

Introduction to Finite Volume Methods - II
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Lecture – 27
Temporal Discretisation – III

So welcome back to the lecture series of Finite Volume and we are in the middle of doing the transient formulation discretization and we have looked at couple of scheme. And now we look at the other transient formulation where we stopped in the last class; so we stopped with the Crank Nicholson forward.

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Unsteady discretization

Forward Euler, Backward Euler, CN

Adams - Moulton Scheme : $\phi(t-\Delta t), \phi(t-2\Delta t)$

$$\frac{\partial \phi(t)}{\partial t} = \frac{3\phi(t) - 4\phi(t-\Delta t) + \phi(t-2\Delta t)}{2\Delta t} \quad \leftarrow \text{2nd order expression.}$$

$$3(\rho_c \phi_c)^t - 4(\rho_c \phi_c)^{t-\Delta t} + (\rho_c \phi_c)^{t-2\Delta t} + L(\phi_c^t) = 0$$

$$\left(a_c^* + a_c \right) \phi_c^t + \sum_{F \in \text{faces}} a_F \phi_F^t = b_c^t - a_c^{t-\Delta t} \phi_c^{t-\Delta t} - a_c^{t-2\Delta t} \phi_c^{t-2\Delta t}$$

$$a_c^* = \frac{3\rho_c V_c}{2\Delta t}, \quad a_c^{t-\Delta t} = -\frac{2\rho_c^{t-\Delta t} V_c}{\Delta t}$$

$$a_c^{t-2\Delta t} = \frac{\rho_c^{t-2\Delta t} V_c}{2\Delta t} > 0 \quad \Rightarrow \text{stable.}$$

So, what we have looked at is forward Euler backward Euler Crank Nicolson; out of that Crank Nicolson is second order accurate now we look at another second order accurate scheme which is Adams Moulton scheme. So, that also uses the value at t minus delta t and value at t minus 2 delta t.

So, it uses the value from 2 step ahead of the present value. So, once we equate them to find out the derivative first derivative of the variable. So, that is written as t minus 4 phi t minus delta t plus phi t minus 2 delta t divided by 2 delta t; which gives a second order expression.

Now once we substitute that the thing become $\rho_c \phi_c(t - 4\Delta t) + \rho_c \phi_c(t - 2\Delta t) + \rho_c \phi_c(t - \Delta t) + \rho_c \phi_c(t) + \rho_c \phi_c(t + \Delta t) + \rho_c \phi_c(t + 2\Delta t) + \rho_c \phi_c(t + 4\Delta t) = 0$. Now once you form the algebraic equation this will give a ϕ_c at time level $t + \Delta t$ plus $FNBC$ a F ϕ_c at time level $t - \Delta t$ plus $a_c \phi_c(t - \Delta t) + a_c \phi_c(t) + a_c \phi_c(t + \Delta t) = 0$; where a_c is $3\rho_c V_c$ by $2\Delta t$; a_c equals to $\frac{3\rho_c V_c}{2\Delta t}$; $a_c \phi_c(t - \Delta t)$ equals to $\frac{3\rho_c V_c}{2\Delta t} \phi_c(t - \Delta t)$.

So, it is also very much clear this guy has a positive sign which is also positive implying that an increase in this value would lead to a decrease of ϕ_c . So, this scheme can be mitigated by the large coefficient of this one which has the right influence; that is the scheme is also a stable scheme. And it is not bounded with any unphysical oscillation which can be expected in certain circumstances.

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Unsteady discretization

In Finite Volume Approach

$t - \frac{\Delta t}{2}$ to $t + \frac{\Delta t}{2}$

$t + \Delta t/2$

$\int_{t-\Delta t/2}^{t+\Delta t/2} \frac{\partial(\rho_c \phi_c)}{\partial t} V_c dt$

Term I

$+ \int_{t-\Delta t/2}^{t+\Delta t/2} L(\phi_c) dt = 0$

Term II

$V_c = C \Delta t$

$V_c (\rho_c \phi_c)^{t+\Delta t} - V_c (\rho_c \phi_c)^{t-\Delta t} + L(\phi_c^t) \Delta t = 0$

Element (temporal domain)

$\phi(x_c, t + \delta t) = \phi_c^{t+\Delta t}$

$\phi(x_c, t) = \phi_c^t$

$\phi(x_c, t - \delta t) = \phi_c^{t-\Delta t}$

$L(\phi^t)$

δt

Element in transient domain

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So, now once we look at these things we can look at the similar implementation in terms of ϕ_c ; so these are the element, so that implementation in finite volume approach; so, which will be written in terms of those coefficients; so this is an element in transient domain, so it shows the schematic of element in the transient domain. So, you have this is the difference from this to this is Δt ; we have the special operator and then these elements are in the temporal domain, how they move along that. Now the transient term it will be

the discretization in final volume system would be similar to the convection term except now the integration is carried over the i mean time.

