Laboratório Nacional de Energia e Geologia, I.P.
UNIDADE DE ENERGIAS RENOVÁVEIS E INTEGRAÇÃO DE SISTEMAS DE ENERGIA

Differential Equations and Courant Number

Relatório Interno

Margarida Giestas

LNEG June/July 2019

DifferentialEquationsandCourantNumber Systems of Differential Equations Numerical Integration Methods

Stability and Convergence Courant Number

A short study

June/July 2019

Summary

The considerations presented in this report result from the analysis performed in the context of the project NewSol.

Even if it is not pertinent to the development of the work, they were needed to obtain a correct modelling.

While modeling is being done, a theoretical support was carried on.

To give support to the chosen method, or going in some direction, several methods were presented for comparison.

Conteúdo

1.Diferential Equations

1.1. Definitions

A partial differential equation (EDP) is a relation *L* which interviews are the independent variables $(x, y, \dots)$ an unknown function of these variables, $u\,(x, y, \dots)$, and the partial derivations of the function:

$$u\left(u_x, u_y, \dots, u_{xx}, u_{xy} \dots .\right);$$

$$L\left(x, y, , , , u, u_x, u_y, \dots, u_{xx}, u_{xy} \dots\right) = 0 \qquad (1)$$

$$u_x = \frac{\partial u}{\partial x} \qquad\qquad u_{xx} = \frac{\partial_u^2}{\partial_x^2}$$

Definition: By order of an EDP one means the order the order of the higher, derivate that appears in that equation.

1.1.1 Initial and boundary conditions

Considering the independent variables $(x, y, \dots)$ in a domain $\Omega \subset R^n$ the objective is to find if the functions $u\,(x, y, \dots)$ satisfy (1) identically in Ω: these functions are the solutions of the equation.

According Hadamard rules a *"well posed problem"* must always satisfy three points:

- Existence of solution.
- Unicity of solution. It is a necessity that results from the determinism on which most physical explanations rest. The same causes always produce the same effects.
- Continuous dependency from solution relatively to initial and/or boundary and other parameters of the problem. In practice, errors occur in measurement processes. For the mathematical model to be cautious about those errors, it is necessary that the "small" variations in the data correspond to "small" variations in the solution.

The initial conditions also called Cauchy conditions are imposed at an $t = t_0$

Boundary condition are imposed over the value of the function, or its derivatives.

In a part Γ of a domain Ω, called boundary, or in a part of it.

Considering a solution *u* defined in a domain Ω, the boundary conditions are classified as:

- Dirichlet Conditions: Occur when the value of the solution *u* of the problem is fixed in the boundary Γ of the domain Ω.
- Neumann Conditions: occur when the solution *u* derivation is imposed in the boundary of the domain.
- Mixed Conditions (also called Robin Conditions): result when there are a) and b) conditions at the same time.

The classical methods of analysis allow developing satisfactorily the theory of the equations with partial derivatives of first order. However, were the methods of functional analysis that allowed to develop the correct formulation of classical analysis. (formulating his theory only in the linear case).

1.2. Classification of EDP

The modeling of the problems of physics are based on the second order differential equations, an act by which it is sufficient to consider the classification of the EDP for the case of the quasi-linear equation of second order given by:

$$au_{xx} + bu_{xy} + cu_{yy} = l \qquad (3)$$

With *a, b, c* and *l* functions of $x, y,. u_x , u_y$.

The fact of consider a second order equation does not seem restrictive being this hypothesis easily generalized.

Now the problem consists in finding the sufficient conditions to u, u_x and u_y always given to satisfy in a unique u_{xx}, u_{xy}, u_{yy} with the objective of satisfy (3).

If these derivations exist, it becomes:

$$du_x = u_{xx}dx + u_{xy}dy$$
$$du_y = u_{xy}dx + u_{yy}dy$$

From this system and equation (3) it becomes

$$\begin{bmatrix} a & b & c \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix} = \begin{bmatrix} l \\ du_x \\ du_y \end{bmatrix}$$

The solution for u_{xx}, u_{xy}, u_{yy} exists and is unique, if and only if, the determinant of the matrix of this system is nonzero, that is

$$a(dy)^2 - b(dy)(dx) + c(dx)^2 \neq 0$$

Otherwise, one obtains:

$$a\left(\frac{dy}{dx}\right)^2 - b\left(\frac{dy}{dx}\right) + c = 0$$

That have solutions real and different or complex according to the signal of $b^2 - 4ac$
This is also the criteria for EDP classification. The equation (3) is of the type:

- Hyperbolic if $b^2 - 4ac > 0$
- Parabolic if $b^2 - 4ac = 0$
- Elliptic if $b^2 - 4ac < 0$

This definition is extended to an equation of second order with n variables.

1.3. General Definition

If u is a function of **n** independent variables, the linear equations to partial derivations of second order become:

$$\sum_{i=1}^{n} a_i(x_1 \dots, x_n)\frac{\partial_u^2}{\partial x_i^2} + \sum_{i=1}^{n} b_i(x_1 \dots, x_n)\frac{\partial u}{\partial x_i} + c(x_1 \dots, x_n)u + c(x_1 \dots, x_n) = 0$$

Then

- If all the coefficients a_i are nonzero and from the same signal, the partial equation is said to be elliptic.
- If all the coefficients a_i are nonzero and from the same signal, with only one exception, the equation is said to be of the hyperbolic type.
- If only one of the coefficients a_i (designated by a_{i0}) is nonzero, and all the others are of the same signal, with a_{i0} nonzero, the equation is parabolic.

Considering differential operators of second order of type done by:

$$L = \sum_{i,j=n}^{n} a_{ij}(x_1, \dots, x_n)\frac{\partial^2}{\partial_{x_i}\partial_{x_j}} \qquad (4)$$

With a_{ij} a symmetric matrix that is $a_{ij} = a_{j_i}$ for all i j=1

The operator (4) is classified, at the point $x = (x_1, \dots x_n)$ accordingly the symmetric matrix a_{ij}.

