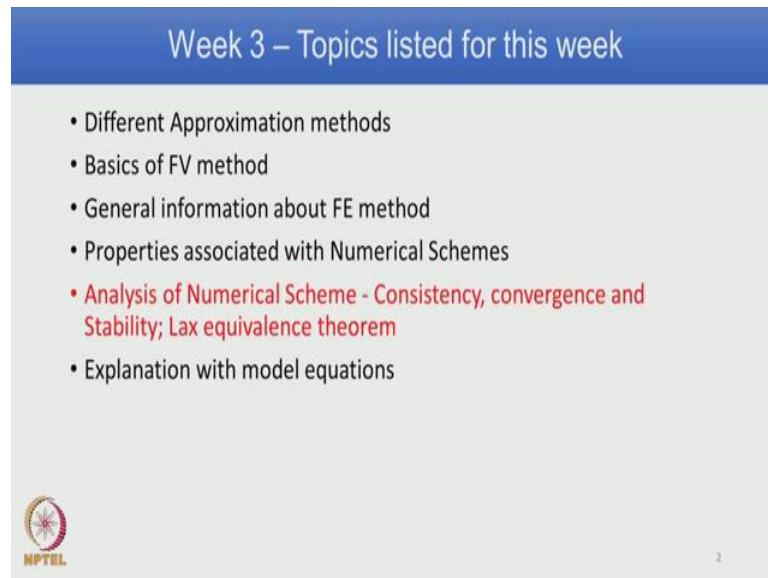


Foundation of Computational Fluid Dynamics
Dr. S. Vengadesan
Department of Applied Mechanics
Indian Institute of Technology, Madras


Lecture - 13

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Week 3 – Topics listed for this week

- Different Approximation methods
- Basics of FV method
- General information about FE method
- Properties associated with Numerical Schemes
- Analysis of Numerical Scheme - Consistency, convergence and Stability; Lax equivalence theorem
- Explanation with model equations

 2

It is my pleasure to welcome you all for this course on CFD. We are now into the module three of this week. So, far, we have done different approximation method, introduction about finite volume, finite difference, finite element methods, then we talked about properties associated with numerical schemes, mainly three properties conservativeness, transportiveness, boundedness. Today's class, we will particularly talk about analysis of numerical scheme, there are again three aspects – consistency, convergence and stability, particular theorem called Lax equivalent theorem that relates or connects all the three aspects while doing the numerical analysis. We will talk about these aspects in detail with example. Then it will be followed by explanation by taking different model equations.

(Refer Slide Time: 01:31)

Numerical errors

- Approximations are made at different stages
- Errors arise due to these approximations
- Error at the stage of computational modelling of physical problem along with proper choice of BCs.
- Error due to coding
- Errors due to numerical approximation
 - Truncation error
 - Round off error
 - Discretization error



3

While doing CFD approximations are made at different stages. And you get errors arises due to these approximations. First step in CFD is computational modeling of physical problem, either we take a physical problem in Ω or we simplify the physical problem and then solved. So, in any one of this stage, there is a possibility some assumptions are made or there is an error in the conversion of computational modeling from physical problem. Second aspect is appropriate choice of boundary condition, again ill posed boundary condition may result additional error. There is also possibility that you have computationally modeled properly, there is a problem in coding. So, you may have index, for example, i at j replaced with j i , in such problem, you may not be able to identify so easily, the program may run, but it may give wrong results after sometimes or after some iteration. So, one has to go back and check the code and it is possible to debug and fix the code for the correct coding. One more type of error is due to numerical approximation. There are three possibilities, one is truncation error, other one is round-off error, and third one is discretization error. So, we will now focus mainly on this numerical approximation error associated due to the numerical approximation.

(Refer Slide Time: 03:46)

Numerical errors

- Round-off errors:
 - Number of significant digits considered
 - Single precision – usually up to 8 digits after decimals
 - Double precision – up to 16 decimals
- Truncation error:
 - Numerical approximation by neglecting leading terms
- Discretization error:
 - Numerical error neglecting round-off error



So, round-off error is the number of significant digits considered. So, we know there are a lot of mathematical operations, subtraction, addition, multiplication and division. And each of these arithmetic operations, we handle numbers, and number of digits, significant digits considered after the decimal make the difference in the solution. So, there is something called single precision; in this we usually consider 8 digits after decimals. If someone decides to have higher accuracy then you go for double precision, where we consider 16 digits after decimals. So, there is a repeated calculation in terms of iteration or in terms of unsteady calculation and over so many nodal points in a computational domain, so though this appears this kind of error appears very small over cumulative this error will affect the results. And next important error is a truncation error. This is resulting by considering or neglecting leading terms while writing finite difference approximation. Now, there is a third error what is known as a discretization error, this is a numerical error without considering the round-off error.

