**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] (2p) Assume that 4 compute nodes of an HPC-cluster where each node offers 2 CPUs with 20 physical cores each (=40 physical cores per node) are available to you as computational resources. Discuss the differences and give explanatory examples between a hybrid OpenMP-MPI parallelization concept and an "MPI-only" parallelization concept considering above listed computational resources. Make necessary assumptions and explain them.

2. [MPI] (3p) Consider the implementation of a stencil-based Jacobi solver for a two-dimensional elliptic PDE on a square two-dimensional domain using a ghost-layer-based domain decomposition. Do you expect any deviations in the serial and parallel results for the global L2-norm of the residual? Do you expect any deviations in the Maximum-norm of the residual? Provide arguments/explanations in your answers.

3. [ODE] (2p) Explain the "classic Runge-Kutta" method. Discuss whether this is a single- or a multi-step method.

4. [ODE] (3p) Explain how ODE methods (for first order ODEs) can be applied to higher order ODEs.

5. [FVM] (2p) Comment on advantages and disadvantages of a discretization using the Finite Volume Method (FVM) compared to a discretization using the Finite Difference Method (FDM).

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6. [FVM] (2p) Explain the divergence theorem and explain its importance for the FVM. Apply the theorem to a PDE of your choosing.

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

8. [PDE] (3p) Is the operator $Lu(x) := u''(x) + u(x)$ an elliptic operator? Justify your answer.

9. [MD] (2p) Give two reasons why the fourth-order Runge-Kutta integrator is not a good choice in the context of molecular dynamics.

10. [MD] (3p) What are the indispensable features that a potential energy function and a molecular dynamics integrator must have to be acceptable on physical grounds?

11. [MD] (4p) Describe what a combination rule for multicomponent systems is in the context of molecular dynamics, why they are necessary and what they are based on.

12. [FD] (2p) Diffusion or advection, which process is more efficient to transport a given species away from a source? Motivate your answer with the help of a qualitative plot showing the time (T) it takes to transport a targeted species away from a source as a function of the distance from the source (L).

13. [FD] (3p) Assume you want to approximate the first derivative of a function, at location $x_i$ and time $n$, with the three-point formulation

$$\left[\frac{\partial f}{\partial x}\right]_i^n = af_{i-1}^n + bf_i^n + cf_{i+1}^n \ ,$$

where subscript $i - 1$ refers to the location $x_{i-1}$, subscript $i$ to the location $x_i$ and subscript $i + 1$ to the location $x_{i+1}$. Find the value of $a$, $b$ and $c$, and the expression of the truncation error.

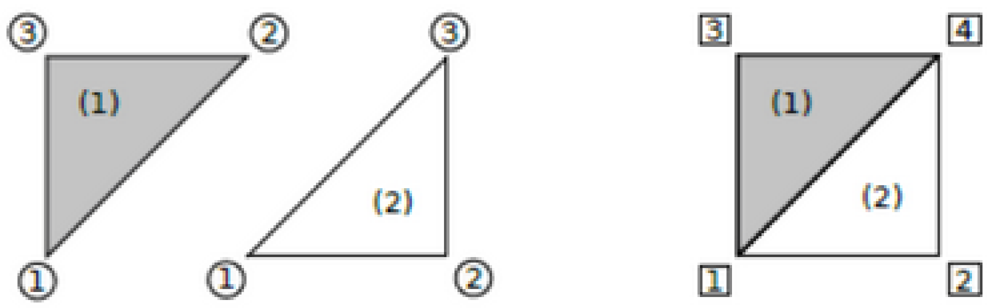
14. [FD] (4p) Show that the Central discretization in Space (CS) for the first derivative of a given function $f(x)$, evaluated at point $x_i$ and at a given time step $n$, is second order accurate in space. Assume that the grid spacing $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$ is constant. Help yourself with the Taylor series expansions.

15. [FEM] (2p) Explain "compatibility" by words.

16. [FEM] (3p) Explain the term "completeness" by words, equation, and sketch; show the check for completeness at the example of one element edge with bi-quadratic interpolation functions in 2D.

17. [FEM] (4p) Assembly of the total stiffness matrix by considering the triangulation and the element stiffness matrices below.

    Elements (1) and (2) with local node numbers are given on the left, the assembly with global node numbers is given on the right.




The element stiffness matrices are:

$$\mathbf{H}^{(1)} = \begin{pmatrix} H_{11}^{(1)} & 0 & H_{13}^{(1)} \\ & H_{22}^{(1)} & H_{23}^{(1)} \\ \text{sym.} & & H_{33}^{(1)} \end{pmatrix} \qquad \mathbf{H}^{(2)} = \begin{pmatrix} H_{11}^{(2)} & H_{12}^{(2)} & 0 \\ & H_{22}^{(2)} & H_{23}^{(2)} \\ \text{sym.} & & H_{33}^{(2)} \end{pmatrix}$$

Compute the total stiffness matrix.