So the operator is:

- Elliptic if the matrix (a_{ij}) is defined positive at the point x.
- Parabolic if the matrix (a_{ij}) has a zero determinant at the point x.
- Hyperbolic if the matrix (a_{ij}) is negative defined at the point x.

This definition say that well posed problems arise:

- For elliptic equations (for example potential equation) with the addition of boundary conditions.
- For hyperbolic equations (for example vibrant string) with the addition of initial conditions and boundary conditions.
- For parabolic equations (equation of heat diffusion) with the addition of initial and boundary conditions.

1.4. Physics Problems

Most of the problems of Physics and Engineering are classified in problems of balance, problems of eigenvalues or problems of propagation.

An example of the first is Laplace Equation that represents the stationary state of temperature in an isotropic mean and at two dimensions is:

$$u_{xx} + u_{yy} = 0$$

As examples of eigenvalues, problems there are stability problems there are problems of structures or resonance in electric circuits and acoustic.

Propagation problems analyses de time evolution of a certain phenomenon from an initial known

time (initial state).

The objective is to solve a differential equation:

$$L[\phi] = 0$$

Subjected to an initial condition and to a set of boundary conditions defined in a boundary Γ of the domain Ω.

Mathematically speaking propagation problems are problems of initial value and are described by equations of the parabolic or hyperbolic type.

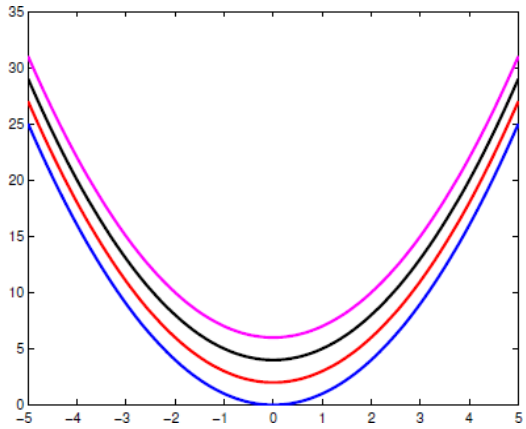
1.4.1. Parabolic Equations in Physics

These equations are of the form $\boldsymbol{u_t = L[u]}$ with L a differential operator of second order.

It can be the case of

$$\boldsymbol{u_t = \nabla.[f\ \nabla\ u]}$$

Where f can be or constant, or spatial function, or function of u or $\nabla\ \mathrm{u}$.



The Heat Equation

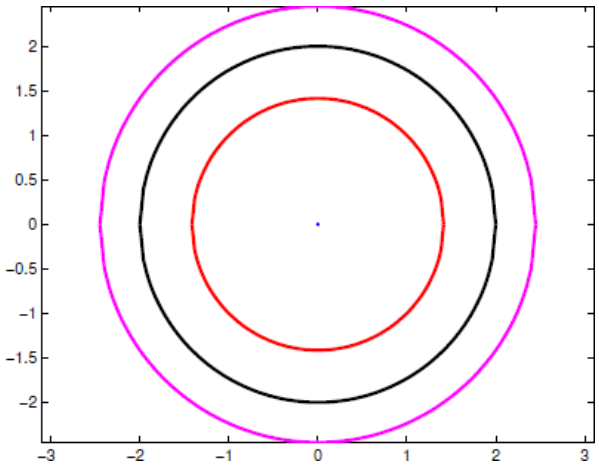
$$u_t - u_{xx} = 0$$

1.4.2. Hyperbolic Equations in Physics

The wave propagation is the example most known of this type of equation:

$$u_{tt} - u_{xx} = 0$$

While the solution of a boundary value problem depends on the values across the boundary, (equilibrium problems) in the case of a propagation problem, the solution at a given interior point of the domain may depend only on the conditions of a part of the boundary.



Poisson equation: $u_{xx} + u_{yy} = f$

1.5. Partial Differential Equations

(The Navier Stokes System)

1.5.1Compressible and incompressible flows

1. Compressible flows:

The mass conservation is a transport equation for density. With an additional Energy equation, *p* can be specified from a thermodynamic relation (ideal gas law)

2. Incompressible flows:

Density variation is not linked to the pressure. The mass conservation is a Constraint on the velocity field; this equation (combined with the momentum) is used to derive an equation for the pressure.

1.5.2. Stokes Set of Equations Escreva uma equação aqui.

Conservation of mass:

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho v_i)}{\partial x_i} = 0$$

Conservation of momentum:

$$\frac{\partial(\rho v_i)}{\partial t} + \frac{\partial(\rho v_j v_i)}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_j}$$

Conservation of energy

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho v E)}{\partial x_j} = \partial_{x_j}\left(k\frac{\partial T}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\tau_{ij} v_i)$$

$$\tau_{ij} = \mu\left[\frac{\partial(v_i)}{\partial x_j} + \frac{\partial(\rho v_j)}{\partial x_i} - \frac{2}{3}\frac{\partial v_k}{\partial k}\right]$$

In 3D we have 5 equations and 6 unknowns: *p*, ρ, *vi*, *E(T)*

so for supplemental information we need the equation of state.

NS equations are considered the appropriate conceptual model for flows. However, they contain three major approximations:

1) Continuum hypothesis
2) Form of the diffusive fluxes
3) Equation of state

Simplified conceptual model can be derived introducing additional assumptions: incompressible flow.

a) Conservation of mass: continuity:
b) Conservation of momentum.

As difficulties there are non-linearity, coupling role of pressure.

The continuity equation is combined with the momentum and the divergence-free constraint becoming an elliptic equation for the pressure:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial x_i}\right) = \frac{\partial}{\partial x_i}\left[\partial\left(\rho\frac{\partial v_i v_j}{\partial x_j}\right)\right]$$

The possible methods to solve these are SIMPLE, SIMPLEC and PISO.

