A1-NUMERICAL SOLUTION OF CONVECTION-DIFFUSION EQUATIONS

1 Governing Equations [1, 2]

The governing equations of the heat transfer by convection are a state equation (relation among pressure, temperature and density) and conservation equations of mass, linear momentum and energy. A constitutive relation are also required: Stokes' law, Fourier law, Fick law,...

Assuming:

- Bidimensional model
- Mono-component and mono-phase fluid
- Incompressible flow
- Newtonian fluid
- Boussinesq hypothesis (constant physical properties everywhere except in the body forces term)

the governing equations written in Cartesian coordinates are:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{1}$$

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} = -\frac{\partial p_d}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \tag{2}$$

$$\rho\frac{\partial v}{\partial t} + \rho u\frac{\partial v}{\partial x} + \rho v\frac{\partial v}{\partial y} = -\frac{\partial p_d}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + \rho g\beta(T - T_\infty) \tag{3}$$

$$\rho\frac{\partial T}{\partial t} + \rho u\frac{\partial T}{\partial x} + \rho v\frac{\partial T}{\partial y} = \frac{\lambda}{c_p}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \frac{\Phi}{c_p} \tag{4}$$

where,

β	Coefficient of volumetric thermal expansion.
c_p	Specific heat.
k	Conductivity.
g	Gravitational acceleration.
μ	Viscosity.
p_d	Dynamic pressure.
ρ	Density.
t	Time.
T	Temperture.
u, v	Velocity components.
x, y	Spatial coordinates.
Φ	Heat source.

They are partial coupled partial differential equations. The 4 unknowns are the pressure, temperature, and the two velocity components u and v. An appropriate boundary and initial conditions are required to close the problem.

Two strong coupling characterise this equation system:

- pressure-velocity. There is no specific pressure equation. For incompressible flows, the pressure is the field that makes the velocity accomplish the mass conservation equation.
- temperature-velocity. This coupling is only present for natural convection, mixed convection or temperature dependent physical properties. In forced convection and constant physical properties, the velocity field does not depend on the temperature field.

All the equations written above (1-4) can be summarized in the convection-diffusion equation:

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \vec{v} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S \tag{5}$$

or in Cartesian coordiantes, incompressible flow and constant physical properties:

$$\rho \frac{\partial \phi}{\partial t} + \rho u \frac{\partial \phi}{\partial x} + \rho v \frac{\partial \phi}{\partial y} = \frac{\lambda}{c_p} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + S \tag{6}$$

The accumulation of ϕ, plus the net convective flow has to be the net diffusive flow plus the generation of ϕ per unit of volume. The diffusive term flows from greater to smaller value of ϕ.

According to the convection diffusion equation, we can write a table with the appropiate parameters in order to reproduce the governing equations. See Table 1.

Equation	ϕ	Γ	S
Coninuity	1	0	0
Momentum in x direction	u	μ	$-\partial p_d/\partial x$
Momentum in y direction	v	μ	$-\partial p_d/\partial y + \rho g \beta (T - T_\infty)$
Energy (constant c_p)	T	λ/c_p	Φ/c_p

Table 1: Parameters to replace in convection - diffusion equation in order to reproduce the governing equations.

2 Finite-Volume Discretization [3, 4, 5, 6]

Integrating the convection-diffusion equation into a rectangular finite volume (see Fig. 1), the discretized equation can be written:

$$\frac{(\rho\phi)_P^{n+1} - (\rho\phi)_P^n}{\Delta t} \Delta x \Delta y + \left[(\rho u \phi)_e^{n+1} - (\rho u \phi)_w^{n+1}\right] \Delta y + \left[(\rho u \phi)_n^{n+1} - (\rho u \phi)_s^{n+1}\right] \Delta x$$
$$= \left[\left(\Gamma \frac{\partial \phi}{\partial x}\right)_e^{n+1} - \left(\Gamma \frac{\partial \phi}{\partial x}\right)_w^{n+1}\right] \Delta y + \left[\left(\Gamma \frac{\partial \phi}{\partial y}\right)_n^{n+1} - \left(\Gamma \frac{\partial \phi}{\partial y}\right)_s^{n+1}\right] \Delta x +$$
$$S_P^{n+1} \Delta x \Delta y \tag{7}$$

where the following hypothesis are done:

1. In the integration process, the convective and diffusive flows have been considered constant through each face of the control volume.
2. (spatial deviation)^n=(spatial deviation)$^{n+1}$
   (spatial deviation)$_w$=(spatial deviation)$_e$
   (spatial deviation)$_s$=(spatial deviation)$_n$
3. The source term: $\int_n^{n+1} \int_w^e \int_s^n S dy dx dt = S_P^{n+1} \Delta x \Delta y \Delta t$

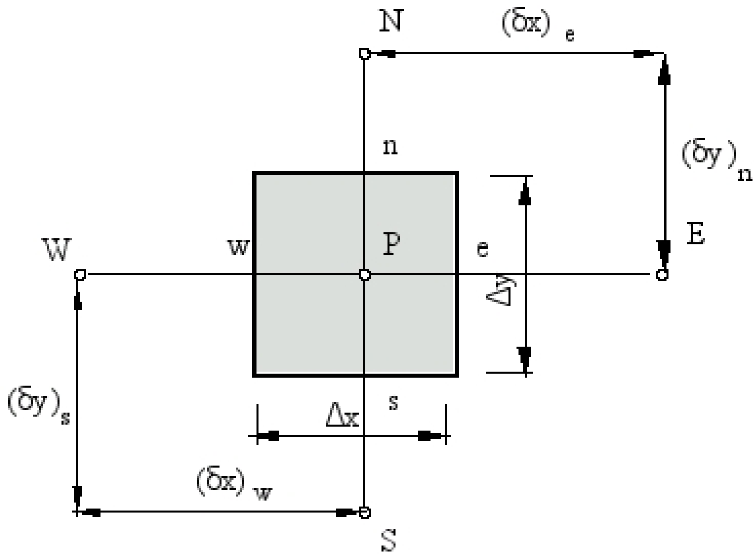

Figure 1: Finite volume

3 Consistency, stability and convergence

A numerical approximation is **consistent** when the discretized equations are solution of the differential equation when the spatial and temporal grid tend to zero. Thus, as the grid is refined, truncation errors must tend to zero.

A numerical approximation is **stable** if the solution obtained is the solution of the discret equations. Possible roundoff errors, equations couplings, etc can produce inestabilities.

A **convergent** solution is a stable solution that tends to the solution of the differential equations as the the meshes are finer. So, **consistency** and **stability** are two necessary and sufficient conditions to get **convergence**.

4 Analytical solution of the convection-diffusion equation. Onedimensional,null source term and steady state solution [3]

For this case the convection - diffusion equation is:

$$\frac{\partial\rho\phi}{\partial t} + \nabla\left(J\right) = S \tag{8}$$

where $J = \rho v\phi - \Gamma\nabla\phi$ and is the total flow: convective and diffusive. Rerwritting J for the specified conditions:

$$J = \rho u\phi - \Gamma\frac{d\phi}{dx} \tag{9}$$

Assuming a nul source term S, equation (8) reduces to:

$$\frac{dJ}{dx} = 0 \tag{10}$$

and integrating over the control volume of figure 2:

$$J_e - J_w = 0 \tag{11}$$

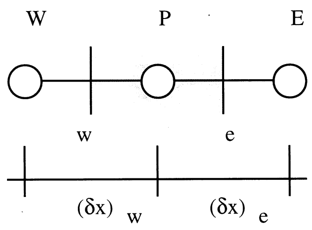

Figure 2: Finite control volume for one dimensional problem.

The resulting discrete equation can be easly solved imposing the following boundary conditions:

in $x = 0 \longrightarrow \phi = \phi_0$

in $x = L \longrightarrow \phi = \phi_L$

The analytical solution is:

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{exp(Px/L) - 1}{exp(P) - 1} \tag{12}$$