So, if we integrate over $t - \frac{\Delta t}{2}$ to $t + \frac{\Delta t}{2}$; then what we get that $t - \frac{\Delta t}{2}$ to $t + \frac{\Delta t}{2}$ $\rho_c \phi_c V_c dt$ plus $t - \frac{\Delta t}{2}$ to $t + \frac{\Delta t}{2}$ $L \phi_c dt$ equals to 0. So, this is a term II, this is term I. Now here V_c is treated as constant when time integration is done. So, term I can be turned into a difference of face fluxes and term II can be evaluated as a volume integral using the midpoint rule. So, the semi discretized equation will look like $V_c \rho_c \phi_c t + \frac{\Delta t}{2} - V_c \rho_c \phi_c t - \frac{\Delta t}{2} + L \phi_c t \frac{\Delta t}{2}$ equals to 0; so, that is the expression for semi discretized equation.

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Unsteady discretization

$$\frac{(\rho_c \phi_c)^{t+\frac{\Delta t}{2}} - (\rho_c \phi_c)^{t-\frac{\Delta t}{2}}}{\Delta t} V_c + L(\phi_c^t) = 0 \quad \begin{matrix} t-\frac{\Delta t}{2} & - & t+\frac{\Delta t}{2} \\ t, & t-\Delta t. \end{matrix}$$


$$\text{Flux}_T = \text{Flux}_c^t \phi_c^t + \text{Flux}_c^{\frac{t+\Delta t}{2}} \phi_c^{\frac{t+\Delta t}{2}} + \text{Flux}_V^t$$

$$a_c^t \leftarrow a_c^t + \text{Flux}_c^t$$

$$b_c^t \leftarrow b_c^t - \text{Flux}_c^{\frac{t+\Delta t}{2}} \phi_c^{\frac{t+\Delta t}{2}} - \text{Flux}_V^t$$

1st order Explicit Euler Scheme

$$\frac{(\rho_c \phi_c)^{t+\Delta t} - (\rho_c \phi_c)^t}{\Delta t} V_c + L(\phi_c^t) = 0 \quad \left\{ \begin{array}{l} (\rho_c \phi_c)^{t-\Delta t} = (\rho_c \phi_c)^{t-\Delta t} \\ \text{Flux}_c^+ = \frac{\rho_c^+ V_c}{\Delta t} \\ \text{Flux}_c^{t-\Delta t} = -\frac{\rho_c^{t-\Delta t} V_c}{\Delta t} \\ \text{Flux}_V^t = 0 \end{array} \right.$$


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Now, one can write in a slightly different format by 2 minus $\rho_c \phi_c t - \frac{\Delta t}{2}$ by 2 ; $\Delta t V_c$ plus $L \phi_c t$ equals to 0. Now to derive the full discretized equation the interpolation profile which is equating the face values between this time $t - \frac{\Delta t}{2}$ by 2 to $t + \frac{\Delta t}{2}$ by 2 . So, information of the current time level previous time level and these are required. So, the choice will obviously affect the accuracy and the robustness of the method.

So, in this context it would be important to note that the integration of the spatial operator is second order in time, but the accuracy of the operator itself is determined by the option used in discretization. So, independent of the profile used the flux could be

linearized as the total flux is flux c ϕ c plus flux c ϕ c t minus Δt this is at present time level. So, this would be t minus Δt t plus flux V at present time level. So, with the linearization completed the coefficient of the algebraic equations can be obtained like a c plus flux c and like the time instant; if you consider then b c t could be b c t minus flux c t minus Δt t ϕ c t minus Δt t minus flux V at t .

So, that is a kind of a interpolation; now what we can look at the first order Euler implicit Euler scheme. So, transient term discretization will lead to this, but it is a first order interpolation. So, what one can do that you can have a stencil of 1 D stencil and I can write $\rho c \phi c t$ plus Δt by 2 equals to $\rho c \phi c t$ and $\rho c \phi c t$ minus Δt by 2 equals to $\rho c \phi c t$ minus Δt .

So, just using this current and previous time iteration then my equation system would become t minus $\rho c \phi c$; t minus Δt divided by Δt $V c$ plus $L \phi c t$ is 0; where one can see the flux c is ρc ; $V c$ by Δt which is at the current time level; flux $c t$ minus Δt is minus $\rho c t$ minus Δt $V c$ by Δt and flux V at current time level is 0.