2.Numerical Models

Turbulent flow is a type of fluid flow in which the fluid undergoes irregular fluctuations, in contrast to laminar flow. In turbulent flows, the speed of the fluid at a point is continuously undergoing changes in both magnitude and direction.

To model turbulence, it is necessary to concern with an unsteady irregular motion in which transported quantities (mass, momentum, scalar properties) fluctuate in time and space. It is also necessary to consider fluid properties, velocity, and variations.

Energy transfer is performed from larger eddies to smaller eddies and in smallest eddies turbulent energy is converted to internal energy through viscous dissipation.

To model this kind of flows there are several types of numerical models.

The main classes of computational models approach for modeling turbulent flows are.

1 Reynolds-Averaged Navier-Stokes Models (RANS)
2 Large Eddy Simulation (LES)
3 Direct Numerical Simulation (DNS)

The first category, RANS, solves time-averaged N-S equations and allows all turbulent length scales. They are used in the case of industrial flows.

The second type of models, LES, solves spatially averaged N-S equations. Large eddies are directly solved and eddies smaller than the mesh is modeled. This category is less expensive than DNS but most expensive tan RANS.

DNS models can simulate all turbulent flows by numerically solve the full N-S equations. This process is not implemented in the dynamic numeric program FLUENT.

With the two first classes of models FLUENT presents several possible combinations of computational models:
Transition models- used to predict boundary layer development and calculate transition onset.

1 Coupling models.

2 Reynolds Stress Model (RSM).

3 Scale-Adaptive Simulation (SAS) Model Reynolds Averaged N-S Equations (RANS);

5 Detached Eddy Simulation (DES).

6 Near Wall Treatment for Wall Bounded Turbulent Flow

2.1. Reynolds -Averaged Navier Stokes (RANS) Equations

The Closure Problem: Boussinesq Approach versus Reynolds stress

Boussinesq Hypothesis (B-H) is applied by eddy viscosity models. Here Reynolds (Re) stresses is modeled using a turbulent (or eddy) viscosity. This Hypothesis is used in Spalart-Allmaras Model (one equation), and all k-ε and k-ω models (two equations).

- The disadvantage is that this hypothesis assumes the viscosity to be an isotropic quantity, which is not strictly true. The B-H works well for shear flows dominated by Re of the turbulent shear stresses which covers wall boundary layers, mixing layers, round jets and channel flows.
- RANS with Reynolds stresses requires modeling for many terms in the transport

equations.

- The only advantage is in the presence of turbulent flow with large streamline curvature and swirl, being more difficult to converge.

2.2. k-ε Turbulence Models

These models, when a nonzero gravity and temperature gradient are simultaneously present, account for the generation of k due to buoyancy and the corresponding contribution to the production of ε.

In transport equation for k turbulent kinetic energy for k tends to be augmented in unstable stratification. For stable stratification, buoyancy tends to suppress the turbulence.

In ANSYS, the effects of buoyancy on the generation of k are always included when considering both a nonzero gravity and a nonzero temperature or density gradient.

There are three differences in the k-ε models:

- the calculating method of turbulent viscosity.
- the Prandtl numbers that are present in k and ε;
- The generation and destruction of terms in equation in ε.

Convective Heat and Mass Transfer Modeling uses an analogy to turbulent momentum transfer. Energy equation may have additional terms depending on the underlying physical model.

2.3. Standard k-ε (SKE) Models (Launder and Spalding)

(SKE) model is the most used model for industrial applications. It is robust and accurate. Contains sub models for compressibility, buoyancy combustion among other.

Limitations

- One term of ε equation cannot be calculated at the wall.
- The performance for flows with strong separation is poor.

2.3.1 Renormalization k-ε (RNG) Models

Equations are derived using the statistical technique called renormalization group theory. It is more accurate than SKE model, for more complex shear flows and flows with high strain rates swirl and separation.

- RNG has an additional term in the equation in ε that improves the accuracy for strain flows.
- Re effect on turbulence is induced enhancing accuracy for swirling flows.
- Differential viscosity to account for low Re effects.
- Analytically derived algebraic formula for turbulent Prandtl number.

2.3.2 Swirl Modification k-ε (RNG) Model

This model is applied when turbulence is affected by rotation or swirl in the mean flow.

RNG provides an option to account for the effects of the swirl or rotation by modifying the turbulent viscosity appropriately. This model is applicable to asymmetrical swirling flows and 3D flows when RNG is chosen. The principal difference between RNG and SKE is in the fourth term in ε equation. RNG models yields a lower turbulence viscosity than SKE.

2.3.3. Realizable k-ε Model

The term realizable means that the model satisfies certain mathematical constrains on the Re stresses, consistent with the physics of turbulent flows: positivity of normal stresses and Schwarz inequality for Re shear stresses. This model contains an alternative formulation for the turbulent viscosity. In the equation of transport, the fourth term represents better the spectral energy transfer and the third term does not have a singularity as in previous models. It has a modified transport equation for the dissipation rate ε, which has been derived from an exact equation for the transport of the mean square vorticity equation.

Limitations:

- Produces non-physical turbulent viscosities in situations when the computation domain contains both rotating and stationary fluid zones. This is due to the fact of this model includes the effects of mean rotation in the definition of the turbulent viscosity.
- This extra rotation effect has a behavior that must be taken in account.
- Turbulent viscosity is modeled in a different way being not a constant.

Advantages:

- Predicts more accurately the spreading rate of both planar and round jets.
- Also, provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation.

2.4. k-ω Turbulence Models

In this class, there are Standard, (BSL)-Baseline, and (SST)-Shear Transfer models.

All of them have similar transport equations for k and ω. Turbulence damping is available only in with k- ω models.

The k- ω of turbulent models have gained popularity mainly because:

- The model equations do not contain terms which are undefined at the wall that is they can be integrated to the wall without using wall functions.
- They are accurate and robust for a wide range of boundary layer flows with pressure gradient.

k- ω of turbulent models are divided in:

2.4.1 Standard k- ω (SKW) model

- Most adopted in the aerospace and turbo-machinery problems Compressibility effects, transitional flow and shear flows corrections.

