

# Scientific Computing

## Exam questions

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Exam questions on lectures materials  
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# Questions (Lecture 1)

- ▶ Traditional scientific and engineering approach includes only theory and experiment. Provide a reasoning on disadvantages/limitations of such approach. How the mathematical modelling might help to manage it?
- ▶ Formulate the Moore's Law. Provide a reasoning on its value for science, industry, and every-day life.
- ▶ List the computational approaches in terms of physical sizes scale (macro to nano). Explain the main idea meshed/meshfree approaches. Does the computational complexity of the problem depend on usage of concrete kind of methods with respect to the scale?
- ▶ List the HPC units; explain the meaning of each one.
- ▶ What will happen when the transistor size shrinks by some factor  $x$ ? Explain in terms of clock rate, unit area, raw computer power and shrinkage of performance of the program.
- ▶ Explain the terms of parallel speedup and parallel efficiency. Might the parallel efficiency metric be equal to 1?
- ▶ Formulate the Amdahl's law and provide reasoning on it: which overheads lead to limitation of the speedup?
- ▶ List all overheads of Parallelism you know. Reason on the ways of overcoming some of them.
- ▶ List the limitations of serial computing. Explain each one in a few words.
- ▶ Explain what do the terms "load balance" and "load imbalance" mean? By what can be the imbalance caused? Provide examples.
- ▶ What kind of parallel computing resources do you know? List them and justify the answer: why the listed resources can be considered parallel?
- ▶ List at least five applications demanding parallel computations. Justify your answer.
- ▶ Describe the main idea of the von Neumann architecture.
- ▶ Which kinds of software we have to use in order to write a solver for a complicated problem? Which ways (in relation to these kinds of software) can be used for optimization of your program?
- ▶ Explain the meanings of shared and distributed memory. Explain the OpenMP and MPI paradigms. Compare them and analyse advantages and drawbacks/risks. Provide reasoning on when it is better to use one or another.

## Questions (Lecture 2)

- ▶ What is the mathematical model of the phenomenon? How can it be represented in the operator form? Describe all parts of the latter in terms of possible representation.
- ▶ What is the forward problem, and what is inverse problem? What is the difference between them? Reason on relativity of this classification. Explain with examples.
- ▶ List several applications of both Forward and Inverse problems. Justify on why the concrete problem is Forward or Inverse.
- ▶ Give the definitions and describe with examples the Top-Down and Bottom-Up approaches.
- ▶ Give the definitions and describe with examples direct and iterative approaches to solution of any problem.
- ▶ List three points J.Hadamard proposed to consider in order to classify problems in terms of well- and ill-posedness. What do these points mean mathematically?
- ▶ List the possible issues for the inverse operator in case of ill-posed problems.
- ▶ What does the continuous dependence of the solution on input means? Prove that derivative of noised function might depend discontinuously on the small error (noises) of the function to be differentiated.
- ▶ What is ill-conditioned problem? Define it mathematically and give reasoning on behaviour of the solution with respect to changes in input data. Give any example of ill-conditioned problem. Explain it.
- ▶ Which additional research and additional steps should or might be done in case of ill-posed problems? Reason on all possibilities you know.
- ▶ Define static and dynamic problems. Give at least two examples of each and explain these examples. List the cases in which a dynamic problem may be considered to be a static one. Explain these cases.

## Questions (Lec 3)

- ▶ Write down the forms of differential operator for Ordinary Differential Equation and for Partial Differential Equation. Explain the difference between them.
- ▶ Explain the meaning of terms: Linear differential equation, Quasi-linear differential equation, Non-linear differential equation. Provide examples of these equations.
- ▶ How the ODE of  $k^{th}$  order can be replaced with a system of ODE of the first order?
- ▶ Give the definitions for three kinds of problems for differential equations (Cauchy problem, BV problem, eigenvalue problem). Explain each of them in a few words; provide a reasoning on how much initial/boundary conditions are needed to make each of these problems well-determined?
- ▶ What is the Cauchy problem? Describe it with an examples. When it has the solution, and when this solution is unique?
- ▶ What is the boundary value problem? Describe it with an example.
- ▶ What is the eigenvalue problem? Describe it with an example.
- ▶ List three general approaches for solution of the Cauchy problem. Explain in few words advantages and disadvantages of them.
- ▶ What is explicit and implicit schemes for solving the Cauchy problem? Explain advantages and disadvantages for all of them.
- ▶ Explain the idea of Euler's method.
- ▶ Explain the idea of Shooting method.
- ▶ Write at least three real-world examples of problems leading to the partial differential equations of the first order. Analyze your examples in terms of linearity.
- ▶ Can the Cauchy problem be stated for the partial differential equation? If yes, give an example of it.
- ▶ Describe the main idea of statement of N-body problem.
- ▶ Describe the main idea of the Molecular dynamics method.
- ▶ Describe the main idea and general pipeline for the Galerkin method.