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Numerical errors

- Truncation error:
 - Numerical approximation by neglecting leading terms

- Dissipative error:
 - Neglecting leading odd order term
 - Smoothens the gradients
 - Called numerical or artificial viscosity

- Dispersive error:
 - Neglecting leading even order term
 - Instability – under or overshoots



5

So, this truncation error, we mentioned how many or what terms you are considering while writing the finite difference form of governing equation. So, you can neglect or you will consider up to some terms in the expansion then you will neglect the remaining terms. Remaining terms can be odd order or even order. So, accordingly the error can be two types, one is the dissipative error, here the leading neglecting term is of odd order. Now, this also behaves like a viscosity, so you know in basic fluid mechanics viscosity helps in diffusion. So, this dissipative error, where you are neglecting leading term; and if the leading term is of odd order, then it functions like numerical viscosity or artificial viscosity, but that helps in smoothing the problem, and other hand, you may not get very peak or accurate results. Second type is the dispersive error, where the leading term neglected leading term is even order term and that results in what is known as a overshoots or undershoots. So, you may have a solution with vigils.

Now, let us get explanation of these two types of errors with some illustration. So, in this figure, what you see, there is a there are three curves; now there is a black line which is going like a step function and that is the expected solution or exact solution obtained by analytical way. Then if you are solve that equation with leading neglecting term as odd order, and you mentioned it is a dissipative error and you get a solution, which is represented by the red line here, so you see here it is smoothens, and you are not able to get the peak here, or you are not able to get the peak here. It connects very smoothly without any problem.

Of course, you can increase the leading term, for example, instead of first term, you can take the second term or third term then you may have a slightly improved solution, but still it never captures the peak that is the property associated with the dissipative error. The second error is the dispersive error and that is due to leading even order term, and the solution obtain will exhibit vigils that is overshoots and undershoots, so you can see here light blue color and that is the type of solution you will get. So, you can see up and down then and so on. So, you have a problem either because of the dissipative error or because of the dispersive error.

(Refer Slide Time: 09:15)


FDE formulae

- Evaluating $\left(\frac{\partial f}{\partial x}\right)$ by forward difference,

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x+\Delta x)-f(x)}{\Delta x} - \frac{\Delta x^1}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) - \dots$$
- Evaluating $\left(\frac{\partial f}{\partial x}\right)$ by central difference,

$$f(x+\Delta x) - f(x-\Delta x) = 2\Delta x \left(\frac{\partial f}{\partial x}\right) + \frac{2\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots$$

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x+\Delta x)-f(x-\Delta x)}{\Delta x} - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots$$



Now, we will try to get the explanation of this from finite difference formula. So, we already did how to obtain forward differences scheme for the first derivative. And without going to the steps in details, we write down the final expression here, so $\frac{df}{dx}$ is given like this. Now, you have consider only the first term, the remaining terms are not consider. So, this is the neglected term $\frac{\Delta x^1}{2!} \frac{d^2 f}{dx^2}$ and so on and followed by many other terms. So, this is the leading term that is not consider and this is of odd order and we mentioned, this is the dissipative error.


We also learned how to write the same first derivative by central difference formula, and you get after a simplification, we are interested only in the $\frac{df}{dx}$, so we rewrite $\frac{df}{dx}$ equal to like this. And you observe this is the leading term which you

are not consider, and this leading term is of even order Δx^2 is of even order and that results is what is known as a dispersive error. So, the leading term if it is odd order, it will be dissipative error; leading term if it is off even order, it will results in dispersive error. You will get smooth solution, but you will not capture the peak. In the second case, we will get a wiggle, but it may be accurate. So, there is a though why not we combine both that is you take advantage of forward difference or backward difference and central difference. So, such a scheme combination of both is what is known as hybrid scheme, and we will use that also to get solution.

