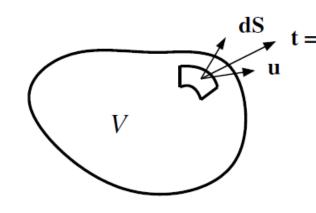
#### Conservation Equations of Compressible Flows

(Integral Form)



$$T = -pI + \tau$$

Stokes: 
$$\mathbf{\tau} = \mathbf{T} \cdot \mathbf{n}$$
Cauchy Stress Tensor:  $\mathbf{T} = -p\mathbf{I} + \mathbf{\tau}$ 
Stokes:  $\mathbf{\tau} = -\frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} + \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ 

Fourier heat flux:  $\mathbf{q} = -\kappa \nabla T$ 

$$\mathbf{q} = -\kappa \nabla T$$

Mass:

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_{V} \rho \mathrm{dV} + \int_{S} \rho \mathbf{u} \cdot \mathrm{d}\mathbf{S} = 0$$

Momentum (**f** body forces):

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} \rho \mathbf{u} \mathrm{d}V + \int_{S} \rho \mathbf{u} (\mathbf{u} \cdot \mathrm{d}\mathbf{S}) = \int_{V} \rho \mathbf{f} \mathrm{d}V - \int_{S} \mathbf{T} \cdot \mathrm{d}\mathbf{S}$$

Energy (Q heat sources):

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} \rho E \mathrm{dV} + \int_{S} \rho E \mathbf{u} \cdot \mathrm{d}\mathbf{S} = \int_{S} \mathbf{u} \mathbf{T} \cdot \mathrm{d}\mathbf{S} + \int_{V} \rho \mathbf{f} \cdot \mathbf{u} \mathrm{dV} - \int_{S} \mathbf{q} \cdot \mathrm{d}\mathbf{S} + \int_{V} \rho Q \mathrm{dV}$$

## Navier-Stokes Egns for Compressible Flows

(Differential Form)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) = -\nabla \rho + \nabla \cdot (\boldsymbol{\tau}) + \mathbf{f}$$

Energy: 
$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = -\nabla \cdot (\rho \mathbf{u}) + \nabla \cdot (\mathbf{u} \boldsymbol{\tau} - \mathbf{q}) + \rho(\mathbf{f} \cdot \mathbf{u}) + \rho Q$$

**Boundary Conditions:** *no-slip* on wall, ....

#### **Constitutive Laws:**

Stokes Viscous stress: 
$$\boldsymbol{\tau} = -\frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} + \mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{T}\right)$$

$$E = e + \frac{\mathbf{u}^2}{2}$$

$$p = R\rho T$$

$$e = c_v T$$

constant specific heat

$$\mathbf{q} = -\kappa \nabla T$$

## 4A2: Euler Equations in 2D: $\mu=0$ and $\kappa=0$

Mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0 ,$$

Momentum:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} = -\frac{\partial p}{\partial x} ,$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} = -\frac{\partial p}{\partial y} ,$$

Energy:

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial\left((\rho E + p)u\right)}{\partial x} + \frac{\partial\left((\rho E + p)v\right)}{\partial y} = 0.$$

**Boundary Conditions:** *slip* on wall, ....

Ideal gas:

$$p = R\rho T$$

Polytropic gas:

$$e = c_v T$$

constant specific heat

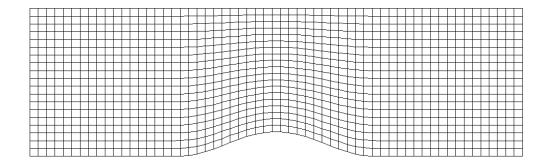
Speed of Sound:

$$a^2 = \frac{\gamma p}{\rho} = \gamma RT$$

#### What is CFD?

CFD is the art of replacing the integral or the differential derivatives in the governing equations with discetized algebraic forms.

First step: discretization of the physical domain



Test 0 : mesh for subsonic flow over bump

Differential equation: finite-difference

Integral equation : finite-volume

Weak formulation : finite-element

Finite Difference Methods (solving differential equations by approximating them with difference equations, in which finite differences approximate the derivatives). For example,

$$\frac{df}{dt} \approx \frac{f(t + \Delta t) - f(t)}{\Delta t}$$

Finite Volume Methods (based on conservation laws. Volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, popular in Fluid Mechanics, especially with hyperbolic equations).

$$\int_{\Omega} 
abla \cdot oldsymbol{q} dV = \int_{\partial \Omega} oldsymbol{q} doldsymbol{S}$$

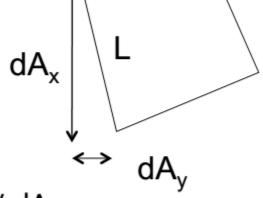
The method has the important physical property that certain conservation laws are maintained.