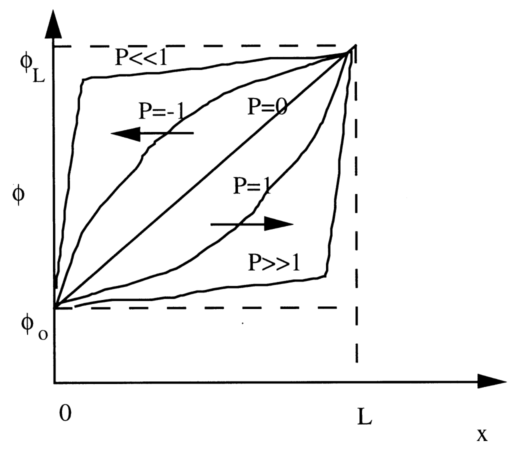

Figure 3: Graphical representation of equation (12).

where P is the Peclet number and is defined as $P = \rho u L/\Gamma$. Graphical representation of equation (12) can be seen in figure 3.

Taking into account this exact analytical profile available, the flows in the faces of the Control Volumes are:

$$J_e = F_e(\phi_P + \frac{\phi_P - \phi_E}{exp(P_e) - 1}) \tag{13}$$

where $P_e = \frac{(\rho u)_e \delta x_e}{\Gamma_e} = \frac{F_e}{D_e}$.

Substituing this flows in the discrete equation, we get an equations like:

$$a_P \phi_P = a_E \phi_E + a_W \phi_W \tag{14}$$

The solution of this equation gives the exact solution of the differential convection-diffusion equation in the nodal points whatever the discretization mesh is.

5 General case. Bidimensional and Transient [3]

The convection-diffusion equation in this situation reads:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S \tag{15}$$

where $J_x = \rho u \phi - \Gamma \frac{\partial \phi}{\partial x}$ and $J_y = \rho v \phi - \Gamma \frac{\partial \phi}{\partial y}$.

Integrating this equation over a control volume, assuming and implicit criteria for the temporal integration and a constant flow at each face of the control volume:

$$\frac{(\rho\phi)_P - (\rho\phi)_P^0}{\Delta t}\Delta x\Delta y + J_e - J_w + J_n - J_s = S_P^{n+1}\Delta x\Delta y \tag{16}$$

In order to assure convergence, is better to introduce the continuity equation in the discretized equation:

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho u}{\partial x} + \frac{\partial\rho v}{\partial y} = 0 \tag{17}$$

which is integrated over a control volume:

$$\frac{\rho_P - \rho_P^0}{\Delta t}\Delta x\Delta y + F_e - F_w + F_n - F_s = 0 \tag{18}$$

where $F = \rho v\mathcal{S}$; $\mathcal{S}$ is the surface vector of the control volume.

Then, we can substract Eq.19 and 18$\cdot\phi_P$, and obtain:

$$\begin{aligned}\frac{(\phi_P - \phi_P^0)\rho_P^0}{\Delta t}\Delta x\Delta y &+ (J_e - F_e\phi_P) - (J_w - F_w\phi_P)\\ &+ (J_n - F_n\phi_P) - (J_s - F_s\phi_P) = S_P^{n+1}\Delta x\Delta y\end{aligned} \tag{19}$$

6 Numerical Schemes

It can be seen that in the discretizated convection-diffusion equation (7) convective and diffusive terms are evaluated at the cell faces, whereas dependent variable ϕ is known at the cell center. The evaluation of the variable at the cell face is carried out by numerical schemes.

Conductive flux is calculated as an arithmetic mean:

$$\left(\frac{\partial\phi}{\partial x}\right)_e = \frac{\phi_E - \phi_P}{\delta x_e} \quad \text{or} \quad \left(\frac{\partial\phi}{\partial y}\right)_n = \frac{\phi_N - \phi_P}{\delta y_n} \tag{20}$$

The *order* of a numerical scheme is the number of neighbouring nodes that are used to evaluate dependent variable at the cell face.

6.1 Low order numerical schemes [3]

These numerical schemes evaluate the variable using nearest nodes: east (E), west (W), north (N) and south (S). Their order is 1 or 2.

Most significant low order numerical schemes are:

- Central Difference Scheme (CDS): It is a second order scheme, variable at the cell face is calculated as an arithmetic mean. That is:

$$\phi_e = \frac{1}{2}(\phi_P + \phi_E) \tag{21}$$

- Upwind Difference Scheme (UDS): It is a first order scheme and the value of ϕ at the cell face is equal to the value of ϕ at the grid point on the *upwind* side of the face. That is:

$$\phi_e = \phi_P \qquad \text{if} \quad F_e > 0 \tag{22a}$$

$$\phi_e = \phi_E \qquad \text{if} \quad F_e < 0 \tag{22b}$$

- Hybrid Difference Scheme (HDS): Uses CDS for low velocities and UDS for high velocities.