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Analysis of discretized equations

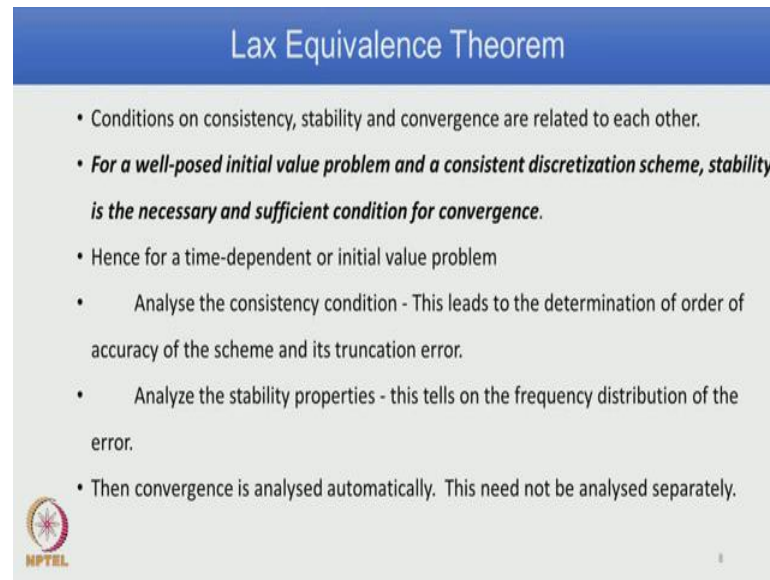
- Consistency
- Convergence
- Stability
- Consistency: Defines the relation between the differential equation and its discrete formulation. Condition on structure of the numerical formulation
- Convergence: It connects the computed solution to the exact solution of the differential equation. Condition on solution of the numerical scheme
- Stability: It establishes a relation between the computed solution and the exact solution of the discretized equations. Condition on the behaviour of numerical scheme

 7

Next, we go to the analysis of discretized equation. We mentioned there are three aspects, one is the consistency, second convergence, third stability. Definition of consistency – it defines the relationship between differential equation and its discrete formulation. So, we have an original or given PDE then we rewrite or we replace the PDE with the discretized and we get the discrete formulation. Now, whether the discrete formulation actually represent the original PDE is the question. And that property or that condition is what is known as a consistency. So, it is a condition on structure of the numerical formulation. Second aspect is convergence, which connects the computed solution to the exact solution of the differential equation, so what scheme you are using and how it is convergent that information is obtained or analyzed by a property or aspect called convergence. Third one is the stability, it establishes a relation between computed solution and the exact solution of the discretized equations. This puts the condition on


behavior of the numerical scheme. So, next few lectures, we are going to get definition and explanation with a model equation on these aspects, consistency, convergence and stability.

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Lax Equivalence Theorem

- Conditions on consistency, stability and convergence are related to each other.
- ***For a well-posed initial value problem and a consistent discretization scheme, stability is the necessary and sufficient condition for convergence.***
- Hence for a time-dependent or initial value problem
 - Analyse the consistency condition - This leads to the determination of order of accuracy of the scheme and its truncation error.
 - Analyze the stability properties - this tells on the frequency distribution of the error.
 - Then convergence is analysed automatically. This need not be analysed separately.

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There is a particular theorem called Lax equivalence theorem, which connects or relates all these three aspects consistency, stability and convergence. The theorem reads like this; for a well-posed initial value problem and a consistent discretization scheme, stability is the necessary and sufficient condition for convergence. To get some more explanation on this theorem, for a time-dependent initial value problem, if you analyze the consistency and if you analyze the stability then convergences need not be analyzed, it is satisfied automatically. So, when you are analyzing consistency, this leads to the determination of order of this scheme as well as the truncation error. Similarly, when you analyze the stability this tells on the frequency distribution of the error. So, if these two are satisfied or analyzed properly then convergence need not be checked and it is automatically satisfied by this theorem. The one point that is to be noted all these are applicable particularly the stability is applicable for a linear problem, but in any practical situation, all the problems are of non-linear, hence to do analysis on stability of a particular scheme for a non-linear problem, one can locally linearize and carry out the stability analysis. Similarly, stability analysis cannot be applied near boundaries.

(Refer Slide Time: 14:57)

Consistency

Consistency

- Measure of equivalence between PDEs and FDEs
- Truncation error as length and time step tends to zero
- Taylor series expansion

Consider 1D Temperature diffusion equation

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} \right) \dots \dots \dots (1)$$

If $\alpha=1$, Forward in Time Central in Space (FTCS) we give,

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \left(\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \right) \dots \dots \dots (2)$$



Let's perform Taylor series expansion of each term in the equation

Now, let us look at each of this in detail. First we take consistency, which measure equivalence between original PDE and the finite difference equation, which replaces the original PDE. So, when you replace the original PDE by a finite difference equation as we know very well from Taylor series expansion, we consider only few terms and remaining terms are neglected whatever order of accuracy that you are deciding. So, that puts the truncation error and if the truncation error goes to zero as a function of delta t or delta x, which means if the length delta t and delta x goes to 0, the truncation error also goes to zero then you recover from the finite difference equation the original PDE. If such things happens then, the particular scheme is referred as consistent scheme.

