

Week 12: Coursework (and stoic wisdom)

Convergence, testing, documentation, use of ChatGPT...

Dr K Clough, Topics in Scientific computing, Autumn term 2023

Plan for today

1. The mark scheme for Coursework 1
2. Convergence testing - what to test and how to interpret the result
3. `assert (testing_sufficient)`, “Testing is not sufficient!”
4. What is “documentation”?
5. A critical look at last year’s NOT MODEL exam solution
6. Time for questions on either coursework

**“Such is the madness of ambition
that you will feel you have come in
last if anyone is ahead of you.”**

Seneca, Epistles

Mark scheme

TOTAL MARKS

| Component | Max mark available |
|----------------------------------|--------------------|
| Implementation | 60 |
| Defensive programming | 20 |
| Readability | 10 |
| Documentation | 10 |
| Total as a percentage | 100 |
| Total out of 20 marks for course | 20 |

Marksheet for first coursework MTH739

Completion of physical scenarios - worth 60% total

| Component | Max mark available | |
|---|--------------------|-----------------|
| Implement a two body system made up of two stars with a mass ratio 1:2 undergoing multiple stable orbits | 14 | |
| Use of classes | 2 | |
| Plots of the orbital trajectories of the stars over time | 2 | |
| Phase diagrams for the position and velocities of the component stars. | 2 | |
| Correct use of solve_ivp() including rtol param | 2 | |
| Correct use of midpoint or RK4 method | 2 | |
| Comment on Euler | 2 | 26 total for Q1 |
| Implement a three body system made up of 3 stars of equal mass, and model the stable solution | 8 | |
| Use of classes | 2 | |
| Plots of the orbital trajectories of the stars over time | 2 | |
| Phase diagrams for the position and velocities of the component stars. | 2 | |
| Correct use of solve_ivp() including rtol param | 2 | |
| Correct use of midpoint or RK4 method | 2 | |
| Model 3 body system in which stars display chaotic behaviour, with one star being ejected from the system | 4 | 22 total for Q2 |

“Whatever the ways of the universe may require us to suffer, let us take it up with high mindedness. This is the oath by which we are bound, not to be disturbed by what we do not have the power to avoid.”

Seneca, On the Happy Life

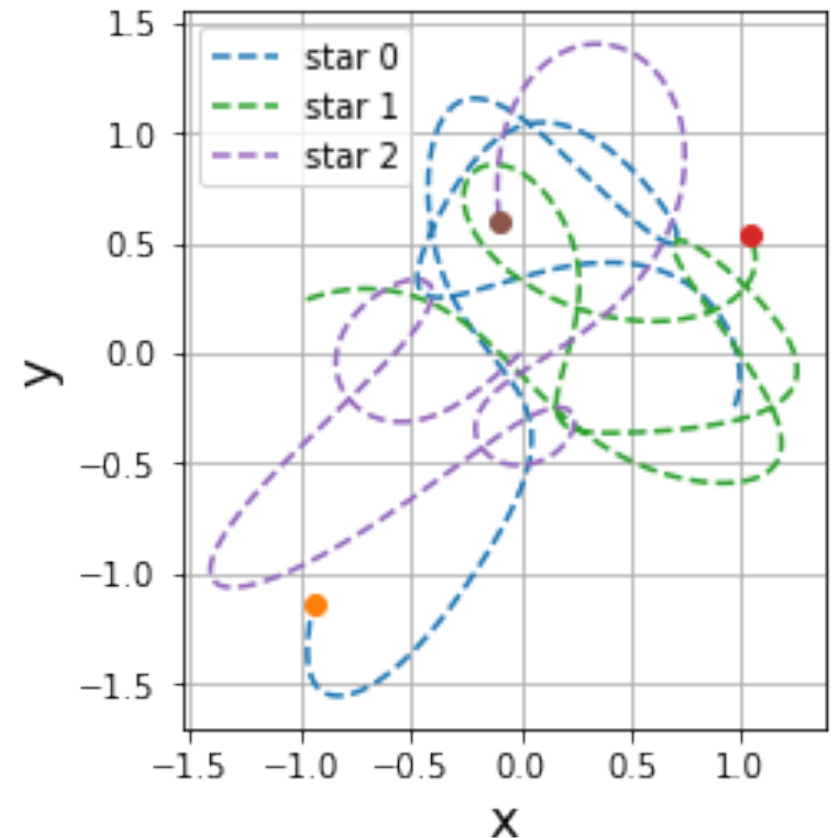
Convergence testing

- What quantity should I convergence test?