- Exponencial Difference Scheme (EDS): It is a second order scheme and the evaluation of the dependent variable at the cell face comes from the exact solution of the convection-diffusion equation in one-dimensional, null source term and steady problem.

- Powerlaw Difference Scheme (PLDS): It is a second order scheme and variable at the cell face is calculated with an approximation of the EDS by a polynomial of fifth degree.

If numerical schemes are introduced in the integrated discretized convection-diffusion equation, it is obtained an algebraic equation for each control volume:

$$a_P\phi_P = a_E\phi_E + a_S\phi_S + a_W\phi_W + a_N\phi_N + b \tag{23}$$

Coefficients a_i can be evaluated with:

$$a_E = D_e \cdot A\left(|Pe_e|\right) + max(-F_e, 0) \tag{24a}$$
$$a_W = D_w \cdot A\left(|Pe_w|\right) + max(F_w, 0) \tag{24b}$$
$$a_N = D_n \cdot A\left(|Pe_n|\right) + max(-F_n, 0) \tag{24c}$$
$$a_S = D_s \cdot A\left(|Pe_s|\right) + max(F_s, 0) \tag{24d}$$
$$a_P = a_E + a_W + a_N + a_S + \rho_P^n \frac{\Delta x\, \Delta y}{\Delta t} \tag{24e}$$
$$b = \rho_P^n \frac{\Delta x\, \Delta y}{\Delta t} \phi_P^n + S_P^{n+1} \Delta x\, \Delta y \tag{24f}$$

where:

$$D_e = \frac{\Gamma_e\, \Delta y}{(\delta x)_e}; \quad D_w = \frac{\Gamma_w\, \Delta y}{(\delta x)_w}; \qquad D_n = \frac{\Gamma_n\, \Delta x}{(\delta y)_n}; \quad D_s = \frac{\Gamma_s\, \Delta x}{(\delta y)_s} \tag{25}$$

$$F_e = (\rho u)_e \Delta y; \quad F_w = (\rho u)_w \Delta y; \qquad F_n = (\rho v)_n \Delta x; \quad F_s = (\rho v)_s \Delta x \tag{26}$$

and the Peclet number evaluated at the face of the control volume (f) is:

$$P_f = \frac{F_f}{D_f} \tag{27}$$

Numerical scheme	$A(\|P\|)$
UDS	1
CDS	$1 - 0.5(\|P\|)$
HDS	$max(0, (1 - 0.5\|P\|))$
EDS	$\|P\|/(e^{\|P\|} - 1)$
PLDS	$max(0, (1 - 0.5\|P\|)^5)$

Table 2: Value of $A(|P|)$ for different low numerical schemes.

6.2 High order numerical schemes

In order to improve accuracy of low numerical schemes, it's useful to use more than two nodal values to calculate dependent variable at the cell face.

These high order numerical schemes are introduced into the general formulation by a deferred term (b_{de}) as if it was a source term, and the coefficients of the equation (23) are calculated using UDS numerical scheme.

By this way, algebraic equation is expressed as:

$$a_P\phi_P = a_E\phi_E + a_S\phi_S + a_W\phi_W + a_N\phi_N + b + b_{de} \tag{28}$$

and deffered term is calculated as:

$$\begin{aligned} b_{de} = F_e(\phi_e^{UDS} - \phi_e^{HS}) - F_w(\phi_w^{UDS} - \phi_w^{HS}) + \\ + F_n(\phi_n^{UDS} - \phi_n^{HS}) - F_s(\phi_s^{UDS} - \phi_s^{HS}) \end{aligned} \tag{29}$$

ϕ_f^{HS} is the variable ϕ evaluated at the cell face f with high order numerical scheme.