So, we know the Taylor series expansion. We take example of one-dimensional temperature diffusion equation and it is given here $\frac{dT}{dt} = \alpha \frac{d^2T}{dx^2}$, where T capital here refers to temperature equal to alpha $\frac{d^2T}{dx^2}$. Now, we know by Taylor series expansion, we can separately write for time derivative and second order spatial derivative. Any scheme we can write, we start off with forward in time and central scheme, so which is otherwise shortly referred as FTCS – forward in time central in space. And for simplification purpose, we will take the coefficient alpha to be one, so it will be only $\frac{dT}{dt} = \frac{d^2T}{dx^2}$.

So, if you substitute forward in time on left hand side, you get finite difference equation as $T_i^{n+1} - T_i^n = \Delta t \left(\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \right)$, this is forward in time. And as I mentioned yesterday's class, subscript i or j stands for spatial and superscript n stands for time, so when you say n plus one, it is forward in

time minus n, so you get forward in time. Now, on the right hand side, we said central in space, but times is at n level, so you can see in the expression superscript n appears, whereas, subscript it is central in space so you get T of i minus 1 minus 2 T of i evaluated known at n and plus T i plus 1 n divided by delta x square. So, this expression we know already; independently we have learned by Taylor series expansion, now we are substituting them together. Now, what we do, we perform Taylor series expansion for each of these terms that is T of i n plus 1, T i minus 1 n, T i plus 1 n.

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Consistency (cont....)

Taylor series expansion of each term in the equation


$$T_i^{n+1} = T_i^n + \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t^2}{2!} \frac{\partial^2 T}{\partial t^2} + \frac{\Delta t^3}{3!} \frac{\partial^3 T}{\partial t^3} + \frac{\Delta t^4}{4!} \frac{\partial^4 T}{\partial t^4} + \dots$$

$$T_{i+1}^n = T_i^n + \Delta x \frac{\partial T}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} + \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} + \frac{\Delta x^4}{4!} \frac{\partial^4 T}{\partial x^4} + \dots$$

$$T_{i-1}^n = T_i^n - \Delta x \frac{\partial T}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} - \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} + \frac{\Delta x^4}{4!} \frac{\partial^4 T}{\partial x^4} - \dots$$

Substitute in the discretized equation,

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \left(\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \right)$$


10

So, if you write the Taylor series expansion for each of the term, I am showing here for each of the term up to certain terms for each term. For example, T of i n plus 1, you can expand in time – forward in time that is why it is n plus one, and I have written up to four terms, remaining terms are not written; similarly for all other terms that is T i plus 1 n, T of i minus 1 n. So, all we have to do, we substitute this expansion in the finite difference equation, in this equation and we will see how to do that.

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Consistency (cont....)

Taylor series expansion of each term in the equation

$$T_i^{n+1} = T_i^n + \Delta t \frac{\partial T}{\partial t} + \frac{\Delta t^2}{2!} \frac{\partial^2 T}{\partial t^2} + \frac{\Delta t^3}{3!} \frac{\partial^3 T}{\partial t^3} + \frac{\Delta t^4}{4!} \frac{\partial^4 T}{\partial t^4} + \dots$$

$$T_{i+1}^n = T_i^n + \Delta x \frac{\partial T}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} + \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} + \frac{\Delta x^4}{4!} \frac{\partial^4 T}{\partial x^4} + \dots$$

$$T_{i-1}^n = T_i^n - \Delta x \frac{\partial T}{\partial x} + \frac{\Delta x^2}{2!} \frac{\partial^2 T}{\partial x^2} - \frac{\Delta x^3}{3!} \frac{\partial^3 T}{\partial x^3} + \frac{\Delta x^4}{4!} \frac{\partial^4 T}{\partial x^4} - \dots$$

Substitute in the discretized equation and rearrange



$$\frac{\partial T}{\partial t} = \left(\frac{\partial^2 T}{\partial x^2} \right) - \frac{\Delta T}{2} \left(\frac{\partial^2 T}{\partial t^2} \right) - \frac{\Delta x^2}{12} \left(\frac{\partial^4 T}{\partial x^4} \right) + O[(\Delta T)^2, (\Delta x)^4]$$

So, if you substitute or rewrite or sum them properly then we get expression like this, which is given $\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$ and there are so many other terms and these terms are coming from, this additional term what we have considered, because of the expansion. Now, while writing this also, we have consider only two terms; one corresponds to time, other corresponds to space, and whatever terms are not consider that decides the leading error term, so this is of order ΔT square and of order four in space Δx .

(Refer Slide Time: 19:56)

Consistency (cont....)