• Finite Element methods are based on weak form of PDE, require a lot of maths (module 3D7)

## Conservation Laws and Finite Volume method

$$Vol\frac{\Delta\rho[?]}{\Delta t} = \sum_{cvs} Flux$$

## Where for edge L:



$$Flux_{mass} = m = \rho V.dA = \rho V_x dA_x + \rho V_y dA_y$$

Flux<sub>mom</sub> = mu = (
$$\rho$$
 V.dA)V  
or  
Flux<sub>x,mom</sub> = ( $\rho$  V<sub>x</sub>dA<sub>x</sub> +  $\rho$  V<sub>y</sub>dA<sub>y</sub>)V<sub>x</sub> + P dA<sub>x</sub>  $\epsilon$   
Flux<sub>y,mom</sub> = ( $\rho$  V<sub>x</sub>dA<sub>x</sub> +  $\rho$  V<sub>y</sub>dA<sub>y</sub>)V<sub>y</sub> + P dA<sub>y</sub>

Flux + Pressure Source -> Strong Conservation Eqn.

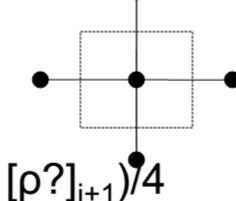
## FINITE VOLUME METHOD

Flux<sub>enthalpy</sub> = 
$$mh_o$$
 =  $(\rho V.dA)h_o$   
or  
Flux<sub>enthalpy</sub> =  $(\rho V_x dA_x + \rho V_y dA_y)h_o$ 

For the RHS terms we have taken a differential eqn and solved it by summing around a control volume – this is the FINITE VOLUME METHOD

## SMOOTHING -> STABILITY

Averaging surrounding data



$$[\rho?]_{i} = ([\rho?]_{i-1} + [\rho?]_{i+1} + [\rho?]_{j-1} + [\rho?]_{j+1})^{7}4$$
(II)

Discrete equivalent of

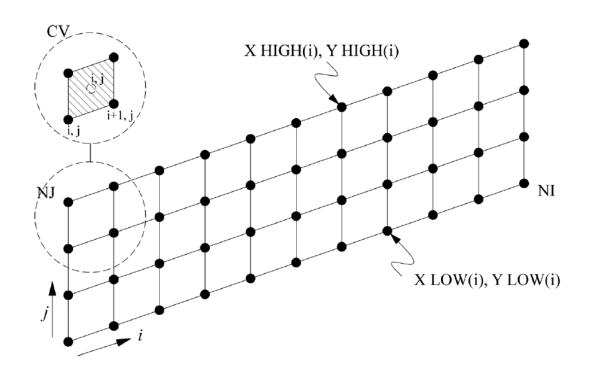
$$\nabla^2 \left[ \rho? \right] = \frac{\partial^2 \left[ \rho? \right]}{\partial x^2} + \frac{\partial^2 \left[ \rho? \right]}{\partial y^2}$$

# Writing the basic solver Pt 1

Tom Hynes

## Task at Hand

Solve for  $\, 
ho, \rho V_x, \rho V_y, \rho E \,$  where  $\, E = c_v T + \frac{1}{2} V^2 \,$ 



## **Initial Calls**

```
program euler
call read_data
call generate_grid
call check_grid
call crude_guess !flow_guess
call set_timestep
```

## Main Loop Calls

```
do nstep = 1,nsteps
 ro_start = ro
 call set others
 call apply_bconds
 call set fluxes
 call sum fluxes
 ro = ro start + ro inc
 call smooth
 call check_conv
end do
```

## Read Data

Need to be able to get information into our program – geometry and flow data

Geometry from file test0\_geom, and flow from file test0\_flow

Geometry (Define the shape of the computational domain): NI, NJ, xhigh(NI), yhigh(NI), xlow(NI), ylow(NI)

Flow (Fluid properties and boundary conditions): R,  $\gamma$ , CFL, NSTEPS,  $P_{0,IN}$ ,  $T_{0,IN}$ ,  $P_{OUT}$ ,  $\alpha$ 

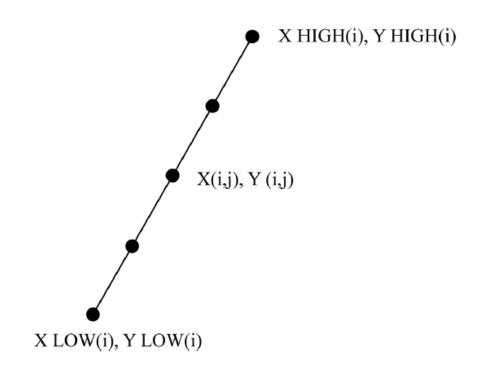
```
-bash-4.2$ more test0_flow
287.1 1.4
100000. 300. 00.0 85000.
0.50 0.50
3000 _0.0001
```