2.4.2 (SSTKW) model (Mentor)

- The SST k- ω model uses a blending function to gradually transition from the SKW near the wall to a high Re number version of the k-ε model in the outer portion of the boundary layer:
- Contains a modified turbulent viscosity formulation to account for the transport effects of the principal turbulent shear stress.

2.4.3. Standard k-ω (SKW) Model (Wilcox)

This model, based on Wilcox formulation, incorporates modifications for low Re numbers of effects compressibility and shear flow spreading.

The weak points of the model are the sensitivity of the solutions to values for k and ω outside the shear layer.

It is also an empirical model based on model transport equation for the turbulence kinetic energy k and the specific dissipation rate ω (That is ε/k).

2.4.4. Baseline (BSL) k-ω Model (Mentor)

The main problem with the Wilcox model is its well-known strong sensitivity to free stream conditions. The BSL model designed by Mentor, was developed to blend the robust and accurate formulation of the k-ω model, in the near wall region within the free stream independence of the k-ε model in the far field. So, k-ε was converted in k-ω formulation.

This model is similar to Standard but includes some refinements.

- Model constants are different.
- Standard k-ω model and transformed k-ε model are both multiplied by a blending function and both models are added together.
- BSL incorporates a damped cross diffusion derivative term in ω equation.

2.4.5. Shear Stress Transport (SST) k-ω Model

This model includes the refinements of the BSL k-ω model and accounts for the transport of the turbulence shear stress in the definition of the turbulent viscosities. The model is more accurate for a class of flows like adverse pressure gradient flows, airfoils transonic shock waves than the standard and the BSL k-ω models.

These models are considered the most important for the work performed dealing directly with Navier-Stokes PDE and Energy Equation. Regarding that, the remaining models that are at the disposal of ANSYS in Fluent will be not subject of attention.

3.Numerical methods of solution

Partial Differential Equations can describe almost all set of things that goes from Nature until Economics, Biomedicine, Physics, Chemistry or even the. Rules of the Human Mind cannot be solved in an analytic way. Only by approximations and there we have several methods from which Galerkin Method must be one of the most known.

Navier-Stokes equations is the set of partial differential equations that describe the behavior of flows.

In most of the cases when the solution is known partials equations are solved by a numerical way.

If we knew the solution of the problem and used it as the first guess of the numerical solver the solution would preserve equal to the initial guess. Moreover, if we introduced a small perturbation over this solution, "perturbation amplitudes would decrease" as time went on if the background flow was stable and the numerical solver was implicit - this stability criteria is obtained from a linear stability analysis and therefore it should be carefully applied to non-linear problems. On the other hand, perturbation amplitudes would increase if an explicit scheme were employed.

The following section present some numerical schemes of integration applied by numerical solvers related to variables suitable to appear in the referred PDE.

4.Procedure to solve Navier-stokes PDEs and Energy Equation

The set of governing transport equations is solved through finite volume element method using software (ANSYS® 17.1). The Initialization method was computed from inlet zone. The solution method was a PISO algorithm coupled with a Pressure Velocity scheme. Pressure, momentum turbulent kinetic energy and time, are discretized by a second order upwind and together with. Presto scheme. This one was necessary to be applied to pressure. These procedures are explained in the next section. Turbulence dissipation rate is discretized by a first order upwind scheme iterations at each time step ended when the dimensionless residual for all equations dropped below 10-5 (accuracy convergence). The solution problem run with double precision. The domain of simulation here studied was first discretized, for ranges of 50,000; 74,000; 92000 cells (mesh). The programmed time-schedule for charge and discharge cycles in a 2D tank. Is defined for a day and have a charge and a discharge that will be not subject of study in this report.

4.1. PISO Algoritm

Momentum equations connects velocity components with pressure gradient; Mass equation, is a constraint on the velocity field calculation.

The PISO algorithm consists in two phases:

1º- predict the velocity that must be computed using the momentum equation where the pressure term is explicitly treated through a time-step solution.

This time step is the "Momentum Predictor" and doesn´t satisfy the free-divergence condition.

2º- Then a "Pressure based" based in mass equation is join to the process and solved.

The pressure field obtained is used to correct the predicted velocity achieving the divergence condition.

For Pressure

4.1.1.The power-law discretization scheme.

Interpolates the face value of a variable using the exact solution to a one-dimensional convection diffusion equation.

4.1.2. The linear scheme

Computes the face pressure as the average of the pressure values in the adjacent cells.

4.1.3. Least Squares and Green Gauss Node Based scheme

Is the most accurate (least squares are slightly cheaper than. Node based).

Is least accurate but much cheaper than least squares. The pressure interpolation scheme is applicable only to the pressure-based solver.

4.1.3. Second order pressure scheme

This method is generally the best. It reconstructs the face pressure in the manner used for second-order accurate convection terms. This scheme may provide some improvement over the standard and linear schemes, but it may have some trouble If it is used at the start of a calculation and/or with a bad mesh. The second-order scheme is not applicable for flows with discontinuous pressure gradients imposed by the presence of a porous medium in the domain

or the use of the VOF or mixture model for multiphase flow.

4.2.PRESTO! (PREssure STaggering Option) scheme

PRESTO! (PREssure STaggering Option) scheme uses the discrete continuity balance for a "staggered" control volume about the face to compute the "staggered" (i.e., face) pressure. This procedure is similar in spirit to the staggered-grid schemes used with structured meshes. Note that for triangular, tetrahedral, hybrid, and polyhedral meshes, comparable accuracy, is obtained using a similar algorithm. The PRESTO! Scheme is available for all meshes PRESTO scheme is the preferred scheme.

For advective fluxes:

4.2.1.First order upwind scheme

First order upwind is the least accurate in terms of order, but generally the most stable. It is used when equations are prone to numerical instabilities.

When first-order accuracy is desired, quantities at cell faces are determined by assuming that the cell-center values of any field variable represent a cell-average value and hold throughout the entire cell; the face quantities are identical to the cell quantities.