-> Ask: What is my “result”?

In the case of stars could be:

- x position of a star at $t=t_{\text{final}}$ (this is only one point, so less informative than...)
- trajectory of star 1 x-position over time (can then repeat for y, star 2 etc).

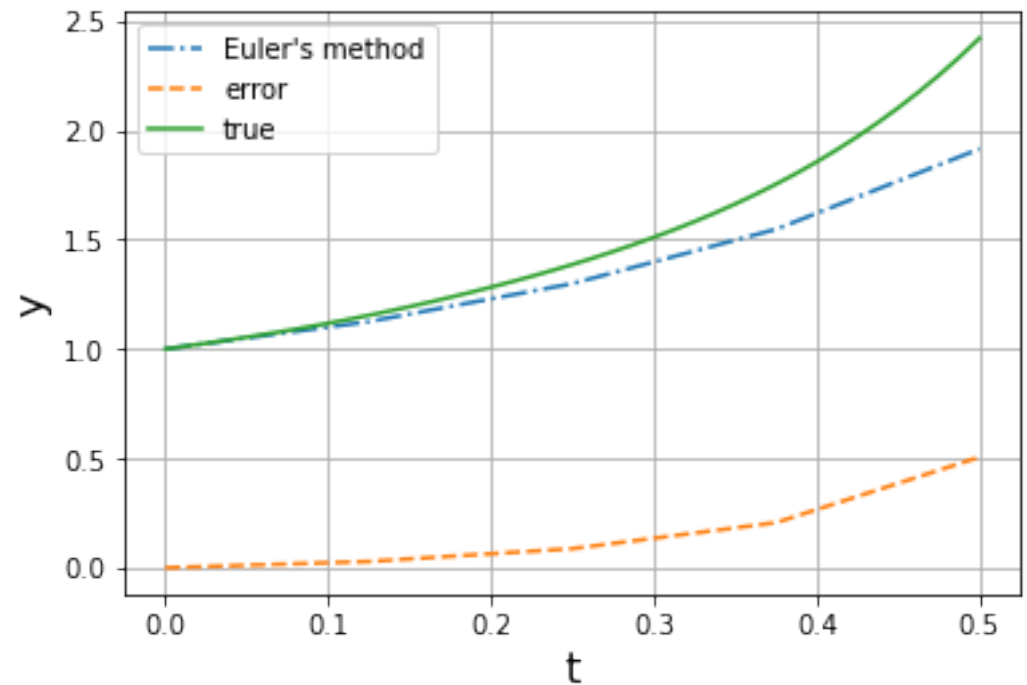


Convergence testing

- What do I compare?
 - Comparison to “truth” only possible if you have analytic solution, usually you don’t otherwise you wouldn’t do numerics.
(NB solve_ivp() or any other numerical solution is not “truth” and so it is morally cheating to use it this way. If you can afford to run at a super high resolution where you know it is right, then why bother to convergence test at a rubbish resolution?)
 - Better: Comparison between 3+ resolutions - easiest to always compare each case to double its resolution, so that expected reduction between two consecutive pairs is $2^{(\text{order})}$. If you use other ratios (or compare all to a single resolution) you need to **rederive the expected ratio**.