Can use FORTRAN's free-format READ command:

```
READ(2,*) RGAS,GAMMA
READ(2,*) PSTAGIN,TSTAGIN,ALPHA1,PDOWN
```

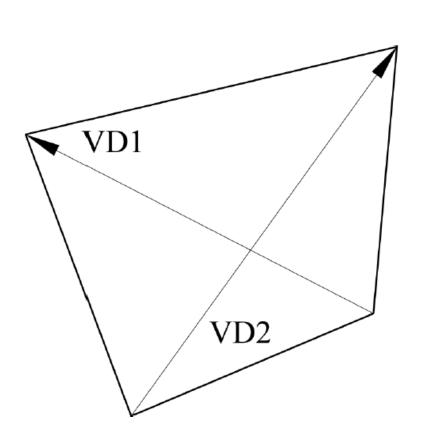
## Generate Grid

First thing GENERATE\_GRID does is interpolate X(NI,NJ), Y(NI,NJ) from XHIGH(NI), YHIGH(NI), XLOW(NI), XHIGH(NI)



## Generate Grid

GENERATE\_GRID also computes the volume (to unit depth) of the control volumes



$$\overrightarrow{A} = \frac{1}{2} \left( \overrightarrow{VD_2} \times \overrightarrow{VD_1} \right)$$

$$\overrightarrow{VD_1} = a_1 \overrightarrow{i} + b_1 \overrightarrow{j}$$

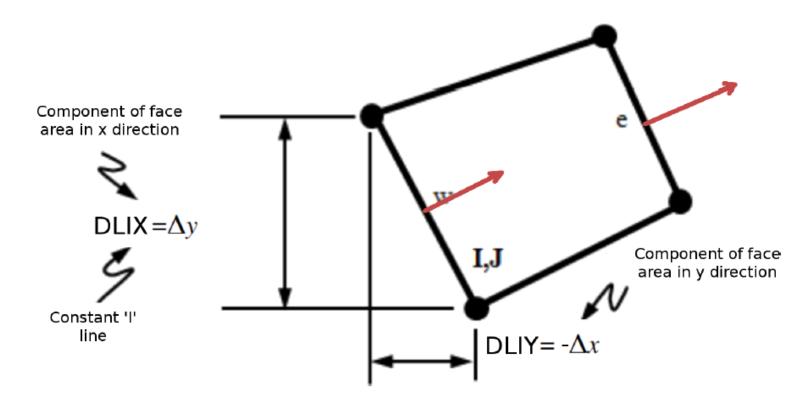
$$\overrightarrow{VD_2} = a_2 \overrightarrow{i} + b_2 \overrightarrow{j}$$

$$A1 = X(I,J+1) - X(I+1,J)$$
  
 $B1 = Y(I,J+1) - Y(I+1,J)$ 

$$A2 = X(I+1,J+1) - X(I,J)$$
  
 $B2 = Y(I+1,J+1) - Y(I,J)$ 

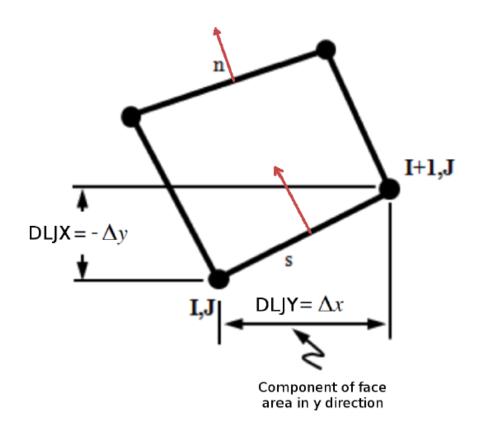
## Generate grid

GENERATE\_GRID also computes the face areas (per unit depth) of the control volumes



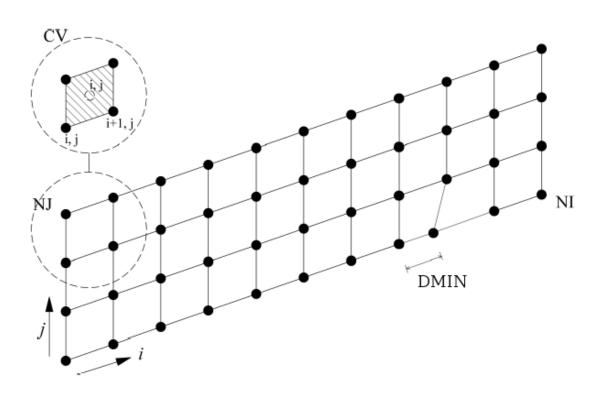
## Generate Grid

GENERATE\_GRID also computes the face areas (per unit depth) of the control volumes



## Generate Grid

GENERATE\_GRID also computes the minimum distance between any two grid points



## Check Grid

If the grid is wrong, nothing else will work properly!