6.2.1 Evaluation of ϕ_f^{HS} according to different high order numerical schemes [7, 8, 9]

It is useful to introduce some variables in order to make calculations independent of the flux direction (figure 4):

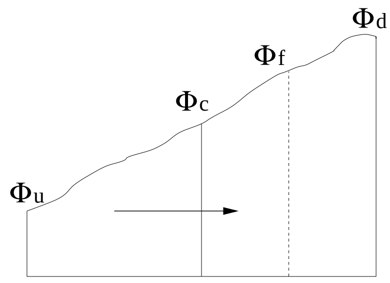

Figure 4: Sketch of original variables profile.

- ϕ_C: Value of ϕ at the nearest grid point on the upwind side of the face.
- ϕ_U: Value of ϕ at the grid point above ϕ_C.
- ϕ_D: Value of ϕ at the nearest grid point on the downstream side of the face.

Then dependent variable at the cell face is evaluated according to table 3.

Numerical scheme	Order	Comments	ϕ_f
UDS	1	-	$\phi_f = \phi_C$
UDS of 2nd order	2	Lineal extrapolation between ϕ_C and ϕ_U	$\phi_f = \frac{(3\phi_C - \phi_U)}{2}$
QUICK	3	Quadratic interpolation among ϕ_C, ϕ_U and ϕ_D	$\phi_f = \frac{(\phi_C + \phi_D)}{2} - \frac{\phi_D - 2\phi_C + \phi_U}{8}$

Table 3: ϕ_f evaluated with different high order numerical schemes.

One of the problems of accurate numerical schemes is the instability. This problem is solved if they are **bounded**, it means that ϕ_f is beween nearest nodal grid points values.

If dependent variable is normalized as:

$$\overline{\phi}_f = \frac{\phi_f - \phi_U}{\phi_D - \phi_U} \tag{30}$$

Then figure 4 becomes figure 5:

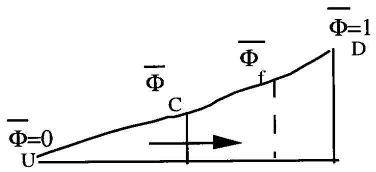

Figure 5: Sketch of normalized variables profile.

And ϕ_f depends on value of normalized nodal grid point variable ϕ_C: $\overline{\phi}_f =$ f($\overline{\phi}_C$).

A bounded numerical scheme must be in the dark zone of the normalized variable diagram, NVD, (see figure 6). According to figure 5, the meaning of this can be seen in figures 7 i 8.

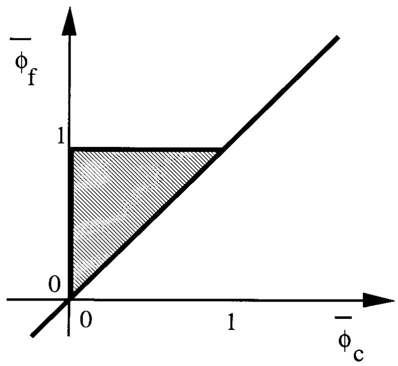

Figure 6: Normalized variable diagram (NVD): graphic of $\overline{\phi}_f$ as a function of $\overline{\phi}_C$, it shows if numerical scheme is bounded

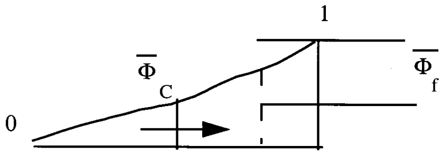

Figure 7: Bounded numerical scheme.

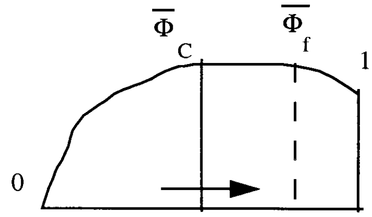

Figure 8: Not bounded numerical scheme.

A second order scheme passes through $(0.5, 0.75)$ coordinate of figure 6. If the slop of the numerical scheme in figure 5 is 0.75 and passes through $(0.5, 0.75)$ coordinate, it is a third order numerical scheme. All this is plotted in the normalized variable diagram of figure 9.