So, this is a first order implicit Euler discretization and so; obviously, when there will be a first order scheme it will associated with numerical diffusion.

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Unsteady discretization

Numerical Diffusion

$$(\phi_c)^{t-\Delta t} = (\phi_c)^t - \frac{\partial(\phi_c)}{\partial t} \Big|_t \Delta t + \frac{\partial^2(\phi_c)}{\partial t^2} \Big|_t \frac{\Delta t^2}{2!}$$

$$\frac{(\phi_c)^t - (\phi_c)^{t-\Delta t}}{\Delta t} = \frac{\partial(\phi_c)}{\partial t} \Big|_t - \underbrace{\left(\frac{\Delta t}{2} \frac{\partial^2(\phi_c)}{\partial t^2} \Big|_t \right)}_{\text{Numerical diffusion term}} - O(\Delta t^2)$$

$$\frac{\partial(\phi_c)}{\partial t} \Big|_t + \frac{1}{V_c} L(\phi_c^t) = \underbrace{\left(\frac{\Delta t}{2} \frac{\partial^2(\phi_c)}{\partial t^2} \Big|_t \right)}_{\text{Numerical Diffusion}} + O(\Delta t^2)$$

1st order Explicit Euler scheme

$$\frac{(\rho_c \phi_c)^{t+\Delta t} - (\rho_c \phi_c)^t}{\Delta t} V_c + L(\phi_c^t) = 0$$

$$\text{Flux } C^t = \frac{\rho_c^t V_c}{\Delta t}$$

$$\text{Flux } C^{t-\Delta t} = -\frac{\rho_c^{t-\Delta t} V_c}{\Delta t}$$

$$\text{Flux } V^t = 0$$

And one can estimate that like the quantity of the numerical diffusion. So, that can be obtained from the expression of rho phi at t minus delta t. So, if you use an Taylor series expression for this and it is like rho phi t minus del del t of rho phi at t delta t plus del 2 by del 2 by rho phi t; t delta t square by factorial 2 like that. And then if you rearrange the term minus rho phi t minus delta t by delta t its gets you rho phi at t minus delta t by 2; del 2 rho phi by del t 2 at t which is numerical diffusion term.

So, this is coming from transient discretization; now if you put this things back in the discretized equation, the discretized equation will get modified like $1 + V_c L \Delta t$ equals to $\frac{\Delta t}{2} \frac{\partial^2 \rho \phi}{\partial x^2}$; which is the numerical diffusion plus order of Δt^2 . So, now, in effect a numerical diffusion term is kind of added to the equation and that scales with the time step in a similar fashion to the upwind scheme of the advection term. So, while the scheme is unconditionally stable the solution it still yields is really a stationary solution for large time steps.

Now, similarly you can find out first order explicit Euler scheme. So, there the equation will become like $\rho_c \phi_c$ and $t + \Delta t$ minus $\rho_c \phi_c$ divided by Δt ; V_c plus $L \phi_c$ equals to 0, which will also lead to the first order scheme. And the linearized coefficients like flux c at t is Δt flux at t minus Δt is minus $\rho_c \phi_c$ minus $\Delta t V_c$ and flux V is 0.

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Unsteady discretization

Numerical Anti-diffusion

$$\frac{\partial(\rho\phi)}{\partial x} \Big|_t + \frac{1}{V_c} L(\rho_c^t) - \underbrace{\left(\frac{\Delta t}{2} \frac{\partial^2(\rho\phi)}{\partial x^2} \right) \Big|_t}_{\text{Numerical Anti-diffusion}} + O(\Delta t^2)$$

CN


$$(\rho_c \phi_c)^{t+\Delta t} = \frac{1}{2} (\rho_c \phi_c)^{t+\Delta t} + \frac{1}{2} (\rho_c \phi_c)^t$$

$$(\rho_c \phi_c)^{t-\Delta t} = \frac{1}{2} (\rho_c \phi_c)^t + \frac{1}{2} (\rho_c \phi_c)^{t-\Delta t}$$

$$\frac{(\rho_c \phi_c)^{t+\Delta t} - (\rho_c \phi_c)^{t-\Delta t}}{2\Delta t} + L(\rho_c^t) = 0$$

$$\text{Flux } c^t = \frac{\rho_c^t V_c}{2\Delta t} \quad \text{Flux } V^t = - \frac{\rho_c^{t-2\Delta t} V_c}{2\Delta t} \phi_c^{t-2\Delta t}$$

$$\text{Flux } c^{t+\Delta t} = 0$$



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So, again this is written in terms; similarly like the, so the numerical anti diffusion that comes from when we actually expand these term in the using Taylor series and express this.