Subroutine check\_grid carries out some tests on your grid to make sure things are right

First – check all the areas (control volumes) are positive

Second – check vectorial sum of control volume faces is effectively zero

```
IF (abs(totx).GT.small_number) THEN
WRITE(6,*) 'X-Grid Not Zero! '
STOP
ENDIF
IF (abs(toty).GT.small_number) THEN
WRITE(6,*) 'Y-Grid Not Zero! '
STOP
ENDIF
```

## Set Time Step

The Courant-Freidrichs-Lewy (CFL) number is defined by information movement:

$$CFL = \frac{\Delta t |\Lambda_{max}|}{\Delta x_{min}}$$

Largest eigenvalue of flux jacobian:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial \mathbf{Q}} \frac{\partial \mathbf{Q}}{\partial x} = 0$$

For the 2D Euler equations, these are:

$$|u|, |u|, |u+a|, |u-a|$$

Max eigenvalue is the forward running acoustic wave

## Set Time Step

Need to estimate the speed of the forward running acoustic wave:

$$|\Lambda_{max}| = |u + a|$$

For subsonic flows, can estimate u pessimistically as the speed of sound:

$$u = a = \sqrt{\gamma R T_0}$$

The CFL number is read from the flow file

Smallest grid spacing is calculated in GENERATE\_GRID as variable DMIN

So:

## Set Others

The SET\_OTHERS subroutine calculates useful secondary variables from the four conserved ones:  $\rho, \rho v_x, \rho v_y, \rho E \rightarrow v_x, v_y, p, h_0$ 

$$v_x = \frac{\rho v_x}{\rho}$$

$$v_y = \frac{\rho v_y}{\rho}$$

$$p = (\gamma - 1) \left(\rho E - \frac{1}{2}\rho V^2\right)$$

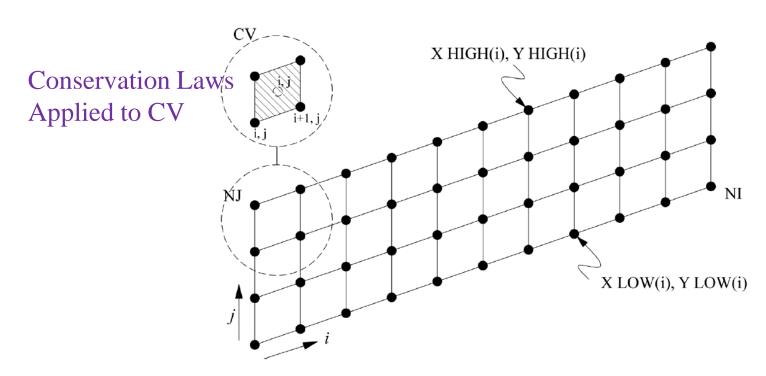
$$h_0 = \frac{\rho E + p}{\rho}$$

There are many ways to compute these variables – this is just a suggestion

## Time-Dependent Euler Solver for Compressible Flows

## Task at Hand

Solve for  $\rho, \rho V_x, \rho V_y, \rho E$  where  $E = c_v T + \frac{1}{2} V^2$  Conservative Variables defined at Cell Vertices

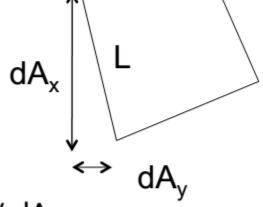


Get Your Hand "Dirty"

## Conservation Laws and Finite Volume method

$$Vol\frac{\Delta\rho[?]}{\Delta t} = \sum_{cvs} Flux$$

## Where for edge L:



$$Flux_{mass} = m = \rho V.dA = \rho V_x dA_x + \rho V_y dA_y$$

Flux<sub>mom</sub> = mu = (
$$\rho$$
 V.dA)V  
or  
Flux<sub>x,mom</sub> = ( $\rho$  V<sub>x</sub>dA<sub>x</sub> +  $\rho$  V<sub>y</sub>dA<sub>y</sub>)V<sub>x</sub> + P dA<sub>x</sub>  $\swarrow$   
Flux<sub>y,mom</sub> = ( $\rho$  V<sub>x</sub>dA<sub>x</sub> +  $\rho$  V<sub>y</sub>dA<sub>y</sub>)V<sub>y</sub> + P dA<sub>y</sub>

Flux + Pressure Source -> Strong Conservation Eqn.