Thus, when first-order up winding is selected, the face value is set equal to the cell-center value of in the upstream cell.

4.2.2. Second order upwind scheme

Second order upwind is much more accurate than first order but has stability issues. However, a first order scheme can have better absolute accuracy than a second order scheme. The order of convergence for a second order scheme is obtained via a loss of absolute accuracy (higher order of accuracy but errors are caused by numerical wiggles). When second-order accuracy is desired, quantities at cell faces are computed using a multidimensional linear reconstruction approach. In this approach, higher-order accuracy is achieved, at cell faces through a Taylor series expansion of the cell-centered solution about the cell centroid. The second-order formulation requires the determination of a gradient in each cell.

4.2.3. QUICK scheme

QUICK is 3rd order accurate for face values and 2nd order accurate for cell values on a hexahedral grid. For non-hexahedral cells. In general, the accuracy of QUICK is similar or slightly better than 2nd order upwind.

4.2.4. The power law scheme

The power law scheme uses the exact power law solution to the advection-diffusion equation to interpolate values. It would be exact on an advection-diffusion problem, but Navier-Stokes is more complicated than simple advection-diffusion.

The power-law scheme is only slightly better than 1st order and is not as accurate as second order and other schemes when all types of flow scenarios are considered.

4.2.3. MUSCL scheme

The Third order MUSCL scheme can be interpreted as a generalization of the QUICK scheme for arbitrary grids (QUICK only works for hexahedral grids). The drawback is the gradient limiter does not work for MUSCL, and this scheme is prone to more pronounced overshoots and undershoots (these limiters do work for second order and QUICK). QUICK and MUSCL schemes. To use these schemes properly requires a high-quality grid so some serious commitments are need to get reasonable results, with these two schemes. There is just very little gain for the cost in effort.

5.Stability and convergence

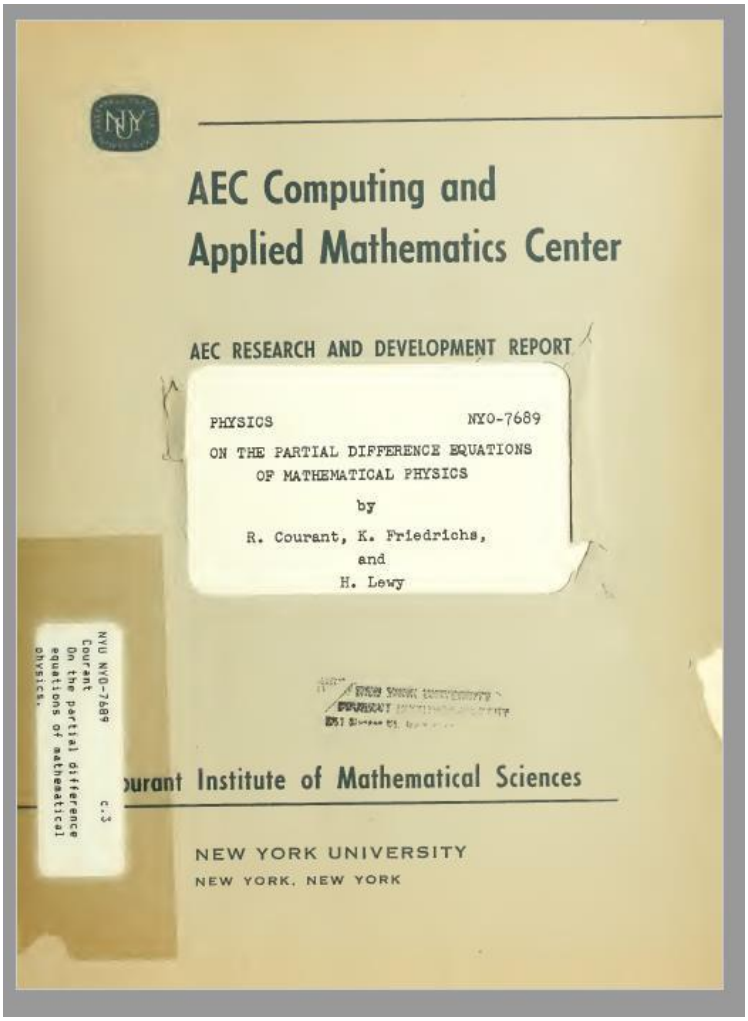
For a transient problem, the solution is obtain changing from one to next time step. In the successive substitution approach, the coupling terms will be evaluated, from the currently available solution.

If the solution changes abruptly in time, successive substitution does not guarantee convergence. This fact is not related to the explicit/implicit character of the numerical scheme. A small Courant number and relaxing the equations would help to stabilize the numerical solution.

For a typical weakly compressible (incompressible or weakly compressible flows) the best method depends on whether you want highest accuracy or cheapest computation or some optimal in-between.

5.1. Courant – Friedrich-Lewy condition

In mathematics, the (CFL) condition is a necessary condition for convergence while solving certain partial differential equations (usually hyperbolic PDEs) numerically.



It arises in the numerical analysis of explicit time-marching computer simulations otherwise the simulation produce incorrect results.

The condition named after Richard Courant Kurt Friedrichs and Hans Lewy, who described it in their 1928 paper.

The principle behind the condition is that, for example, if a wave is moving across a discrete spatial grid and we want to compute its amplitude at discrete time steps of equal duration, then, this duration must be less than the time for the wave to travel to adjacent grid points.

As a corollary, when the grid point separation is reduced the upper limit for the time step also decreases.

In essence the numerical domain of dependence of any point in space and time (as determined by initial conditions and the parameters of the approximation scheme) must include the

analytical domain of dependence (where in the in the initial conditions influence the exact value of the solution at that point).

This is to assure that the scheme can access the information required to form the solution.

5.1.2One-Dimensional case

In this case, the CFL has the form:

$$C = \frac{x\,\Delta t}{\Delta x} < C_{max}$$

C means Courant number.

