PHYS3071
Worksheet 9 Tutor Notes - Active matter I: Passive matter

Week 9, Semester 2, 2024

Learn about the symmetry of indefinite integration and numerical stability for single particle problems. Not all indefinite integration is equal and fails in different ways for reasons plethora. Here we examine second order indefinite integration methods and assess suitability to solve weakly interacting particles.

- Quantify the differences between two second order methods: RK2 (midpoint), and leapfrog using velocity Verlet.
- Assess suitable approximations for modelling single particle systems.
- Fitting as an optimisation problem.

Task 1
Weight on a spring, molecular dynamics... Newton's laws of motion apply. Systems with oscillatory motion.

Task 2

- $x_1 = (t_{i+1} - t_i)$, noting that $(t_{i+1/2} - t_i) = (t_{i+1} - t_i)/2$...
-
$$f''(t_i) = -f'(t_i)\beta/m - f(t_i)\kappa/m \tag{1}$$
$$f'(t_{i+1/2}) = f'(t_i) + (t_{i+1/2} - t_i)f''(t_i) \tag{2}$$
$$f(t_{i+1}) = f(t_i) + (t_{i+1} - t_i)f'(t_{i+1/2}) \tag{3}$$
$$= f(t_i) + (t_{i+1} - t_i)f'(t_i) + (t_{i+1} - t_i)^2 f''(t_i)/2 \tag{4}$$

  Note how $f''(t_i)$ is exact, also pretty much the same result as RK2.
- In leapfrog we've assumed $f'(t_{i+1/2})$ is the average velocity over the entire step, which means we can move the result back in time and obtain the earlier point. We can't with RK2. Both are accurate with errors $\propto \Delta t^3$.

Task 3

- step size. make sure difference equations are correct.
- rk2 will drift, verlet will oscillate near a conserved value.
- verlet is a complete inevitable matrix of coefficients. RK2 has a row of zeros—in other words it is underdetermined.

Task 4

- numerical instability shall occur, step size will need to be small

- i have no idea. seems about the same. they are second order methods with loss... should be the same imo.
- overdamped
- yes. the mass term is way too small, leads to stiff equations from the intertia. in overdamped you don't need double dot to get basically the same thing. you can get them to demonstrate this if you like.

Task 5

- advancing and retarding constants, $C_{\pm}$, and the stiffness, k.
- k/β can be balanced any way you want. this means we get a valley of despair in the optimisation landscape. they can show this in the next exercise.
- you can make $f(C_+, C_-, k) = \|x_{\text{model}}(C_+, C_-, k, t_i) - x_{\text{sim}}(t_i)\|^2 / \|x_{\text{sim}}(t_i)\|^2$. or anything similar or plausible... i don't care what they come up with as long as it works.
- `divdim` (and not `dimdim`) calculates approximations of central finite differences in as many dimensions and times as the stack will take.
- step size! get them to plot each attempt. it is pretty cool how the slide show of fits looks.