Convergence

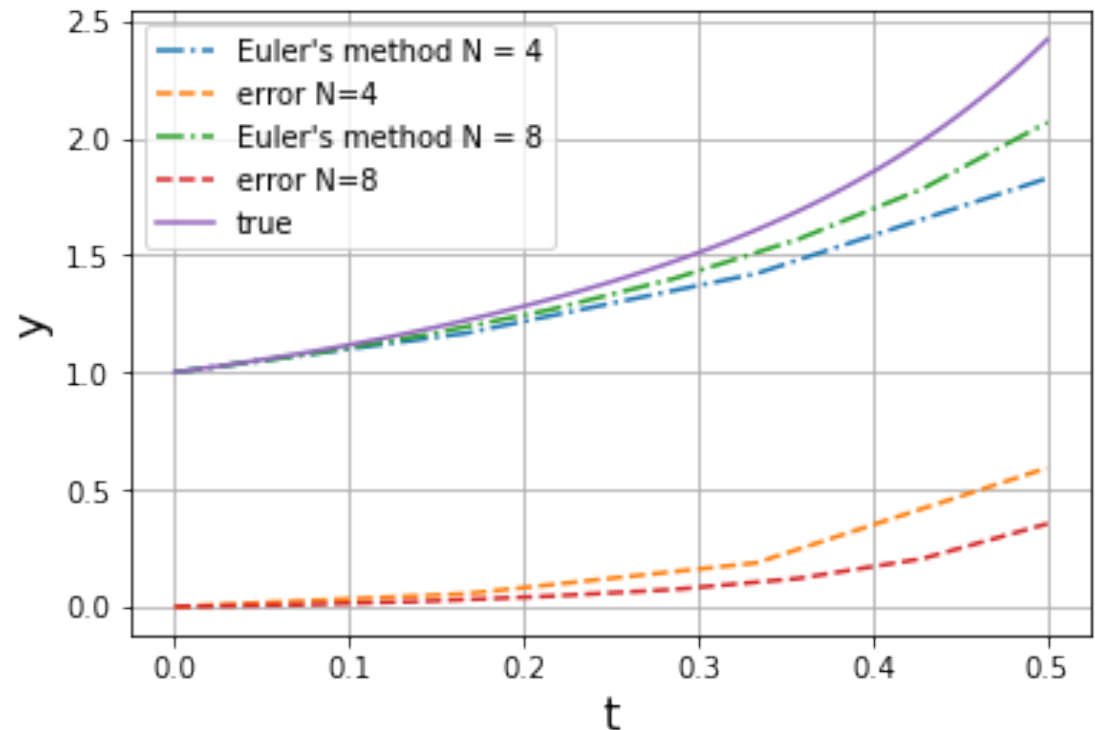
Usually I won't know the solution exactly, so how do I know what I get is right? Should I just trust the solver?



Convergence

For the Euler method which is first order, decreasing the step size by 2 SHOULD decrease the error by 2.

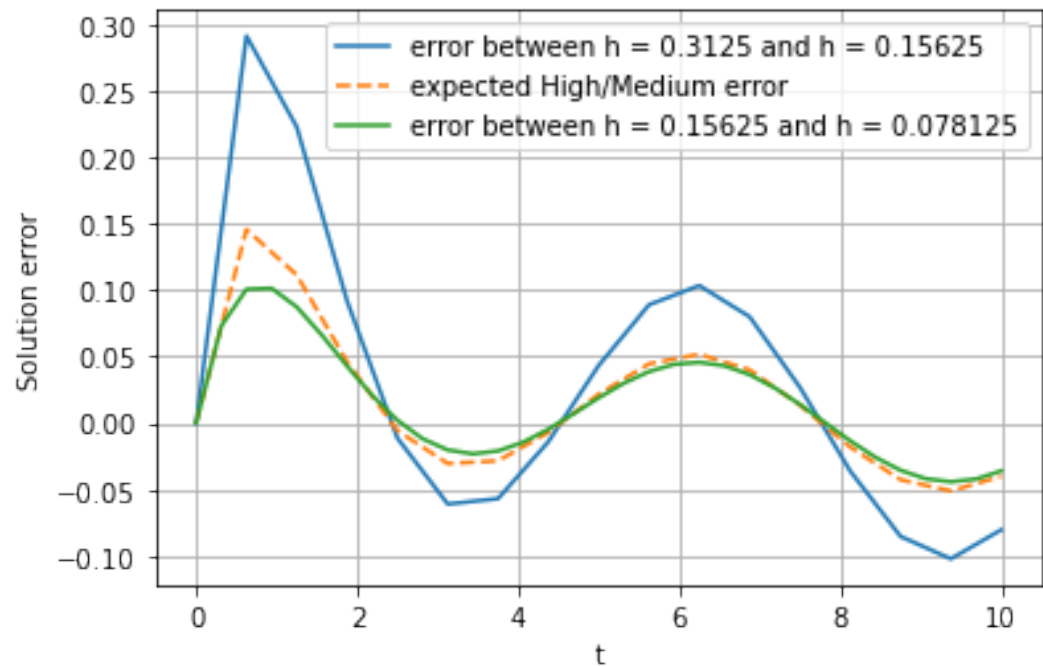
If we can show this, we are
“in the convergence regime”