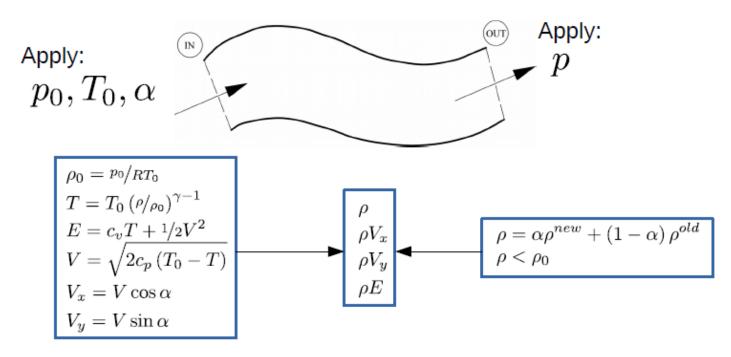
## FINITE VOLUME METHOD

Flux<sub>enthalpy</sub> = 
$$mh_o$$
 =  $(\rho V.dA)h_o$   
or  
Flux<sub>enthalpy</sub> =  $(\rho V_x dA_x + \rho V_y dA_y)h_o$ 

For the RHS terms we have taken a differential eqn and solved it by summing around a control volume – this is the FINITE VOLUME METHOD

## **Apply Boundary Conditions**

The APPLY\_BCONDS subroutine enforces the specified boundary conditions at the inflow and outflow to the domain



Wall boundary conditions are applied implicitly by preventing flux through surfaces where J=1 or J=NJ

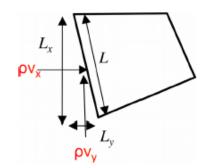
## Set Fluxes

The SET\_FLUXES subroutine computes  ${f F}_{\phi}\cdot{f n}$  for the four Euler equations

#### For i fluxes:

```
FLUXI_PHI(I,J) = 0.5*(ROVX(I,J)+ROVX(I,J+1))*0.5*(PHI(I,J)+PHI(I,J+1))*DLIX(I,J) + 0.5*(ROVY(I,J)+ROVY(I,J+1))*0.5*(PHI(I,J)+PHI(I,J+1))*DLIY(I,J) + 0.5*(SOURCE(I,J)+SOURCE(I,J+1))
```

Conserved Variable	Ф	Source Term
Mass	1	0 – no mass source
x-Momentum	$V_{x}$	pδx – pressure term
y-Momentum	$V_y$	pδy – pressure term
Energy	$h_0$	0 – no internal generation



Similar expressions apply in j

## Sum Fluxes

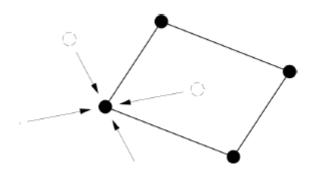
The SUM\_FLUXES subroutine accumulates the fluxes into and out of each control volume, updates the solution, and scatters data to the vertices

$$\Delta \phi = \frac{\Delta t}{\Delta V} \sum_{CV} \left( \mathbf{F}_{\phi} \cdot \mathbf{n} \right)$$

 $del_prop(i,j) = (deltat/area(i,j))*(iflux(i,j) - iflux(i+1.j) + jflux(i,j)-jflux(i,j+1))$ 

## Sum Fluxes

 $del_prop(i,j) = (deltat/area(i,j))*(iflux(i,j) - iflux(i+1.j) + jflux(i,j)-jflux(i,j+1))$ 



Solution stored at vertices, so the change at each is averaged from surrounding control volumes

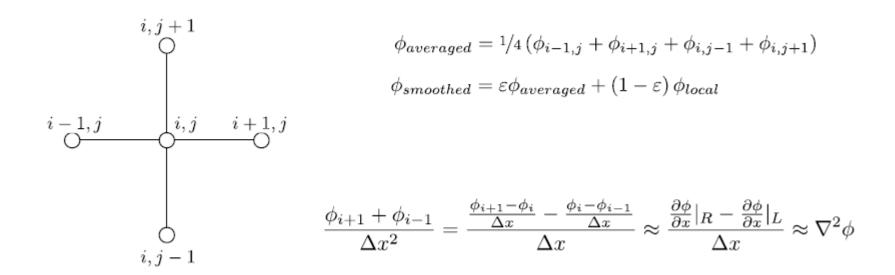
Numeric Trick:

Variable Changes calculated at Cell Centres Interpolate to Anywhere you want

prop\_inc(i,j) =

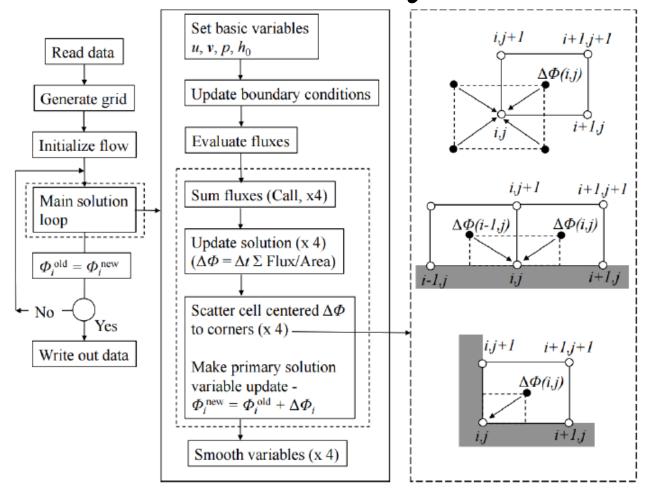
## Smooth

The SMOOTH subroutine smooths the conserved variable fields using their averages from surrounding vertices

