## Advanced Numerical Analysis Prof. Sachin Patwardhan Department of Chemical Engineering Indian Institute of Technology - Bombay

## Lecture - 45 Solving ODE-IVPs: Selection of Integration Interval and Convergence Analysis of Solution Schemes

Methods for solving ODE initial value problems, we have looked at algorithms. We have looked at the way algorithms are derived and now one of the most crucial aspects is how do I select the integration step size okay. I am at some point tn, I want to move to tn+h, what should be integration step size h? It is a crucial decision when you have to implement or when you have to use ODE IVP solver.

Now I was describing 1 approach in which you are not really worried about analysis but a practical approach to deal with this problem is variable step size solver or variable step size implementation.

## (Refer Slide Time: 01:13)



This variable step size approach can be used only when you are going from tn to tn+1 without using the information from the past okay. So Runge-Kutta can be used. Alternatively, you could even tailor orthogonal collocations if you want using variable step size. So variable step size is something that is possible when the method involves only going from only you need information at time tn.

You do not need past information about derivatives, so multi-step methods are difficult to tailor for variable step size but the other Runge-Kutta methods can be easily tailored for variable step size implementation so here I do not have to worry about what should be the right step size. I can just work with a changing step size. I make a on the spot on the fly decision as to what should be my integration step size and next time it could be different.

Next time, it could be you know smaller or larger it depends upon how the system is behaving in a particular region. So let me just write down the steps in the algorithm that way you will understand what is really happening. Yesterday, I tried to explain the philosophy. Now let us look at so my problem is I am given x tn=xn at t=tn and epsilon is the tolerance, this could be 10 to the power -8 or this could be some small value.

Now my first step is to choose step size, let us say we have chosen a step size h1 okay. (Refer Slide Time: 03:54)

tep 2: Compute  $x^{(2)}(n+1)$  using chosen method. at  $t = t_n + h_1 \equiv t_1^{(2)}$ Steps: Define  $h_2 = \frac{h_1}{2}$   $t_{n+1}^{(2)} = t_n + h_2$ ,  $t_{n+2}^{(2)} = t_n + 2$ Compute  $\chi^{(2)}(n+1)$  and  $\chi^{(2)}(n+2)$ the chosen method.

Then now using this step size h1 what I do is I compute x n+1. I am choosing to index it as 1 okay because this is using h1 so using whatever method I have chosen it could be RK method, it could be Runge-Kutta or Euler method whatever Runge-Kutta class of method I have used as I said you could also tailor this for orthogonal collocations so whatever method you have chosen to march from tn to tn+h1.

So you can use that and compute x1 n+1 okay. Now step 3, now I am calling h2 which is h1/2 okay and now what I am going to do is so here just to put the notation correctly here okay. So this one is computed at tn+h1 okay. I am calling it as t1 n+1, n+1, see n is the counter right, n

is the index of time, t is actual time okay and in this first step 2 we have marched from tn to tn+h1 okay.

Now after I define this h2, my counter will see 2 steps of h2 will be=1 step of h1. Is not it? Because I have divided this by 2. So now I have to adjust and redefine my counter, so now I will call tn+1 2=okay the counter will have to advance twice because you are going half step here so counter would have to advance twice okay. Now what I do is I compute x2 n+1 and x2, now this index 2 is given because this is using h2 okay.

This is using h1, this is using h2 that is why I given index 2 here. Now as far as the time is concerned okay t2 n+2 is same as t1 n+1 right. This, this, these 2 are equal. This is equal to this okay. So what should happen is you will be wondering why I have given the tolerance. The tolerance is to check whether the value that you get here and a value that you get here are the 2 different okay.

If they are very, very close what you mean by close? Is using tolerance. If they are very close, I accept h1 as my step okay. If not, I reset my h1 to be equal to you know some fraction of initial h1. You can halve it or you can make it 0.75 or whatever okay.

(Refer Slide Time: 09:16)

Step 4:  $\frac{\|\chi^{(2)}(n+2) - \chi^{(1)}(n+1)\|}{\|\chi^{(2)}(n+1)\|}$ CDEEP

Now what I am going to do here is I am going to check whether this relative error. Remember this is  $x^2 n^{+2}x^1 n^{+1}$  because their time matched okay. You cannot use matching of n and n here okay. So if this relative error is very, very small okay so whether you make 2 steps and

go to that point or whether you make 1 single step it is not making too much difference. So we accept this as the next value else what we do is we shrink h okay.

