**Written Online Exam**

***General Information:***

- *[xxx] and (xp) refer to the question's topic and maximal achievable points.*
- *The total number of achievable points is 46.*
  *You must achieve at least 50%, i.e., 23 points to get a positive grade.*
- *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.*
- *Write clearly using large hand-writing and generously use the available space.*
- *When finished, 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 submit to:*
  *nssc@iue.tuwien.ac.at*
  *Submission should be done within 5 minutes of notifying the exam supervisor.*

***Inform an exam supervisor when***

- *you are finished and want to scan and submit.*
- *you need more paper then initially approved by the supervisor.*

---

1. [MPI] (3p) Consider the implementation of a stencil-based Jacobi solver for a two-dimensional elliptic PDE on a square two-dimensional domain.
   a. Write a pseudocode which shows the key adaption steps required to parallelize the solver using a ghost-layer-based two-dimensional domain decomposition using MPI.
   b. Include the calculation of global residual and error norms.

2. [MPI] (2p) Show via pseudocode and additional explanations the difference between blocking and non-blocking point-to-point communication.

3. [ODE] (2p) Name two numerical methods for ODEs (can be explicit or implicit) together with the respective update rules (including the truncation error) assuming a constant step size h.

4. [ODE] (3p) Single-step and multi-step methods:
   a. Explain the key difference between both methods for the numerical solution of ODEs.
   b. Explain why multistep methods (compared to single-step methods) require special attention regarding the start-up and when considering a dynamic step size.

**Written Online Exam**

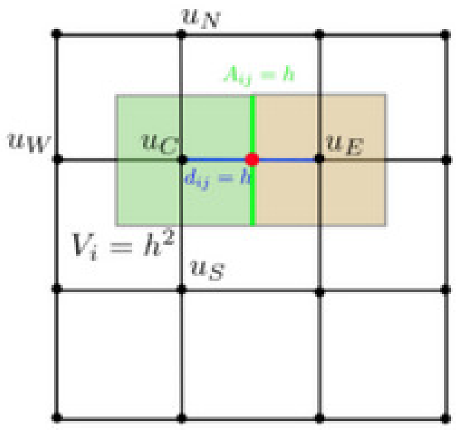
5. [FVM] (4p) Consider the discretization of the two-dimensional Poisson equation

$$u_{xx} + u_{yy} = f$$

and the integral form

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

on a regular equidistant grid spacing $h$ and box control volumes (see figure below). Show that the resulting discretization for an interior point $u_C$ is identical for the FVM (using a central difference for $\nabla u$) and the FDM (using second-order central differences).




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

7. [PDE] (3p) What does it mean that a second order linear operator L is elliptic?

8. [MD] (2p) What sets classical molecular dynamics apart from ab-initio molecular dynamics?

9. [MD] (3p) Describe the minimum image convention.
    a. When is it applicable?
    b. If your simulation box is an axis-aligned straight rectangular prism with side lengths $L_x, L_y, L_z$, how would you calculate the distance between two particles with positions $\boldsymbol{p}$ and $\boldsymbol{P}$ under this convention?

**Written Online Exam**

10. [MD] (4p) The following code snippet contains a naive Python implementation of the velocity Verlet integrator that uses significantly more memory than strictly necessary. Discuss why and how to fix it.
Note: For simplicity, masses are assumed to have a value of 1.

```
def next_step(pos, vel, dt):
    force = -calc_gradient_e_pot(pos)
    pos = pos + dt * (vel + .5 * force * dt)
    newforce = -calc_gradient_e_pot (pos)
    vel = vel + (force + newforce) * .5 * dt
    return (pos, vel)
```

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

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

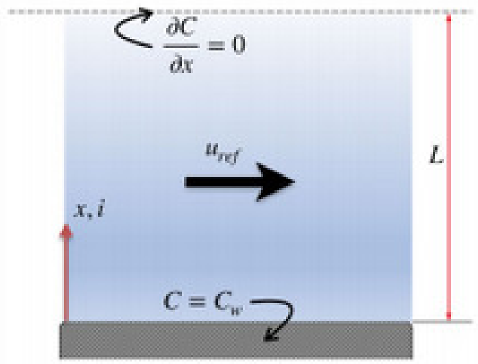
where $D$ is the diffusion coefficient, $C$ is the concentration field, $x$ is the spatial coordinate, and $t$ is the time. Derive the discretized counterpart using a 2nd order implicit scheme in time using Crank-Nicolson and a 2nd order central scheme in space.

12. [FD] (3p) Consider the 1D Advection-Diffusion Equation (ADE) in Cartesian coordinates:

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

where the superscript * indicates variables in dimensional form and $D$ the diffusion coefficient. Assume the flow configuration given in the figure below.

a. Derive the dimensionless counterpart of the above equation and identify the Peclet number.
b. How does the dimensionless equation look like for (1) a diffusion-dominated and (2) for an advection-dominated phenomenon?



13. [FD] (4p) Consider the 1D pure Advection Equation in cartesian coordinates:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = 0,$$

where $U$ is the (uniform and constant) advection velocity, $C$ is the concentration field, $x$ is the spatial coordinate and $t$ is the time. Show that ...

   a. ... when the upwind approximation (1st order in time, 2nd order in space) is used to discretize the equation, a numerical diffusivity is introduced.
   b. ... the numerical diffusivity is null when $Co = 1$ (where $Co$ indicates the Courant number).

14. [FEM] (2p) What is the interpretation of the determinant of the Jacobi matrix of an isoparametric element?

15. [FEM] (3p) The fundamental FEM equation reads: $\underset{\approx}{K}\,\underset{\sim}{U} = \underset{\sim}{F}$

   a. Explain variables and their dimensions (in terms of lin. Algebra) in continuum solid mechanics.
   b. Consider a plane (two-dimensional) mechanical problem with 18 elements and 16 nodes: How many equations has the system?
   c. Consider a three-dimensional heat conduction problem with 27 elements and 64 nodes: How many equations has the system?

16. [FEM] (4p) Consider a FEM heat conduction problem with the global FEM equation

$$H_{ab}\,T_a = P_b$$

with $n$ degrees of freedom and with the known total stiffness matrix. Dirichlet boundary conditions are given for $a = 1 \dots m$; Neumann boundary conditions are given for $b = m + 1 \dots n$.

Write the computation steps by linear algebra manipulations to solve the system, i.e., the unknown $T$- and $P$- entries.

Hint: Start by writing down the FEM equations by using sub-matrices and sub-vectors.