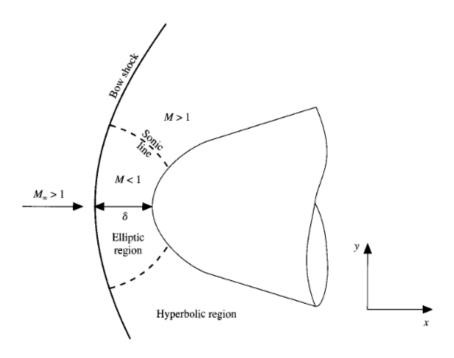


Careful thought needed for smoothing behaviour near the boundaries

Equivalent to add a viscosity (diffusion) term Artificial (numeric) viscosity Summary



## Steady Solutions & Time-Marching Methods

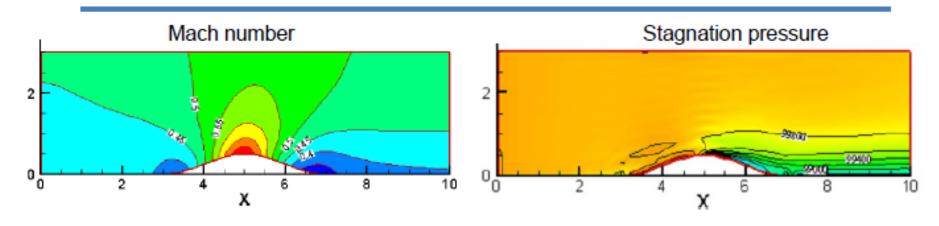


Sketch of the flow field over a supersonic blunt-nose body.

(Courtesy of Anderson, Computational Fluid Dynamics)

- First order in time
- Second order in space
- Numerical viscosity (smoothing)

#### BASIC SOLVER



Converges in ~ 2600 iterations

Not symmetric, Stagnation pressure loss

Maximum stable time step  $\sim 1.6\Delta t$  (CFL = 0.5, SF = 0.5)

#### Scope for enhancing:

Speed

Accuracy (due to smoothing)

Stability

#### Extensions: Enhanced Solver

Time Accuracy (Class A) (enhances stability)

Space Accuracy (Class B)

Speed (Class C) (easiest)

- Adams-Bashforth
- Runge-Kutta

- Deferred Corrections
- High order smoothing
- High order differencing
- Constant stagnation enthalpy
- Spatially varying time steps
- Residual averaging

Pick "at least" one of each class

Propose the *best combination* you have found

Use enhanced solver for all test cases

Previous students liked *Deferred Corrections* + *Runge-Kutta* 

#### ENHANCE STABIL

#### Adams-Bashforth (Multi-Step method) – uses n, n-1 time levels

Taylor series expansion for [?]<sub>i</sub>n+1 in time:

$$\left[ \int_{t}^{n+1} - \left[ \int_{t}^{n} + \frac{\partial \left[ \int_{t}^{n} \right]^{n}}{\partial t} \right]^{n} \Delta t + \frac{1}{2} \frac{\partial^{2} \left[ \int_{t}^{n} dt \right]^{n}}{\partial t^{2}} \Delta t^{2} + O(\Delta t^{3})$$

2<sup>nd</sup> derivative evaluated as one-sided difference in time

$$\left[ \right]_{i}^{n+1} = \left[ \right]_{i}^{n} + \frac{\partial \left[ \right]}{\partial t} \right]_{i}^{n} \Delta t + \frac{1}{2} \frac{\partial^{2} \left[ \right]}{\partial t^{2}} \right]_{i}^{n} \Delta t^{2} + O(\Delta t^{3})$$

$$\frac{\partial^{2} \left[ \right]}{\partial t^{2}} \right]_{i}^{n} = \frac{\partial}{\partial t} \left( \frac{\partial \left[ \right]}{\partial t} \right)_{i}^{n} = \frac{\partial \left[ \right]}{\partial t} \left[ \frac{\partial \left[ \right]}{\partial t} \right]_{i}^{n} + O(\Delta t)$$

Combine:

$$\begin{bmatrix} \\ \\ \end{bmatrix}_{i}^{n+1} = \begin{bmatrix} \\ \\ \end{bmatrix}_{i}^{n} + \frac{\partial \begin{bmatrix} \\ \\ \\ \end{bmatrix}}{\partial t} \Big|_{i}^{n} \Delta t + \frac{1}{2} \left( \frac{\partial \begin{bmatrix} \\ \\ \\ \end{bmatrix}}{\partial t} \Big|_{i}^{n} - \frac{\partial \begin{bmatrix} \\ \\ \\ \end{bmatrix}}{\partial t} \Big|_{i}^{n-1} + O(\Delta t) \right) \Delta t^{2} + O(\Delta t^{3})$$