So we shrink h1 okay, so what I do is if the tolerance condition is not met, I shrink my h1 okay so I shrink my h1 to h2 that is h1/2 okay and then I redo the whole thing. I keep repeating till this condition is satisfied so essentially I keep shrinking, I start with some guess, the initial guess you have to give, I start with some guess okay and then you go on shrinking till you get tolerance satisfied. In MATLAB, you have this Runge-Kutta solver.

There are 2 Runge-Kutta solvers, which can be very easily used RK23 and RK45 okay. Actually, these are very good solvers. They can be used for large class of problems except some stiff equations. What is this stiff business? I will come to that. So these are variable step size solvers. They will ask you maximum integration interval okay and they will also ask you tolerance okay.

The solution when it comes it will not be at 1 solution at the end point. The solution will be profiled because it will have shrunk the integration step size to the point where tolerances are met and then it proceeds. What is the advantage here? Okay the advantage of this approach is this is a practical way of solving the problem when you do not know how to choose an integration step size.

Unfortunately, this will not give you insights into what is happening but it solves your problem. Now of course will go to the point where we start getting insights or we start understanding why this is happening. Before that I have given and described an algorithm which practically solves the problem okay. So when you do not know what the step size you choose, just use variable step size implementation it is safe.

Even if you use Euler with variable step size, it will work because even if you make a wrong guess of the step size, it will keep shrinking the step till this condition is met okay. So you do not accept till this condition is met okay. So that is the practical way out. Now let us start getting into the insights.

Earlier we were talking about linear difference equations arising out of iterative schemes right, xk+1 or ek+1 for some matrix s inverse t times ek where e was the error right and k was

iteration index. Now I am going to talk about difference equations in time okay. We are going to use difference equations in time. So this concept of Eigen values is so fundamental that you know it pervades the analysis that we do.

And those of you who are doing the analytical methods for partial differential equations and ODE's that course also you will appreciate more and more that how this Eigen values play a role and why they are so important. Of course, there you get Eigen functions and Eigen values whereas finite dimensional case you get Eigen vectors and Eigen values. Now let us start getting into this business of convergence analysis.

So this convergence analysis is tightly coupled with selection of step size so 2 things cannot be really separated. How do you choose integration step size? Will decide whether convergence to the true solution occur or not? Okay so these 2 things are not really separate entities okay. Though now we have a fix of how to go about if you do not know anything, we would still like to get insights into what is really going on okay.

It also allows you to compare different methods okay. Now what I am going to do is to do the analysis okay. First of all, I need to know see when can you analyze whether a particular method is converging to the true solution? Only when you know the true solution right. If you do not know the true solution, how will you analyze with the given method is going to the true solution or not okay, it is very difficult to do that.

So the first criteria is that you should start looking at a system for which true solution is known okay. Then only we can start looking at difference between the true and approximate solution and is the first thing. So which are the systems for which we know the true solutions exactly whether it is scalar or whether it is vector case is linear differential equations, ODE initial value problem for linear ordinary differential equations could be scalar or could be vector.

So I am going to use linear ordinary differential equations, initial value problem as a benchmark to understand to get insights into convergence analysis okay. How to extend it to a non-linear case will worry about it little later. Let us first get some insights as to what is happening and then let us see how to extend it to a non-linear case okay.

(Refer Slide Time: 16:51)

 $\frac{dx}{dt} = qx, x \in R,$ x(tn) = x(n) / $x(0) \equiv I \cdot C$ 

So I am going to consider 2 kinds of systems, 1 is dx/dt=ax, x belongs to R and x tn=xn or I have given some you could consider this initial condition, you could consider x0 is initial condition whichever way okay. The nice thing about this is that a is a constant, a is a scalar, x is scalar variable, one variable differential equation initial value problem. I know the solution. I know the true solution okay.

Now I can use Euler method or whatever Runge-Kutta method and see whether you know whether approximation goes to the truth and so on.