X magnitude of the velocity (whose dimensions is length/time)

Δt the time step (time)

Δx *lenght interval* (Length)

The value of C_{max} changes with the method used to solve the discretized equation, especially depending on whether the method is explicit or implicit.

If an explicit solver is used (time-marching) than $C_{max} = 1$.

Explicit solvers are less sensitive to numerical instability and so larger values of C_{max} may be tolerated.

5.1.3.Two and general n-dimensional case:

Two-dimensional case CFL becomes:

$$C = \frac{u_x\,\Delta t}{\Delta x} + \frac{u_y\,\Delta t}{\Delta y} \leq C_{max}$$

5.1.4. General case

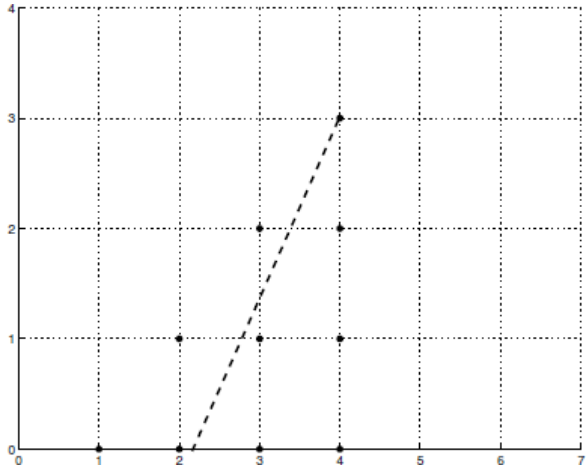
$$C = \Delta t\left(\sum_{i=1}^{n} \frac{u_{x_i}}{\Delta_{x_i}}\right) \leq C_{max}$$

The interval length is not required to be the same for each spatial variable Δ_{x_i} This degree of freedom can be used to somewhat optimize the value of the time step for a particular problem by varying the values of the different interval to keep it not too small.

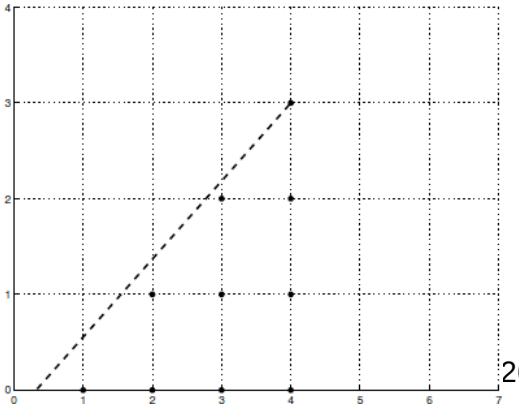
The CFL condition is a necessary condition for the convergence of a finite approximation of a hyperbolic problem.

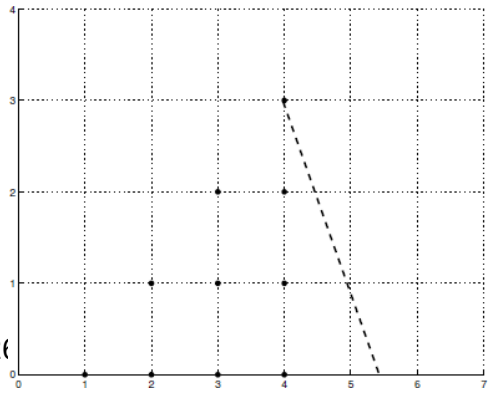
According CFL condition to a convergent scheme the domain of dependence of a PDE must lie within the domain of dependence of the numerical method. (Numerical approximations)

In a very simple way, it must be represented by:



The dashed line represents a solution that is inside the domain of dependence. We have x in x-axes and t in y-axes the points marked in the chart represent the domain. This represents a first order equation of advection.





The schemes above don´t satisfy the CFL condition.

So, what is violated in CFL condition?

The exact solution *u (x, t)* depends on initial values $u_0(x_0)$ which is outside the numerical methods domain of dependence.

The numerical approximation to *u (x, t)* is "insensitive" to the value $u_0(x_0)$ which means that the method cannot be convergent.

CFL is only a necessary condition for convergence.

The great value of this number is its simplicity in helping to reject Finite Differences Schemes in hyperbolic problems with a very little investigation.

For example, considering:

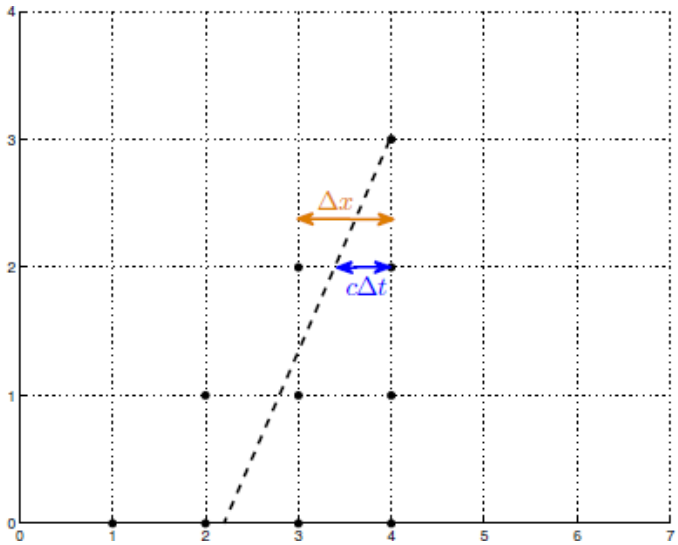
$$u_t + cu_x = 0$$

We must have c < 0 for convergence.

If c > 0 than it will be required that:

$$\mu \equiv \frac{c\Delta t}{\Delta x} \leq 1$$

For CFL be satisfied:



The scheme that satisfies this condition is upwind method according to c< 0 or c>0.

$$|v| \equiv \left|\frac{c\Delta t}{\Delta x}\right| \leq 1$$

The central difference method satisfies CFL satisfies CFL according the sign ( ) Therefore, we should pick a method to reflect the direction of propagation of information.
Hyperbolic equations were analysis in a very simple way. Other type of equations will have an analogous treatment and have no less meaning in what concern Courant Number.

