Written Online Exam

General Information:

- *[xxx] refer to the question's topic and (xp) to the maximal achievable points.*
- *You must answer the questions via hand-written notes on empty sheets of paper.*
- *Show the stack of empty papers at the beginning when asked.*
- *Clearly indicate the respective question number for each answer.*
- *Add page numbers to every sheet of paper.*
- *Note the total number of submitted pages on the top of the first page.*
- *Write clearly using large letters, dark pen color and generously use the available space.*
- *When you want to hand-in your exam let one of the supervisors know: you will be moved to a "breakout room" where a supervisor will guide you to scan all the sheets of paper into a single PDF document. Double-check that the PDF contains all pages and is of reasonable quality and finally submit to: nssc@iue.tuwien.ac.at*

Inform an exam supervisor when

- *You are finished and want to scan and submit.*
- *You need more paper then initially approved by the supervisor.*
- *Something unforeseen happened*

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1. [MPI] (3p) Consider the implementation of an MPI-parallelized numerical integrator in one dimension. Show the pseudocode of a possible implementation and focus on a proper distribution of workload among the MPI processes. Assume variables as needed; ignore implementation specifics of the integration function. Explicitly highlight and discuss the specific, necessary MPI statements, communication strategy and parallel efficiency (specific values for parameters are not important).

2. [MPI] (2p) Explain via drawings and additional explanations the following collective operations: MPI_Bcast() and MPI_Reduce().

3. [ODE] (2p) Explain the Euler method and discuss the implicit and explicit approximations.

4. [ODE] (3p) Explain the key difference between implicit and explicit methods for the numerical solution of ODEs and comment on the consequences with respect to computational demand.

5. [FVM] (4p) Consider Poisson's equation

$$\nabla^2 u = \nabla \cdot \nabla u = f$$

and the integral form

$$\int \nabla \cdot \nabla u = \oint \nabla u dA = \int f dV \ .$$

(a) What theorem was used in the integral form above?
(b) Discuss the steps (and graphically show the discrete gradients!) required for a discretization of the integral form of Poisson's equation using the finite volume method.
(c) Why are finite volume schemes considered *conservative?*

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6. [PDE] (2p) Give an example for a second order linear elliptic operator.

7. [PDE] (3p) What is a second order linear partial differential operator in divergence form? Give an example.

8. [MD] (2p) List the five steps of an entire, practical molecular dynamics simulation.

9. [MD] (3p) Describe (briefly and in words, no implementation needed) the process to detect cluster formation in the post-processing step of a molecular dynamics simulation.

10. [MD] (4p) Describe, schematically, how a neural-network potential works. Use a flow diagram where the inputs are atomic coordinates and the output is the potential energy (ignore forces!).

11. [FD] (2p) Consider the 1D dimensionless Diffusion equation in cartesian coordinates

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2},$$

where D is the diffusion coefficient, C is the concentration field, x is the spatial coordinate, and t is the time. Derive a finite difference discretization using a 1st order explicit scheme in time and a 2nd order central scheme in space.

12. [FD] (3p) Write the forward and backward approximation for the first derivative of a given function $f(x)$, evaluated at point x_i and at a given time step n. Show that these two approximations are 1st order accurate in space. Help yourself with the Taylor series expansions.

13. [FD] (4p) Apply the Thomas algorithm (for tri-diagonal systems) to solve the linear system [A][V] = [R], where the matrix A and the vectors V and R are

$$\begin{bmatrix} a_1 & c_1 & 0 & 0 \\ b_2 & a_2 & c_2 & 0 \\ 0 & b_3 & a_3 & c_3 \\ 0 & 0 & b_4 & a_4 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{bmatrix}.$$

14. [FEM] (2p) What is approximated by the interpolation functions in isoparametric elements in continuum mechanics?

15. [FEM] (3p) What are the advantages to formulate a Ritz Ansatz for small sub-domains (i.e. Finite Elements)?

16. [FEM] (4p) Why is the Jacobi matrix needed when using isoparametric elements and in which form? Show the derivation. What restrictions apply to the Jacobi matrix?