### (Refer Slide Time: 17:52)

 $\frac{dx}{dt} = A x \quad x \in \mathbb{R}^n$  $\alpha(t_n) = \alpha(n)$ A -> nxn real valued matrix

The second thing which I am going to look at the second benchmark which I am going to look at is dx/dt=ax x belongs to Rn and x tn=xn and a here is a n cross n real valued matrix, real valued in the sense, containing all real entries.

#### (Refer Slide Time: 18:22)

(Refer Slide Time: 19:34)

 $\frac{dx}{dt} = qx$ ,  $x \in R$  $\chi(t_n) = \chi(n)$ 7(0) = I.C a is real scalar  $x^{*}(t) = e^{at} x(0)$ CDEEP IIT Bomba

I am taking a short cut and a is the real scalar okay. What is the true solution here for the first case? If I am given x0, what is the true solution? The true solution x star t let us call it star as a true solution. X star t is e to the power at x0. If it is x at tn it will be xn okay, whether it is x0 or xn does not matter. This is a true solution okay. What about this case? If you are attending the other course, this must have been done, analytical methods.

What is the true solution here? Okay if you have not done it, I will derive it in the class, not an issue.

 $\frac{dx}{dt} = A x \quad x \in \mathbb{R}^n$  $\chi(t_n) = \chi(n)$  $A \rightarrow n \times n$  real valued matrix. At $\chi^{*}(t) = C \chi(0)$ CDEEP

So the true solution here well what she is saying also correct but the true solution can be written here as x star t is e to the power At, where A is the matrix. I suppose you have been

introduced to this e to the power exponential of a matrix. Yes, or no? How many of you do not know this? Okay will talk about it, not an issue, into x0 okay, I will derive this not an issue. So you can write this as e to the power At x0.

I will derive it for a special case but the result holds for general case. I will derive this for a case where you have Eigen values or Eigen vectors are linearly independent. So we can derive this very easily. Other cases require little more work okay. So this is my true solution and now I can use this as a benchmark to compare whether my approximate solution is going to the true solution or not okay.

So let us not worry right now about the multi-variable case, let us start looking at the scalar case. It is easier to understand the convergence behavior so this will visit later okay. So my true solution is this okay, typically when I am using some numerical integration method or some solver like RK45 or whatever I want to go from xn to xn+1 right so I will write this solution in that format okay.

(Refer Slide Time: 21:22)



So x star tn+1, let us take right now step size to be constant. Now I am not worried about variable step size and all that. Let us take constant step size h okay, x tn+1 is e to the power a tn+h x0 right and x star tn is e to the power a tn x0 okay. Is this is okay? I can combine these 2 and say that x star t n+1=e to the power ah x star tn just check. Is everyone with me on this? I am just expanding this substituting for right.

I will just expand it and substituted this so these 2 equations I can combine to write this okay. In our notation, this is same as x star n+1=e to the power ah. The notation that we have adapted with that this is x star n+1 is e to the power ah x star n is the true solution. How it should actually evolve? Okay now let us look at explicit Euler method first okay. How will you write explicit Euler method?

### (Refer Slide Time: 23:38)



Explicit Euler method is xn+1, now when I am writing just x no star, this is approximate solution. X star is the true solution. X is the approximate solution okay. Now explicit Euler okay. What is xn+1? xn+1 is at least today you should know because you are supposed to submit Euler's method and h times today or what is the submission data? 4th okay but it is too close right not too far.

So I can expect that you should know what is Euler method today. So h times fn right but what is fn in this case? ax n so this I can write here xn+h ax n right so I can write this as 1+ah xn. Is everyone with me on this? Okay now let us define an error okay. Let us define error which is en this is x star n-xn okay. This is my error so what is this error? This is error between the truth and approximation okay.

(Refer Slide Time: 25:49)

$$x^{*}(t_{n+1}) = e^{a(t_{n}+h)} \pi(0)$$

$$x^{*}(t_{n}) = e^{at_{n}} \pi(0).$$

$$x^{*}(t_{n+1}) = e^{ah} \pi^{*}(t_{n})$$

$$x^{*}(n+1) = e^{ah} \pi^{*}(h) - (A)$$

Now if I take this as my equation B and if I go here and call this equation as my equation A okay then I can subtract the 2 equation and then get the difference equation that governs the error dynamics okay.