6.Consistency

We say that a numerical scheme is consistent with a PDF if its truncation error tends to zero as $\Delta x, \Delta t \longrightarrow 0$

For example, any first or higher order scheme is consistent.

6.1Lax Milgram Theorem

(**Fundamental theorem in scientific computing**)

For a consistent finite difference approximation to a linear evolutionary problem, the stability of the scheme is necessary and sufficient for convergence.

The theorem refers to linear evolutionary analysis that is hyperbolic or parabolic PDES.

7.Performed work

In what follows we consider a 2D tank and present some results of the obtained meshes.

7.1The problem

The problem takes place in a tank where a fluid (molten salt) enters from an inlet to mix with a porous mean (filler) that is at rest inside (the tank) and at a lower temperature of the fluid.

This moisture contributes to a difference of position of the particles inside the tank generating a gradient of temperature called thermocline. The bottom tends to be warm and the temperature stored in the filler particles will be removed throughout an outlet to be transformed. This is a simpler way to describe a molten porous thermocline with a simple (not structured mesh) geometry.

The Thermal Storage Tank with this characteristic has movements of conduction and turbulence inside and thermal fluxes at the boundaries.

This type of problem is described by a PDE set of transfer equations of momentum mass and energy. Each set of PDE equations, is written according to 2D or 3D and has a set of boundary and initial conditions. The model chosen to solve it is a RANS model that can be a k-ε Turbulence Models or a k-ω Turbulence Model. SST k-ω turbulence Model was proposed in this specific problem to give account to the wall effects.

The employed mesh to solve the problem was structured and had into account the Courant Number to avoid numerical instability.

A Courant number is the criteria, like Péclet number where the program decides if the flow and heat equations is calculated in each cell. It governs the rate of information transfer between the cells.

According to the CFL expression:

$$CFL = \frac{U\Delta T}{\Delta x}$$

These criteria will select the time step ΔT to adopted regarding the constructed mesh. To make the best of this formula is chosen, keeping the constraint in Courant number since the mass flow rate inside the tank is fixed hence the velocity.

Most numerical simulation methods like Finite Element Method (FEM) requires stabilization procedures when modeling transport applications.

In these problems numerical instabilities can occur, when approaching the solution, leading eventually to oscillations. Courant number or Péclet number relates the convective and diffusive

effects together with the mesh element size through the no dimensional number CFL or Pe. Pe deals with convection, which is not the case of CFL.

Pe >1 numerical instability can occur as convective effects dominate diffusive activity.

Pe<<1 is diffusion that dominates the process (which is not the case in a thermocline with filler)

The stabilization methods allow the construction of coarser meshes capable to simulate with enough accuracy all physic properties derived from the convective and diffusive phenomena leading to a more robust and faster computational performance.

The governing transport equations were solved through finite volume element method using software ANSYS. The Initialization method chosen was the standard initialization, and the solution was computed from the inlet zone. The solution method was a PISO algorithm coupled with a Pressure Velocity scheme.

Pressure, momentum turbulent kinetic energy, and time were discretized by a second order upwind scheme. Turbulence dissipation rate was discretized by a first order upwind scheme

iterations at each time step ended when the dimensionless residual for all equations dropped below 10^{-3}. The solution problem was obtained with double precision. The domain of simulation here studied, was discretized into 55,000 cells (the mesh).

7.2. Global view

The presented topics in a very simpler way, can be related to show how they are connected to real problems.

The geometry is not subject of this report. However, the mesh relates to the model choose to solve the problem. The numerical schemes for integration of the variables for instances pressures and advection fluxes must be choose with care.

7.3.Meshes for a thermocline 2D

The mesh much obey to certain properties related with the CFL Courant number to have stability in the integration. This fact can conduct to smaller step sizes which is computer time consumer and must be avoid.

To do this mesh must be well done, tested and obey to the parameters of orthogonality, skewness and aspect ratio that indicates what a good mesh is. These parameters vary from domain and accordingly 2D or 3D domain and could be analyzed when the mesh is produced. Is better to lose time doing and testing meshes than after having a program that each run takes more than four days to calculate five real hours. Indicators of a mesh whether it is a good or a bad mesh.

Minimum Orthogonal Quality	ranges from 0 to 1, where values close to 0 correspond to low quality
Maximum Ortho Skew	ranges from 0 to 1, where values close 1 correspond to low quality
Maximum Aspect ratio	where values close to 1 correspond to high quality

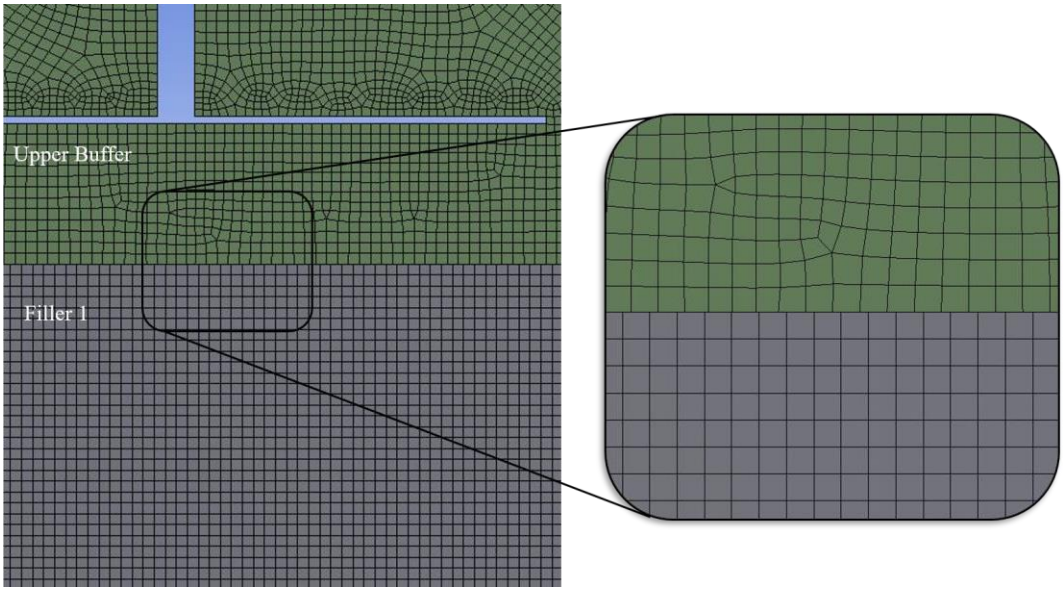
One point to have in mind is that the difference of cells dimensions should not be very big. If that is the case it could result a good mesh but the Courant number (CFL) is very large implying to have a very small step size to achieve convergence.