Convergence

Where we don't know the solution, we need
3 RESOLUTIONS
to test convergence - if we double the resolution, we know that the differences should scale as

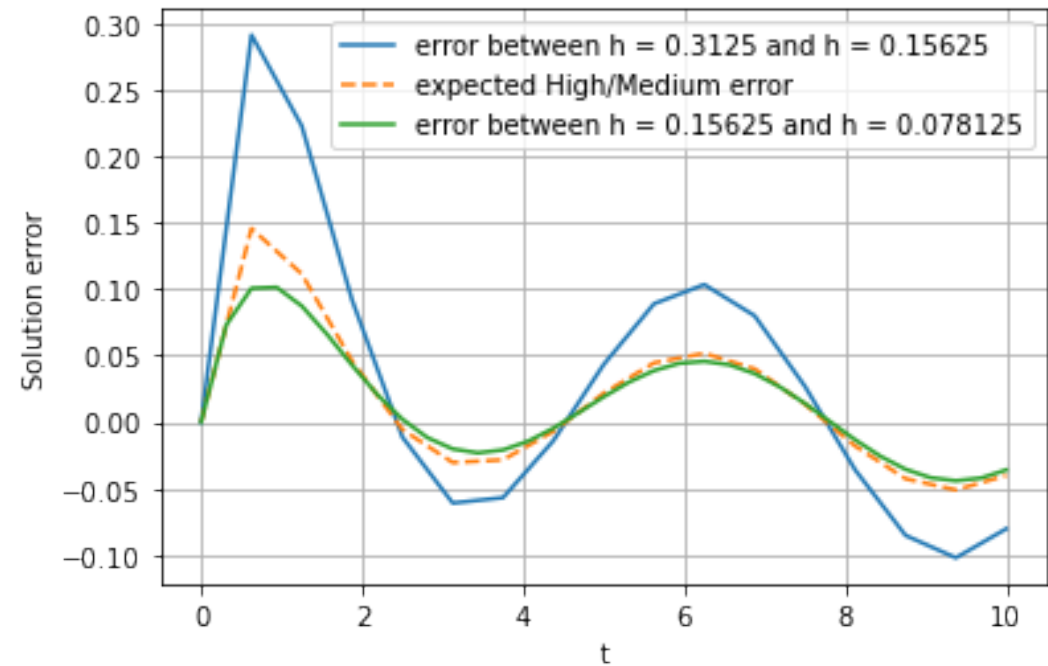
$$\frac{y_{N=8} - y_{N=4}}{y_{N=4} - y_{N=2}} = 1/2$$



Convergence

Because

$$\begin{aligned} & \frac{(y_{N=8} - y_{true}) - (y_{N=4} - y_{true})}{(y_{N=4} - y_{true}) - (y_{N=2} - y_{true})} \\ &= \frac{(y_{N=4} - y_{true})/2 - (y_{N=4} - y_{true})}{(y_{N=4} - y_{true}) - 2(y_{N=4} - y_{true})} \\ &= \frac{1}{2} \end{aligned}$$



Convergence testing

- How do I know it works? Just seeing that error decreases with resolution **tells you nothing**. The expected **order of the convergence must be right**.