# (Refer Slide Time: 26:03)

$$\frac{Fxplicit}{\chi(n+1)} = \chi(n) + hf(n) = \chi(n) + ha \chi(n)$$
  
= (1+ah)  $\chi(n)$  (B)  
 $\mathcal{E}(h) = \chi^{N}(h) - \chi(h)$  (c)  
(A) - (B)  
 $\mathcal{E}(h+1) = e^{ah}\chi^{*}(h) - (1+ah)\chi(h) - (D)$ 

So A-B equation A-B will give me okay now do not confuse between this e exponential or let us do like this to reduce the confusion I will call this epsilon. I will call this error epsilon because you should not confuse with e to the power something okay. This is what I get okay. Now I have to convert this into a difference equation okay. I am going to play a little bit of a trick. I am going to substitute for x star n okay in terms of epsilon+xn. I am going to do some readjustment okay. So this equation let us call it C and this equation let us call it D, so I am going to combine C and D and get a difference equation.

## (Refer Slide Time: 27:44)

$$e(n+1) = (1+ah)e(n)$$
  
+  $[e^{ah} - (1+ah)] x^{*}(n)$   
 $x(n) = x^{*}(n) - \varepsilon(n)$ 

So combining these 2 you get en+1=1+ah+e to the power ah-1+ah okay sorry I forgot about en okay. What I have done is I have eliminated xn on the right hand side of that equation. I have written x star n. I have written x star but I have removed all that I have done is I have written xn is same as x star n-epsilon n. If I just use this, this is my definition. I am just using this definition, substituting and rearranging that equation, I get this equation okay.

So this gives us some idea about how the error behaves okay. It also gives us some insights, will look at the insights and then move on and do some more analysis but this 1 simple insight which you will get here is that error dynamics okay will depend upon this difference. You see something familiar here 1+ah, how do you expand e to the power ah? 1+ah+a square h square/2 factorial+ whatever.

If h is very, very small, okay higher order terms can be neglected and this difference will be very, very small okay. If this difference is very, very small then what will govern the error dynamics? en+1=1+ah right. How 1+ah behaves will decide okay. Whether the error goes to 0, whether error goes to infinity or whatever happens. If this is very, very small, if this can be neglected okay can you just look at this term and say what should happen.

This is the linear difference equation, scalar linear difference equation. What is the Eigen value? 1+ah 1 variable, there is no matrix, is only a scalar okay. How will the difference equation behave?

### (Refer Slide Time: 31:10)



If you can neglect e to the power ah-1+ah, this is approximately=0. This can be neglected okay then you can say that en+1=1+ah en okay. Let us make a simplifying assumption, just to get or understanding correct. Let us assume that a is strictly<0. If a is strictly<0, how should the true solution behave? What is the true solution? True solution x star t is e to the power at x0. What should happen to x star t if t goes to infinity?

If a is<0, exponential-something will exponential decade will go to 0 okay. If a<0 okay when will error go to 0? How will this equation behave? See this equation will behave as you can derive what I am writing here very, very easily en will be 1+ah raise to n e0 right raise to e0. So what will happen to 1+ah? When will it go to 0? When will this go to 0? This quantity should go to 0, error should go to 0 right.

The difference between the truth and approximation should go to 0. When will it happen? Louder, I cannot hear. No, something more than that -5 is<0 then between 0 to 1, no yaar, mod of 1+ah, not 1+ah, mod of 1+ah should be<1. The way you should put mod of 1+ah should be<1 okay. So this will go to 0.

```
(Refer Slide Time: 34:12)
```

 $e^{ah} = (1+ah) \approx 0$  $x^*(t) = e^{at} x(0)$  $e(n) = (1+ah)^{n!}e(1)$ CDE

Now if mod of 1+ah if this is strictly<1, what will happen? en will tend to 0 as n tends to infinity yeah. **"Professor - student conversation starts."** So you start with e1, there will be a mistake committed one step you move right. The moment you take 1 step, there will be a mistake committed from x0, 0 is some initial point okay, which need not be same as.

