Computational Physics
0. Exercise Sheet

SuSe 2023

Handing out: 21.4.2023
Submission: 28.4.2023 8 pm

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Exercise 1: Comprehension questions — 0 Points

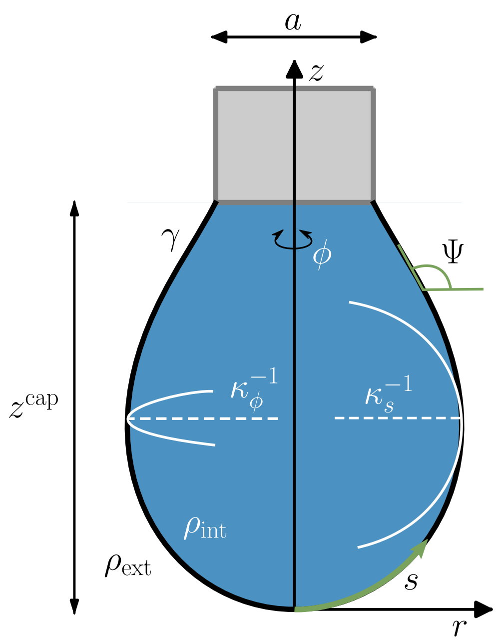
1) What is a symplectic integration method? Which benefits do they offer?

Exercise 2: Formgleichungen eines flüssigen Tropfen — 10 Points

A fluid droplet with density ρ is suspended from a capillary with diameter a.
The force balance between surface tension γ, pressure difference across the interface $p(z)$ and gravity g yields the Young-Laplace equation, which links the principal curvatures of the interface κ_s and κ_ϕ with the pressure and the surface tension:

$$p(z) = p_L - \rho g z = \gamma(\kappa_s + \kappa_\phi) \tag{1}$$

where p_L is the pressure difference across the interface at the drop apex and $\rho g z$ the hydrostatic pressure contribution. We will focus on axisymmetric drops, such that a parametrization of the interface is possible with a line segment that can be rotated around the z-Axis to give the full contour of the drop. The line segement has an arc length coordinate s and an arc angle $\Psi \in [0, \pi]$, which is measured relative to the horizontal plane.



The shape equations thus consist of two purely geometric equations and an additional equation from (1):

$$\begin{aligned}
\frac{\mathrm{d}r}{\mathrm{d}s} &= \cos(\Psi) \\
\frac{\mathrm{d}z}{\mathrm{d}s} &= \sin(\Psi) \\
\frac{\mathrm{d}\Psi}{\mathrm{d}s} &= \kappa_s = \frac{p_L}{\gamma} - \frac{\rho g z}{\gamma} - \frac{\sin\Psi}{r}
\end{aligned} \tag{2}$$

a) Use the surface tension γ and the capillary diameter a as scales to non-dimensionalize the shape equations (2).

b) The shape equation $\frac{\mathrm{d}\Psi}{\mathrm{d}s}$ contains a numerical singularity at the apex ($s = 0$), where $\sin\Psi = 0$ and $r = 0$. Show that the limit of this shape equation is given by:

$$\frac{\mathrm{d}\Psi}{\mathrm{d}s}(s \to 0) = \frac{p_L - \rho g z}{2\gamma} \tag{3}$$

and use this result in your numerical solution.

c) Integrate the (dimensionless) shape equations with a 4th order Runge-Kutta method and solve for the shapes with $p_L a/\gamma = 2$ and $\rho g a^2/\gamma = 0.1$ with the addtional conditions:

$$r(s = 0) = 0 \tag{4}$$
$$z(s = 0) = 0 \tag{5}$$
$$\Psi(s = 0) = 0 \tag{6}$$
$$r(s = s_{\max}) = a/2 \tag{7}$$

Hint: The condition $r(s = s_{\max}) = a/2$ can be satisfied by stopping the integration at an arbitrary point where $r(s) = a/2$. Also include solutions where $r(s) = a/2$ is fulfilled multiple times during the integration.

d) Explore the parameter space of the problem and record a pressure volume curve for the solutions with $\rho g a^2/\gamma = 0.5$ and $p_L a/\gamma \in [0, 5]$.

Exercise 3: Two-body problem - Comparison of two integrators 10 Points

In this assignment, you will compare the the numerical integration of ordinary differential equations using the Euler- and Verlet algorithm.

Consider two masses m_1, m_2 at positions $\vec{r}_1$, $\vec{r}_2$ and velocities $\vec{v}_1$, $\vec{v}_2$ under influence of Newton's law of gravitation

$$\vec{F}(\vec{r}_1, \vec{r}_2) = -G \frac{m_1 m_2}{|\vec{r}_1 - \vec{r}_2|^3} (\vec{r}_1 - \vec{r}_2)\,, \tag{8}$$

where the force $\vec{F}$ acts on the mass m_1 and correspondingly $-\vec{F}$ on mass m_2. The constant of gravitation can be set to 1 by an appropriate choice of units and the motion is considered only in the orbital plane. Use the initial conditions $m_1 = 1$, $m_2 = 2$, $\vec{r}_1(0) = (0, 1)^T$, $\vec{r}_2(0) = (0, -0.5)^T$, $\vec{v}_1(0) = (0.8, 0)^T$, $\vec{v}_2(0) = (-0.4, 0)^T$ and integrate at least up to the time $T = 100$.

a) Implement both mentioned integration methods. Choose one adequate and one too coarse step size for each algorithm and plot the corresponding trajectories $\{(x, y)\}$ in comparison to each other.

b) Choose a reliable step size for each method and compare the resulting run times.

c) After integrating to $T = 100$, reverse time (negative step size) and integrate the trajectories back to $T = 0$. Comment on your result for the different integrators.