This validates that *this specific source of error* (ie, from the numerical integration) is dominating, which is the goal of the convergence test.

If you obtain a different rate, some other error source is dominating, and if you don't know what that is, you are in trouble.

e.g. If you hit a place where you converge slower than expected, it could be that numerical precision error is now dominating. This might be ok, but then it also tells you that you are wasting time resolution, because you have hit a wall where you can't get better by taking smaller dt .

Asserts and testing

1. Asserts require **judgement** and **humility**
2. The usual mistake is to underestimate your/the user's ability to screw things up
3. Every time your code doesn't work, think "can I make this an assert?"
4. Each assert should be tested with a unit test. e.g. if you should not be able to set the mass attribute of the Star class negative, create a class inputting a negative mass parameter and check that it triggers the assert. This may seem overkill, but I refer you back to point (2).
5. Consider also using print statements, which can be helpful to check the code reflects back the values you expect. e.g. "Initial x value of Star 1 is set to 2.0."
6. It is definitely possible to have too many asserts, but in the context of the coursework at least I am unlikely to penalise for it.

What is “documentation”?

- Markdown formatting:
<https://www.markdownguide.org/cheat-sheet/>
- The documentation required depends heavily on the expected user. Usually people make the mistake of **assuming too much prior knowledge of the user**.
- But equally, don't just repeat the question back to me in new words!
- Also do not say things that are manifestly not true. e.g. “Here we see that the convergence test has worked perfectly” when it hasn't. If you aren't sure, best to say it. (Socrates: “I know that I know nothing”)



What is “documentation”?

- Example of documentation for a code: <https://github.com/GRTLCollaboration/GRChombo/wiki>
- Possible components of documentation:

A list of capabilities of the code, and overview of the structure, prerequisites (did you tell the user to active the python environment? What python modules do you need?), list of coding conventions (what order are your variables in the state vector?), what do the parameters do? Do they have expected ranges? What would break the code? How do I know it has worked? What is a phase plot? How does the convergence test work? ...

“The mind is not like a bucket that needs filling, it is like wood that needs igniting - nothing more - to produce an impulse to discovery and a longing for truth.”

Plutarch

“Imagine that someone needing fire from their neighbours, and finding there a big blazing one, just stayed warming themselves until the fire burned out...”

Plutarch

“... it is the same if someone who comes to ChatGPT to get their thinking does not realise that they ought to strike some light of their own and kindle their own ideas, but just sits there enchanted.”

Plutarch

ChatGPT << Your brain

- You are a free human being, with infinite capacity to change, evolve, love, make choices, read and digest information, and use your judgement.
- YOU ARE BETTER THAN CHATGPT (for now at least)
- Take pride in your human ability to not know, to make mistakes and to improve (remember: a mistake is not a sign that you aren't good enough)

ChatGPT how do I hate thee? Let me count the ways...

- ChatGPT generates a horrible mix of bullsh*t and blandness that is maddening to read.

e.g. “In this exercise we understood the intricate dance of celestial mechanics, and learned many useful things that we can apply in the future.”

SAID NO QMUL STUDENT EVER

ChatGPT can of course be useful

- If you already know the answer roughly but you forgot it
- If you want to find the right python function for a specific use
- If you are confident that you can check the output makes sense and modify it if needed
- If you use it to improve your grammar and spelling for pre written text
- ...
- AI is good for reducing effort, but in learning ***effort is the point***

“The impediment to action advances action. What stands in the way becomes the way.”

Marcus Aurelius, Meditations

Plan for today

1. ~~The mark scheme for Coursework 1~~
2. ~~Convergence testing – what to test and how to interpret the result~~
3. ~~assert (testing_sufficient), “Testing is not sufficient!”~~
4. ~~What is “documentation”?~~
5. A critical look at last year’s NOT MODEL exam solution (see QMPlus)
6. Time for questions on either coursework