See because when if you start from the same point okay the moment you take one step okay the approximate solutions will be different from the true solution. You start analysis from e1 okay so let us start from e1. This will be n-1 okay yeah good question, e0 is always be 0. **"Professor - student conversation ends."** 

(Refer Slide Time: 35:18)

|1+ah| < 1  $e(n) \rightarrow 0 \text{ as } h \rightarrow \infty$   $\varepsilon(n) = \chi'(n) - \chi(n) - q$  (A) - (B)

Now let me start from e1 okay. So this will be n-1 right and this is e1. Now e1 is different even if I start from same x0 okay, x1 which is calculated using approximate solution is not

same as x star 1 okay. Now let us see the analysis fine. Yeah good thinking I appreciate your en-1. Is this fine? So this has to go to 0 right otherwise we have trouble. So en will go to 0 only when this is strictly<1 okay.

So this being strictly<1 what does it mean in terms of choice of see this condition is giving you a way to choose h for explicit Euler method. If you violate this condition the difference between the true and the approximate will not vanish okay. If you violate this condition, the difference between the true and but if you obey this condition what you know is that asymptotically the difference between the truth and approximate will vanish okay.

So this is socket condition for explicit Euler. Can we derive a condition for implicit Euler? What is implicit Euler? Just do it. So for implicit Euler my approach is now one thing before you proceed, I just want to point out one more thing here. See look at this, look at this expression here, whether h is small or whether h is large it depends upon a okay. See this is very, very important okay.

What is small h? Somebody might give you some number 10 to the power -6 is small h but that is not the thing whether h is small or h is large, it depends upon what is value of a. So it depends upon the characteristic equation or characteristic constant of the equation a okay which appears in the equation. When we go to the vector case, this a here will get replaced by Eigen values okay.

So what is step size? It depends upon the system, it depends upon the system parameters a, that is also an important take home message that it is not independent of what value a has okay. Of course, this you can write in terms of you can expand this and write this as inequality in terms of but now let us move on to implicit Euler method.

(Refer Slide Time: 38:34)

 $= \pi(n) + h a \pi(n+1)$  $\pi(n+1) = \frac{1}{1-2h} \pi(n).$ 

Implicit Euler method is x n+1 will be f n+1 okay. For the linear case, you do not have to do iterations to compute the solution. So this is nothing but xn+h ax n+1 right okay. So I can write that xn+1=what 1/1-ah. I am just taking this on left hand side 1-ah xn right. If a is<0, 1-ah this will always be positive, your integration step size is positive okay, 1-ah is always positive so 1+a positive number this is always going to be a fraction okay.

This is very nice okay. Now if I am doing analysis for this method how will this equation change? What will appear here?

### (Refer Slide Time: 40:21)

$$e(n+i) = \frac{1}{1-qh} e(n)$$

$$+ \left[e^{qh} - \frac{1}{1-qh}\right] x^{*}(n)$$

$$\chi(n) = x^{*}(n) - \varepsilon(n)$$
CDEEP

1/1-ah, 1/1-ah okay. There are things called Pade approximants and this is a type of Pade approximation of e to the power ah 1/1-ah is a type of Pade approximation. This is the better

approximation than Taylor series and truncating okay. So now again if this is very, very small you could just look at this okay.

(Refer Slide Time: 41:17)

e(n+1) = (1+ah) e(n) e(n+1) = (1+ah) e(n)Ealer

You could look at this and the equation for error will change to see this is explicit Euler. This is my implicit Euler okay, a is<0, when a is<0 okay the true solution asymptotically goes to 0 e to the power -at that asymptotically goes to 0. What can you say about the error in this case? What is our criteria for convergence? This coefficient should be<1 strictly<1 right. Now for implicit Euler will this always be<1 for any choice of h?

You see why implicit Euler is better. Well if you make a wrong guess of h, you are still you know you do not have to worry whereas here you have to be very, very careful. Explicit Euler you better be careful about how you choose your integration step size. Implicit Euler when if you make a wrong choice eventually the error will go to 0 okay. That is why implicit methods okay are many times perform much better than the explicit methods yeah.

**"Professor - student conversation starts."** If a is positive no matter what will happen but if a is positive, it is a difficult problem because the solutions are going to infinity. So matching 2 infinities, both will go to infinity actually but the difference between the 2 infinities can grow blow so difficult to get insights into what is happening if you make an assumption about if you say something about if you take a to be>0.