## questions: Lec 4

- ▶ Give the definition of convolution. Explain its meaning in terms of point spread function. Provide real-world examples.
- ▶ Write the generalized form of an integral transform; describe its parts. Why do we use the integral transforms? What are we expecting of usage of them?
- ▶ Write the definition of the Fourier transform and inverse Fourier transform. Explain the differences of real domain and reciprocal (frequency) domain. Provide examples.
- ▶ What is the Fourier convolution theorem? Describe why, where and when this property is useful.
- ▶ Explain the pipeline of the spectral analysis with the Fourier transform. Which properties of Fourier Transform are meaningful in this context? Explain with examples.
- ▶ How do we use Fourier transform for calculation of cross-correlation of two functions?
- ▶ How the derivatives of some function could be explained with its Fourier image? How can we apply this property to the differential equations? Explain with example.
- ▶ What is Parseval's theorem? When is it important?
- ▶ Why FT is that important? List all the applications of FT you know. Provide at least two examples.
- ▶ What is the Wavelet Transform? Give the definition and describe motivation.
- ▶ Write the definition of the STFT. Write its advantages and disadvantages. Provide at least one possible application.
- ▶ Describe step-by-step the idea of wavelet analysis. What is similar between the Fourier and continuous wavelet transforms?
- ▶ Write the general classification of integral equations. Which integral equations are well-posed, and which type of them is often ill-posed?

# Questions: Lec 5

- ▶ Describe four steps for computational solution of the scientific computing problem with usage of a mesh.
- ▶ Suppose the computational domain is covered with a uniform mesh. How can you approximate first and second derivatives of some function (defined in this domain) with FDM?
- ▶ Describe the "cross" template for approximation of second derivatives; write the approximation of the boundary value problem for the Poisson equation using this template. Analyze the obtained SLAE with respect to number of equations and variables.
- ▶ When should you use non-uniform meshes in FDM? When it is not reasonable to use them (in FDM)? What are disadvantages of this approach?
- ▶ Describe the procedure (steps) of reduction the problem for differential equation to SLAE using FDM.
- ▶ Describe general properties of FDM matrix for the elliptic equations, obtained using the Cross template.
- ▶ Why it is better to avoid usage of inverse matrices in real computations of Poisson equation with the Cross template?
- ▶ Explain the meaning of terms 'implicit scheme' and 'explicit scheme'. Which advantages and drawbacks has each of these schemes? Provide an example of implicit and explicit schemes for some differential equation.
- ▶ Compare FDM and FEM in terms of advantages and drawbacks of each method.
- ▶ Define the FEM approximation with basis functions. List necessary properties of the basis functions. Write the approximations or derivatives and integrals.
- ▶ What is the weak formulation? Describe with the example.
- ▶ Describe the procedure of reduction of the Poisson equation to the SLAE using FEM.
- ▶ List the properties of the matrix of SLAE, obtained using the FEM for the Poisson equation.

## Questions: Lec 6

- ▶ Write the general concept of Optimization problem. Define linear and non-linear optimization.
- ▶ List and give explanations of the applications of the optimization from point of view of mathematical problems reduction.
- ▶ Define the unconstrained and constrained optimization. Give a simple examples and think on where it can be applied.
- ▶ Write the definition of minimum and minimizer. Provide the classification of them and explain this classification with examples.
- ▶ Write the definition of the differentiable function and the Frechet derivative.
- ▶ Write the necessary and sufficient conditions for the functional  $f(u)$  to have a local minimum at the point  $u_0$ . Give an example.
- ▶ What is a convex functional? Which kinds of convex functional do you know?
- ▶ Prove that the functional  $f(x) = ||x||^2$  is strongly convex
- ▶ What is convex programming? What is the advantage of it?
- ▶ Describe the Least Squares Method, construct the cost functional and discuss on its derivatives.
- ▶ What is the pseudosolution and normal pseudosolution?
- ▶ Describe the main idea of the Golden Section Method.
- ▶ Describe the main idea of the Gradient Descent.
- ▶ What is the k-step method? Which 2-steps methods do you know?
- ▶ Give the description of the heavy-ball method.