7.4. Problems with meshes.

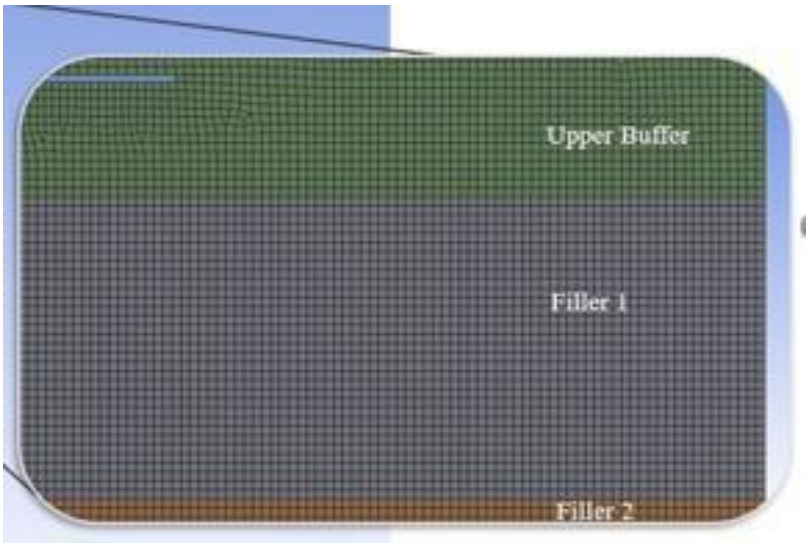
There are some problems to solve concerning mesh quality.

7.4.1. Conformal mesh

A less good mesh can result from several things. The boundaries between cell zones are not identical. So it is not possible to the flow to have a continuously dislocation. The following type of meshes are non-conformal.



In the case of non-conformal mesh the results of an integration are not very realistic. There is a more effort to the part of the fluid to go from one cell zone to another that makes simulation time to increase. When this occur, it is necessary to convert the mesh in a conformal one.

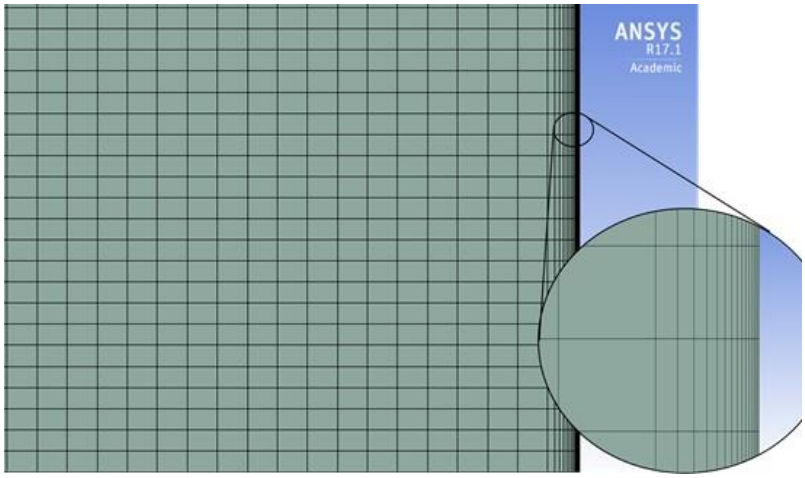


Conformal mesh

Now cell boundaries are continuous between cell zones. This quality of mesh will improve all the performance of the simulation. The fluid do not have a big resistance to pass and a higher time step can be used.

7.4.2. Inflation

The SST k-ω Turbulence Model uses a specific function at the wall to deal with stability An inflation near the wall is proposed to better analyze adverse fluxes and thus instabilities.



The figure shows the effect of the inflation near the wall.

In the transient case, a slight problem arises due to such imposition. The ratio of the sides of cells tends to decrease closing to the boundary of the tank wall, making the aspect ratio to increase drastically. This affects the quality of the mesh and so the mesh size. In terms of time-step, the result hugely decreases to a range of 0.005s. It would be impractical to simulate a daily cycle with this time-step.

Therefore, a compromise could be achieved with y+ values. This number accounts for stability near walls. Although the inflation is removed, and y+ does not show too many abnormal values considered values near the walls can be taken into to account.

To overcome it the more obvious solution is not to use inflation with the method but a smaller cells size in the mesh.

References

ANSYS 16, ANSYS 17.1 manual (turbulence methods and meshes)

Introduction to Conputational PDES Hans De Sterck, Paul Ulrich

http://fluent-time-step-size-transient-implicit-solver

Numerical solution of ordinary and Partial Differential Equations L. Fox. Macmillan (Pergamon), New York, 1962

Partial Differential Equations of Parabolic Type. Prentice Hall Inc., A. Friedman Englewood Cliffs, N.J. 1964

R. Courant, K. Friedrichs and H. Lewy. *On the Partial Difference equations of Mathematical Physics*. AEC computing and Applied Center, N.Y U-7689

Newsol Project (720985). Implementation and validation tests for fluent case 0. Victor Seram, Margarida Giestas, Pedro Azevedo, 2018.