That is why I have taken the case where a is<0, we basically want to get insight into how error behaves. **"Professor - student conversation ends."** The system is truly unstable system

okay then getting the true unstable solution is a difficult problem computationally not an easy problem even a small difference can blow up. **"Professor - student conversation starts."** In this case, not here. Why?

(Refer Slide Time: 44:00)

$$|1+ah| < 1$$
  
-1 < 1+ah < 1  
 $\pi(n+i) = \pi(n) + \frac{h}{2} [f(n) + f(n+i)]$ 

So I have to make sure in this case I have to make sure that -1 is<1+ah is<1 right. So I have to choose my h carefully so that this inequality is not violated. Can you do analysis for the trapezoidal rule? Just do it. See what expression that you get. See trapezoidal rule is xn+1=xn+h/2 fn+1, this is the trapezoidal rule okay. "**Professor - student conversation ends.**" What will be equivalent difference equation for en?

(Refer Slide Time: 45:03)

$$e(n+1) = \frac{(1+\frac{b}{2}a)}{1-\frac{b}{2}a} e(n) + \left[e^{ab} - \frac{1+\frac{b}{2}}{1-\frac{b}{2}}\right] \pi^{*}(n)$$
  
$$\pi(n) = \pi^{*}(n) - \varepsilon(n)$$
  
CDEEP

If I do the algebra okay I will get this thing here is just check whether you are getting the same thing 1+h/2\*a/1-h/2a right okay.

### (Refer Slide Time: 45:35)

And again the same thing we can say, we can argue that if this 1+ha/2/1-ha/2 if this is close to 0 okay you could only look at how well I do not have exact equation when it is not close to 0 but right now this is approximate analysis just so in that case this is 1+ha/2, this is 1-ha/2 right and the condition becomes mod of this should be<1 so this is trapezoidal rule or Simpson's method or whatever okay.

## (Refer Slide Time: 46:34)

Itahl <

And in this case it will become right in fact this ratio is always going to be a fraction why? Of course if a is<0 then this ratio is going to be a fraction. This is always going to be higher than this okay. So we are assured that this is a fraction so trapezoidal rule will converge, the error will you know the error will go to 0 asymptotically, it will become smaller and smaller okay. Actually, the way you should do analysis is I am doing a very handwavy kind of analysis.

The way I should look at this problem is I will write it down a little more, I will write an exact expression.

(Refer Slide Time: 47:27)



The exact expression I should write is  $en+1 \ x \ star \ en+1 \ x \ star \ n+1=1+ah/2 \ 1-ah/2 \ e$  to the power  $ah-1+ah/2 \ 1-ah/2 \ 0$  and e to the power ah. Well right now when I am writing this equation, I am not doing any hand waving business, I am not saying this is close to 0 and all that okay. This is a linear difference equation okay. This is my let us call this z, let us call this vector as z, zn+1=if you call this matrix as B and if you call this as zn.

This is a linear difference equation, zn+1=b times zn okay. What is the criteria for convergence? Spectral radius of this should be=you can find out a spectral radius of this. This is a triangular matrix okay and then you can argue about that. So basically we are using this fundamental concept of analyzing qualitative behavior of linear difference equations in this context to understand how the error goes to 0, same idea.

In fact, those are few who will probably continue to work in area of digital control, will find the same idea you come back there. When you talk about you know design of controllers, digital controllers, there again you will use spectral radius of the closed loop dynamic should be inside unit circle same idea, linear difference equations that is the fundamental, applications are different, iterative processes or analyzing behavior of integration methods or you know solving some control problem the same idea. In a context of iterative methods, we had k+1 as b times k, where k was iteration index, here n is time okay.

(Refer Slide Time: 50:23)



And my condition still is spectral radius of B should be strictly<1 okay. One thing you can see is that if a is<0 okay, this part is going to go to 0 anyway asymptotically because x star is going to 0 okay. Everything will depend upon this and this, of course this is going to 0, a is<0 so e to the power –ah is going to 0. So everything finally boils down to this term. If this term is strictly<1 approximation error will go to 0 asymptotically okay.

This is what gives us insight into what happens. Now when I extend this to multivariate case, Eigen values of A matrix will appear and will have to analyze them, we will see that later.