So, the equation which becomes like $\frac{\partial}{\partial t} \rho \phi$ at $t + \Delta t$ by V_c equals to $\frac{\partial}{\partial t} \rho \phi$ by Δt ; $\frac{\partial^2 \rho \phi}{\partial x^2} \Delta t^2$ which is the numerical anti diffusion term plus order of Δt^2 square; so, this is the term which gets added to the system. Now the second order differential term has the negative sign; so which will lead to a negative diffusion or anti diffusion, so which compresses the effects on profile and very similar to that downwind scheme in convective flows.

This anti diffusion timescales with the time step; so, when used in combination with the upwind convection scheme and a Courant number of 1, one can show that the numerical diffusion of these convection scheme and the numerical anti diffusion of the explicit Euler for a CFL equals to 1 are of equal magnitudes and of opposite sign.

So, they cancel each other and produce in L_n exact solution, but nevertheless this is not a practical as ensuring a CFL criteria for convection to 1. And another problem which may arise due to this anti diffusion is the numerical instability; so which can be increasing with Δt . So, that can put a strong restriction on your Δt option.

Now similarly one can talk about the Crank Nicholson's scheme. So Crank Nicholson's scheme now if you have a uniform time step; so that can be written as $\rho_c \phi_c(t + \frac{\Delta t}{2})$ expressed as half of $\rho_c \phi_c(t + \Delta t)$ plus half of $\rho_c \phi_c(t)$ and $\rho_c \phi_c(t - \frac{\Delta t}{2})$ is written as half of $\rho_c \phi_c(t)$ minus half of $\rho_c \phi_c(t - \Delta t)$.

Now, this once we put in the semi discretized equation; it will become $(t + \Delta t) \rho_c \phi_c(t + \Delta t) - \rho_c \phi_c(t) - \Delta t \frac{\partial}{\partial x} (\rho_c \phi_c)$ plus $L \rho_c \phi_c(t) = 0$. Here the flux is $\rho_c V_c$; $\frac{\partial}{\partial x} (\rho_c \phi_c)$ by Δt flux $\rho_c \phi_c(t) - \rho_c \phi_c(t - \Delta t)$ is 0, but the flux V at t is minus $\rho_c \phi_c(t) - \rho_c \phi_c(t - \Delta t)$ by Δt . So, that is how it gets modified and the, if you carry out the accuracy the numerical accuracy of the scheme would be.

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Unsteady discretization

$$\frac{\partial(\rho\phi)}{\partial t} \Big|_t + \frac{1}{V_c} L(\phi_c^t) = - \frac{\partial^3(\rho\phi)}{\partial t^3} \Big|_t \frac{\Delta t^2}{6} + O(\Delta t^3)$$


dispersion error

Second Order Upwind Euler (SOUE) scheme

$$\left. \begin{aligned} (\rho_c \phi_c)^{t+\Delta t} &= \frac{3}{2} (\rho_c \phi_c)^t - \frac{1}{2} (\rho_c \phi_c)^{t-\Delta t} \\ (\rho_c \phi_c)^{t-\Delta t} &= \frac{3}{2} (\rho_c \phi_c)^{t-\Delta t} - \frac{1}{2} (\rho_c \phi_c)^{t-2\Delta t} \end{aligned} \right\}$$

$$3(\rho_c \phi_c)^t - 4(\rho_c \phi_c)^{t-\Delta t} + (\rho_c \phi_c)^{t-2\Delta t} + L(\phi_c^t) = 0$$

$$\text{Flux}_c^t = \frac{3\rho_c^t V_c}{2\Delta t}, \quad \text{Flux}_c^{t-\Delta t} = -\frac{2\rho_c^{t-\Delta t} V_c}{2\Delta t}, \quad \text{Flux}_c^{t-2\Delta t} = \frac{\rho_c^{t-2\Delta t} V_c}{2\Delta t}$$


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So, once you use the Taylor series expansion and carry out this the modified equation for this guy will become plus 1 by V c phi c t minus del 3 rho phi; t delta 2 square by 6 order of delta t 3; so that is the modified equation.

So, essentially one has to just use the Taylor series expansion in the previous equation. So, here just use the Taylor series expansion and get the modified equation as we have done earlier and the modified equation will look like that. Now what it confirms that it is also a second order scheme, but it returns a third order derivative with a negative sign; this also can lead to some sort of an instability and this is the dispersion error and it can lead to some instability to the system.