**FACSEC** 

 $0 \rightarrow 1^{st}$  order  $0.5 \rightarrow 2^{st}$  order > 0.5 → Further increases stability



Truncation error

#### ENHANCE STABILITY

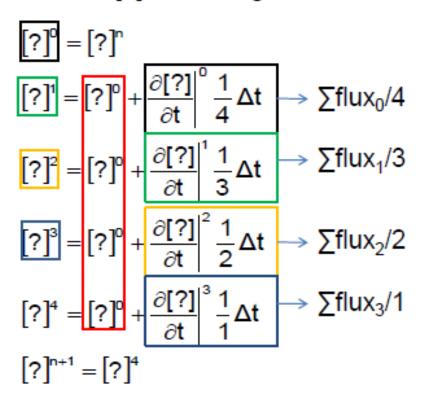
#### Adams-Bashforth (Multi-Step method)

- Since not solving unsteady problems the 2<sup>nd</sup> order temporal accuracy will not give an accuracy benefit
- Modified Eqn analysis shows the method adds a diffusive error term in time (Vanishes at convergence)
  - This improves stability and much lower values of smoothing coefficients can be used

#### ENHANCE STABILITY

#### Runge-Kutta (Multi-stage method) – uses only nth time level

Unlike multi-step, progress from time level 'n' to 'n+1' using 'm' sub-stages
[?]n = starting value of variable at time level 'n' i.e.



Always add to starting value

Use new values to find changes in next sub-stage

- Significantly larger time steps
- •More CPU time per iteration!
- Low values of artificial viscosity!
- Minimum complexity & memory



#### Deferred Corrections

- In classic CFD form would involve say making a stable 1<sup>st</sup> order estimate of the solution and then adding on a correction based on a high order spatial discretization to vield <u>Accuracy & Stability</u>
- Estimate in basic code:

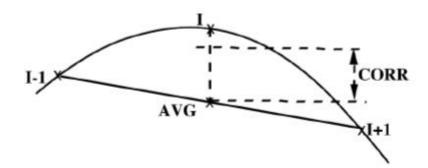
$$[?]_I = (1-\epsilon)[?]_{unsmoothed} + \epsilon[?]_{smooth}$$

Too much smoothing :smooth factor between 0 and 1

Improve accuracy by adding the correction:

$$[?]_{I} = (1-\epsilon)[?]_{unsmoothed} + \epsilon([?]_{smooth} + correction)$$
 

Unstable



#### Deferred Corrections

- In classic CFD form would involve say making a stable 1<sup>st</sup> order estimate of the solution and then adding on a correction based on a high order spatial discretization to vield <u>Accuracy & Stability</u>
- Estimate in basic code:

$$[?]_{I} = (1-\epsilon)[?]_{unsmoothed} + \epsilon[?]_{smooth}$$

Too much smoothing smooth factor between 0 and 1

Improve accuracy by adding the correction:

$$[?]_I = (1-ε)[?]_{unsmoothed} + ε([?]_{smooth} + correction)$$

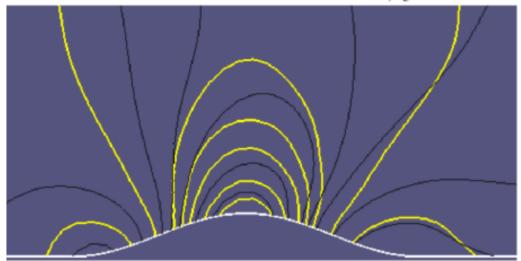
Correction =  $[?]_{unsmoothed}$  -  $[?]_{smooth}$ 

Unstable

$$[?]_{I} = (1-\epsilon)[?]_{unsmoothed} + \epsilon([?]_{smooth} + grad\_correction)$$

#### **Deferred Corrections**

Contours of M. Black = Basic LAX, yellow = DC.



Much more symmetric!

fcorr : proportion of artificial viscosity we want to cancel, typically about 0.9 Effective smooth\_fac = (1-fcorr)\*smooth\_fac = 0.1 \* smooth\_fac

#### **High-Order Smoothing** (Further minimize smoothing!)

We have been explicitly adding as smoothing

Smoothing = 
$$\nabla^2 \left[?\right] = \frac{\partial^2 \left[?\right]}{\partial x^2} + \frac{\partial^2 \left[?\right]}{\partial y^2}$$
  $\leftarrow$  2<sup>nd</sup> order smoothing

For greater accuracy we can use

Smoothing = 
$$\nabla^4 \left[?\right] = \frac{\partial^4 \left[?\right]}{\partial x^4} + \frac{\partial^4 \left[?\right]}{\partial y^4}$$
  $\leftarrow$  4<sup>th</sup> order smoothing

Commercial CFD codes generally have

Smoothing = 
$$\varepsilon_1 f_1[?] \nabla^2[?] + \varepsilon_2 f_2[?] \nabla^4[?]$$
 Blend!