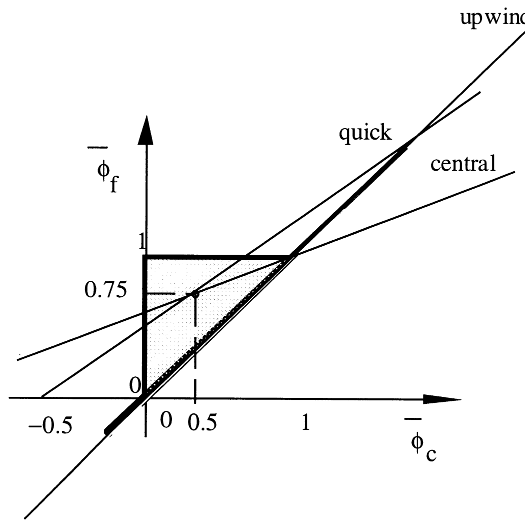

Figure 9: Normalized variable diagram plots for several linear schemes.

In figure 9 it can be seen that second and third order numerical schemes will have problems of instability. "Esquemes a la carta (??)", like SMART, try to solve these problems.

Using equation (30), the normalized dependent variable at the cell face is evaluated using table 4.

Numerical scheme	Order	$\overline{\phi}_f$
UDS	1	$\overline{\phi}_f = \overline{\phi}_C$
UDS2	2	$\overline{\phi}_f = \frac{3}{2}\overline{\phi}_C$
QUICK	3	$\overline{\phi}_f = \frac{3}{8} + \frac{3}{4}\overline{\phi}_C$
SMART	$2-4$	$\overline{\phi}_f = 3\overline{\phi}_C$ if $0 < \overline{\phi}_C < \frac{1}{6}$ $\overline{\phi}_f = \frac{3}{8} + \frac{3}{4}\overline{\phi}_C$ if $\frac{1}{6} < \overline{\phi}_C < \frac{5}{6}$ $\overline{\phi}_f = 1$ if $\frac{5}{6} < \overline{\phi}_C < 1$ $\overline{\phi}_f = \overline{\phi}_C$ otherwise

Table 4: $\overline{\phi}_f$ evaluated with different high order numerical schemes.

If cell face is not at the middle between two nodal points, it is necessary to introduce geometric variables. Thus, distances are normalized in a similar form to ϕ:

$$\overline{x} = \frac{x - x_U}{x_D - x_U} \tag{31}$$

Then problem only depends on three variables:

$$\phi_f = \mathrm{f}(\phi_U, \phi_C, \phi_D, x_U, x_C, x_f, x_D) \quad \Rightarrow \quad \overline{\phi}_f = \mathrm{f}(\overline{\phi}_C, \overline{x}_C, \overline{x}_f)$$

According to (31), table 4 is transformed to table 5.

Numerical scheme	Order	$\overline{\phi}_f$	
UDS2	2	$\overline{\phi}_f = \frac{\overline{x}_f}{\overline{x}_C}\overline{\phi}_C$	
QUICK	3	$\overline{\phi}_f = \overline{x}_f + \frac{\overline{x}_f(\overline{x}_f - 1)}{\overline{x}_C(\overline{x}_C - 1)}\left(\overline{\phi}_C - \overline{x}_C\right)$	
SMART	2 - 4	$\overline{\phi}_f = \frac{\overline{x}_f(1-3\overline{x}_c+2\overline{x}_f)}{\overline{x}_c(1-\overline{x}_c)}\overline{\phi}_C$	if $0 < \overline{\phi}_C \leq \frac{\overline{x}_C}{3}$
		$\overline{\phi}_f = \frac{\overline{x}_f(\overline{x}_f - \overline{x}_C)}{1-\overline{x}_C} + \frac{\overline{x}_f(\overline{x}_f - 1)}{\overline{x}_C(\overline{x}_C - 1)}\overline{\phi}_C$	if $\frac{\overline{x}_C}{3} < \overline{\phi}_C \leq \frac{(1+\overline{x}_f-\overline{x}_C)\overline{x}_C}{\overline{x}_f}$
		$\overline{\phi}_f = 1$	if $\frac{(1+\overline{x}_f-\overline{x}_C)\overline{x}_C}{\overline{x}_f} < \overline{\phi}_C \leq 1$
		$\overline{\phi}_f = \overline{\phi}_C$	otherwise

Table 5: $\overline{\phi}_f$ evaluated with different high order numerical schemes and using normalized distances.

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