Now one can have a second order upwind Euler. So, this is second order upwind Euler which second order upwind Euler scheme. So, it would be the again look like an it is going to be the scheme where the value what you approximate at rho c; phi c, t plus delta t by 2 equals to 3 by 2 rho c phi c t minus half rho c phi c t minus delta t. And the other term t minus delta 2 by is 3 by 2 rho c phi c t minus delta t minus half rho c phi c t minus 2 delta t.

And this once we put it back in the semi discretized equation; this will look like an 3 rho c phi c t minus 4 rho c phi c t minus delta t plus rho c phi c t minus 2 delta t divided by 2 delta t plus operator phi c t equals to 0; which is a implicit second order Euler scheme and this scheme is also stable independent of time step. So, which now if you linearize

the coefficients the coefficients; if you linearize then it gets you the flux at time level t is $3 \rho c V c$ by Δt and flux at previous level which is $t - \Delta t$ would be $2 \rho c$ by Δt .

And flux V at this time instant would be ρc ; $t - 2 \Delta t$ $V c$ by $2 \Delta t$ and also this will have $\phi c - 2 \Delta t$. And same thing for this particular scheme one actually can do the Taylor series expansion.

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Unsteady discretization

$$\frac{(p\phi)^{t-\Delta t} - (p\phi)^{t-2\Delta t}}{2\Delta t} = \frac{\partial(p\phi)}{\partial t} \Big|_t - \frac{\partial^2(p\phi)}{\partial t^2} \Big|_t \frac{\Delta t^2}{3} + O(\Delta t^3)$$

$$\frac{\partial(p\phi)}{\partial t} \Big|_t + \frac{1}{Vc} L(\phi_c^t) = \frac{\partial^2(p\phi)}{\partial t^2} \Big|_t \frac{\Delta t^2}{3} + O(\Delta t^3)$$

Initial Condition


$$\phi_c^{t_i + \frac{\Delta t}{2}}, \phi_c^{t_i}$$

t_i initial time

at the boundary

$$\frac{(\rho_c \phi_c)^{t_i + \frac{\Delta t}{2}} - (\rho_c \phi_c)^{t_i}}{\Delta t} Vc + L(\phi_c^{t_i + \frac{\Delta t}{2}}) = 0$$

$\rho\phi$ at $t_i + \frac{\Delta t}{2}$ & $t_i + \frac{\Delta t}{2}$


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Like each term $\rho \phi$ $t - \Delta t$; one can get the Taylor series expansion. Similarly $\rho \phi$ $t - 2 \Delta t$ you once you get that then if you put $3 \rho \phi$ $t - 4 \rho \phi$ $t - \Delta t$ plus $\rho \phi$ $t - 2 \Delta t$ divided by $2 \Delta t$ equals to $\frac{\partial^2 \rho \phi}{\partial t^2}$ at t $\frac{\Delta t^2}{3}$ minus Δt cube.

And if you recover the original equation; so the equation that we are solving for that gets modified like 1 by Vc ; ϕc at t equals to $\frac{\partial^3 \rho \phi}{\partial t^3}$ by $\frac{\Delta t^3}{3}$ plus Δt cube. So, it also does not have any; so here is the third order derivative which sits there. So, this is also does not have any diffusion, but it it does have some dispersion error.

So, see third order derivative term will actually return you back the dispersion error. Now there are some issue which are like initial condition because we are doing all transient case. So, the solution has to start with a some initial; I mean implementation of this transient discretization in finite volume framework is state forward; except for some

initial time step. And the first temporal element which is essentially at the boundary ; it does not have an upwind neighbor.

So, rather the value at the lower element face is used directly at the face and resulting a gradient that is half the correct numerical value. So, this comes about because it is computed as difference between the values of $\phi_c; t_i + \Delta t/2$ and between $\phi_c; t_i$ which are kind of a difference between 2 time steps and so that happens with the initializations of the system. So, this easily can be demonstrated by considering the first temporal element in the discretized equation.

Let us say if you consider the first order Euler the equation looks $\rho_c \phi_c; t_i$; t_i is the initial time plus $\Delta t/2$ minus $\rho_c \phi_c; t_i$ you get by Δt multiplied with V_c plus $L \phi_c$ at $t_i + \Delta t/2$. So, the first temporal element the upwind interpolation yields a gradient; a computed as a difference between $\rho_c \phi_c$ as $t_i + \Delta t/2$ and t_i divided by Δt .

However, case for the regular element the gradient is actually between $\rho_c \phi_c$ at $t_i + \Delta t/2$; $3 \Delta t/2$ and $t_i + \Delta t/2$ which is divided by Δt . So, we will stop here today and we will take from here in the follow up lectures.

Thank you.