PDE considered $\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} \right) \dots \dots \dots (1)$

Discretized Eqn. $\frac{T_i^{n+1} - T_i^n}{\Delta t} = \left(\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \right) \dots \dots \dots (2)$

- Upon substitution of Taylor series expansion for each term and then rearranging terms,

$$\frac{\partial T}{\partial t} = \left(\frac{\partial^2 T}{\partial x^2} \right) - \frac{\Delta T}{2} \left(\frac{\partial^2 T}{\partial t^2} \right) - \frac{\Delta x^2}{12} \left(\frac{\partial^4 T}{\partial x^4} \right) + O[(\Delta T)^2, (\Delta x)^4]$$

- If ΔT and Δx tends to zero, then Eq.2 is equal to Eq.1.



We get back the original partial differential equation from the Finite difference equation.

The scheme is said to be consistent.

Now, I put all the things together, so original PDE considered is given here. Discretized equation is forward in time and central in space is also given here. Then upon Taylor

series expansion for each of the term substituting and rearranging, you get equation like this. Now, what do we do to understand consistency, consistency definition if delta T and delta x goes to zero, then original PDE should be recovered. So, we can understand that from this. If you make delta T going to 0 and delta x going to 0, then original PDE that is appearing here itself dou T by dou t equal to dou square T by dou x square. We get back the original PDE from the finite difference equation, hence this particular scheme that is forward in time central in space for this PDE said to be consistent. So, one can analyze any PDE by this way, this is the very straight-forward procedure.

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Convergence

- Essential condition to quit the iterative procedure


Let $A\phi = b$ is the equation to be solved.

If $\epsilon^n = \phi - \phi^n$ is defined as the iteration error where ϕ is the converged solution.

Then equation for residual is given by

$$A\epsilon^n = \rho^n$$

where ρ^n is the residue error at n^{th} iteration


11

Now, we will take the next criteria, what is known as the convergence, so this is a essential condition for any iterative procedure where to quit the calculation. Let say usually end up in a algebraic equation, which is given here as A into phi equal to b, this is set of equation that we will be solved. A is a coefficient matrix; and phi is the variable, which you are interested, and b is the known coefficient, which is on the right hand side. Let say you are doing iteration then, you get phi value pervious level, you get phi value from the present level. The difference between the two is what is referred here as epsilon and this is evaluated for the current level, so epsilon to the power of n is what for the current level and based on this, we decide whether to quit the particular iterative procedure. So, one can setup a equation for residual; if you substitute epsilon into the solution matrix that we have put, we replace phi by epsilon n and then you get residue,

residue mean equation is not satisfied some is remaining and that is given by rho, because it is evaluated at nth level superscript n is given.

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Convergence criterion


Convergence limit is defined as

$|\Delta\phi_{i,j}^{n+1}| < \epsilon$ for all i, j where $\Delta\phi$ is the difference in numerical solution $\Delta\phi = \phi^{n+1} - \phi^n$

$(|\Delta\phi_{i,j}^{n+1}|) < \epsilon$

$\sum_{i,j} |\Delta\phi_{i,j}^{n+1}| < \epsilon \quad \dots(L_1 \text{ norm})$

$\left[\sum_{i,j} (\Delta\phi_{i,j}^{n+1})^2 \right]^{\frac{1}{2}} < \epsilon \quad \dots(L_2 \text{ norm})$

 14

There are many ways where you can use this epsilon to decide terminating a calculation. So, if you take a absolute, so that is what is given here as modulus of delta phi which is evaluated for the case of two-dimensional nodal location that is why it is subscript here i comma j and for the current level superscript n plus one is given. If the modulus of it is less than specified value, so one can specify error limit, say ten power minus five or ten power minus seven, some particular value for epsilon can be said, whenever you are doing such calculations. And once that difference delta phi at the current level n plus one and at all i comma j location is less than convergence limit of epsilon then you can say we can terminate calculation at that step and proceed the next stage.

There also other methods, for example, the first one I written here, it is also possible to write based on summation all the errors absolute errors and you say it is less than some value prescribed value and such as called L one norm or you take summation, you take a summation of the square all the error, so when you do square, there is no minus sign, automatically everything goes to positive and you take a summation over the entire domain and then you take a square root of it. And that also can be used as a criteria is less than prescribed value epsilon and such is called L 2 norm. And we will talk about

these convergence criteria later classes also with different explanation. So, convergence is also decided based on previous value and present value.

So, in today's class, we talked about numerical analysis, particularly consistency and convergence with some example. We will see you again with another important aspect of this numerical scheme.

Thank you.