformation. Streamlines and pathlines. Kinematic condition for material surface. Lagrange and Euler description. Compatibility conditions for linearized strain tensor. Isotropic tensor functions, representation theorem for isotropic tensor functions.

(b) Dynamics

Balance equations (mass, momentum, angular momentum, total energy) in Euler and Lagrange description. Integral form for the balance equations, localization principle. Cauchy stress tensor, first Piola–Kirchhoff stress tensor, Piola transformation. Balance equations in non-inertial reference frame.

(c) Simple constitutive relations

Compressible and incompressible Navier–Stokes–Fourier model (viscous heat conducting fluid), equation of state for ideal gas. Geometric linearization, linearized elasticity. Boundary conditions, displacement and traction boundary conditions.

(d) Non-newtonian fluids

Balance equations in the case of non-newtonian fluids, identification of entropy production. Clausius–Duhem inequality. Assumption on the maximization of the entropy production and its application in the design of mathematical models for fluids, concept of natural configuration. Overview of non-newtonian phenomena – shear dependent viscosity, normal stress differences, activation/deactivation criteria, stress relaxation, non-linear creep. Principle of frame indifference and its consequences, frame indifferent quantities in fluid mechanics, frame indifferent rates. Application of representation theorem for isotropic tensorial functions. Overview of standard models for non-newtonian fluids. Power-law fluids, fluids with pressure dependent viscosity, Bingham type fluids. Viscoelastic fluids and simplified spring-dashpot models. Korteweg fluids.

(e) Solids

Principle of frame indifference and its consequences, frame indifferent quantities in solid mechanics. Elastic materials in finite elasticity theory, linearized elasticity. Incompressible materials in finite elasticity and in linearized elasticity. Elastic material as a material that does not produce entropy, relation between the stress tensor and free energy. Hyperelastic materials, examples of hyperelastic materials, behaviour with respect to the determinant of deformation gradient. Variational formulation of the static problem for deformation of hyperelastic solids. Viscoelastic solids – Kelvin–Voigt model – and simplified spring-dashpot models.

(5) **Molecular dynamics**

The topics are covered mainly in courses Simulations in many-particle physics, Advanced Simulations in many-particle physics and Computer modelling in plasma physics I. It is expected that the student is also familiar with basic concepts of statistical physics at the level of course Thermodynamics and statistical physics II.

(a) Basics of statistical physics

Statistical description of thermodynamics. Liouville equation. Basic statistical ensembles, micro canonical, canonical and grand canonical ensemble. Quantum statistical mechanics. Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein distributions. Basic formulas of statistical mechanics for simulations (calculation of thermodynamic variables, ergodic theorem) and role of numerical simulations.

(b) Basics of Monte Carlo simulations of physical systems

Basics of the Monte Carlo method (integration using MC method, Markov chains, error estimate of MC integration). Implementation of Monte Carlo step (natural and preferential sampling, Metropolis method). Methods of random number generation. MC simulation of discrete models (Ising model, percolation threshold). MC simulation of simple models of liquids.

(c) Basics of molecular dynamics

Principles of the method of molecular dynamics. Equations of motions of the classical many-body system. Interaction potentials and boundary conditions. Simulations in different statistical ensembles – NVE, NVT, NPT and grand canonical.

(d) Determination of thermodynamics and structural properties from simulations

Calculation of specific heat and susceptibility using fluctuations. Radial distribution function.

(e) Advanced methods of many-particle simulations

Phase transitions and critical phenomena. Phase and reaction equilibria. Simulation of growth processes. Quantum simulations. Calculation of kinetic coefficients. Kinetic Monte Carlo. Determination of energy barriers using molecular statics. Optimization methods.

(f) Basics of modelling in plasma physics

Characterization of plasma and types of plasma. Quasineutrality and Debye screening length. Theoretical description of plasma, kinetic description, Boltzmann equation, conservation laws, magnetohydrodynamic description.