Tricky at boundaries, Leave it 2nd order!

#### **High-Order Differencing**

In basic code: Assumed properties to vary linearly between grid points

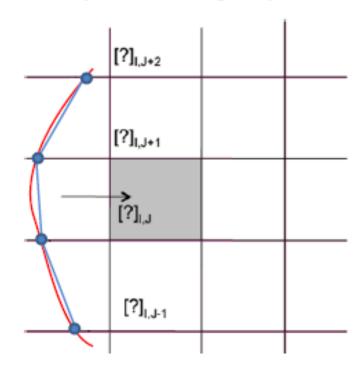
Construct high-order fluxes using:

Finite difference formula

Compact schemes

Simple high-order interpolations

Eg: Cubic variation in interior domain
Parabolic variation at boundaries
Uniform grid spacing to simplify algebra



#### ENHANCE SPEED

#### Constant stagnation enthalpy

Assumptions: Flow is adiabatic, Not time accurate

Get rid of Energy Equation, set  $h_o = c_p T_{o,in}$ 

#### Spatially adaptive time-step

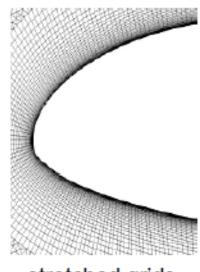
Different time steps for different elements

Not time accurate

Use local dmin, cell velocity and sound speed:

$$\Delta t = dmin_{loc}/(U+c)_{loc}$$

Any benefit? Limited benefit on uniform grids

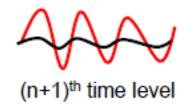


stretched grids

#### ENHANCE SPEED

#### Residual Averaging

Have smoothed solved for variables, Φ, for stability



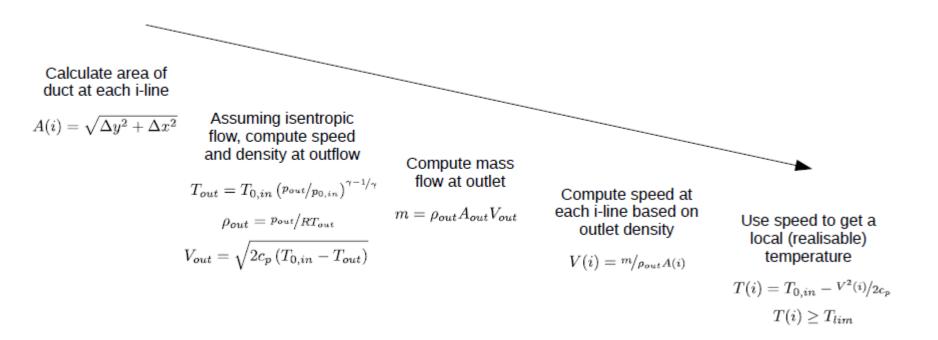
- Essentially solving ΔΦ/Δt=Residual(=Σflux)
- At convergence Residual = 0. Hence, can smooth R like did for
  Φ and not change answer.
- More <u>stability</u> allowing bigger Δt

- (n+1)<sup>th</sup> time level
- In practice, for convenience, we smooth ΔΦ (ΔΦ α R)

Any Benefit with default schemes? - Try with Runge Kutta!

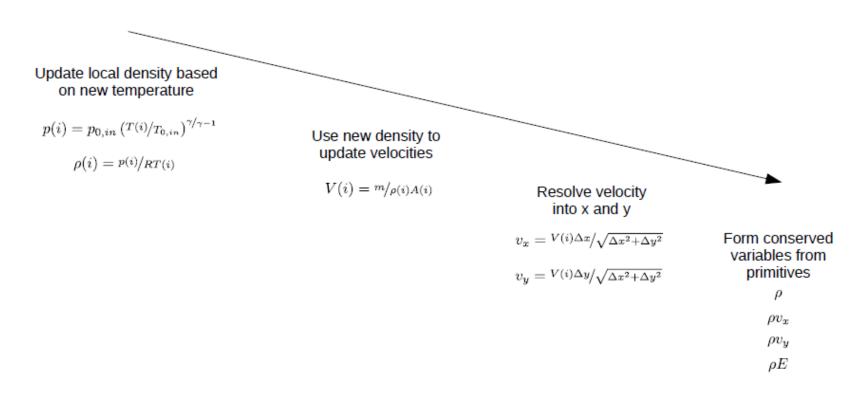
## Flow Guess

The FLOW\_GUESS subroutine improves on CRUDE\_GUESS as an initial estimate of the flow



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The FLOW\_GUESS subroutine improves on CRUDE\_GUESS as an initial estimate of the flow



Summary