(6) **Quantum systems**

The topics are covered mainly in courses Quantum scattering theory, Theory of collisions of atoms and molecules. It is expected that the student is also familiar with quantum mechanics which is covered by any of the courses Quantum mechanics II (NTMF067) or Quantum mechanics II (NJSF095) or Quantum theory II and their first parts.

(a) Basics of quantum mechanics

Description of states and observable quantities. Operators, commutation relations. Time dependence in quantum mechanics. Description of measurement. Stationary states and integrals of motion.

(b) Solvable systems

Particle in potential well, linear harmonic oscillator, Coulomb field.

(c) Angular momentum and spin

Definition of angular momentum, spectrum and eigenfunctions. Addition of angular momenta, Clebsch-Gordan coefficients. Vector and tensor operators, irreducible components and Wigner-Eckart theorem.

(d) Basic approximation methods

Variational method and perturbation theory. Many-particle systems: symmetrization postulate, bosons, fermions, Slater determinant, role of spin.

(e) Scattering theory

Møller operators and S-matrix. Scattering cross section. Time independent formulation of scattering, Lippmann-Schwinger equation. S-matrix poles and eigenphases. Basics of multichannel scattering theory.

(f) Basic methods of many-particle quantum physics

Mean field approximation, correlation energy and methods for its calculation. Second quantization. Basics of theory of atoms and molecules: electronic structure, vibrational and rotational states of molecules, application of group theory, optical transitions.

(g) Methods for scattering calculations

Partial wave expansion. Born series. Variational principles. R-matrix theory.

(7) **General theory of relativity**

The topics are covered in courses General theory of relativity, Relativistic physics I and Foundations of numerical study of spacetimes.

(a) The underlying principles of special and general theory of relativity

Spacetime, four-vector formalism, coordinate transformations. Metric, affine connection, covariant derivative. Parallel transport and geodesic equation. Gravitational redshift. Lie derivative and Killing vectors, tensor densities. Integration on manifolds (densities, integral theorems). Spacetime curvature.

(b) Einstein law of gravitation and its consequences

Energy-momentum tensor, conservation laws and equations of motion. Einstein gravity field equations. Schwarzschild and Reissner-Nordström metric. Kerr and Kerr-Newman metric.

(c) Relativistic astrophysics and cosmology

Relativistic models of stars. Gravitational collapse and black holes. Critical behavior of gravitational collapse. Relativistic cosmology FLRW models.

(d) Properties of Einstein equations

Linearized theory of gravitation and gravitational plane-waves. Lagrangian formalism in general relativity, conservation laws. Hamilton formalism in general relativity, initial value problem. Conformal decomposition of constraints, initial-value data. Einstein equations as hyperbolic system of partial differential equations.

(8) **Particle physics**

The basic theoretical information is partially covered by course Elementary particle physics, and practical topics in Software and data processing in particle physics II, Neural nets in particle physics.

(a) Basic concepts and methods of quantum field theory

Equations of relativistic quantum mechanics. Quantization of free fields. Interaction of fields, Feynman diagrams.

(b) Classification and properties of elementary particles

Leptons, hadrons and force carriers. Spin, parity, charge parity, strangeness, isospin. Conservation laws.

(c) Structure of hadrons

Quark model, color charge, partons, distribution functions.

(d) Basics of standard model of elementary particles

Electroweak interaction. Higgs mechanism. Quantum chromodynamics.

(e) Interaction of particles with environment and particle measurement methods in experiments

Measurement of energy, momentum and time of flight of particles. Identification of particles. Monte Carlo simulation of particle motion in detector.

(f) Methods of data analysis in particle physics experiments

Software tools. Selection rules and multivariate analysis. Neural networks.

3. Contact

If you have any further questions, please contact Martin Čížek (cizek@mbox.troja.mff.cuni.cz) or Vít Průša (prusv@karlin.mff.cu We are looking forward to see you at the exam!