Meshfree methods for conservation laws using kinetic approach and alternate least squares procedures

Praveen. C

TIFR Center for Applicable Mathematics, Bangalore
praveen@math.tifrbng.res.in

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Outline

Kinetic schemes

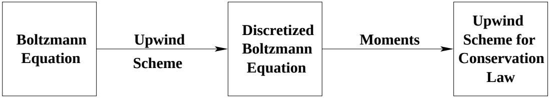
- Exploit connection between Boltzmann and Euler/Navier-Stokes equations

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \nabla F = 0$$

$$\Downarrow$$

$$\frac{\partial U}{\partial t} + \text{div } G = 0$$

- Kinetic scheme



Kinetic Meshless Method

- 2-D Boltzmann equation

$$\frac{\partial F}{\partial t} + v_x F_x + v_y F_y = 0$$

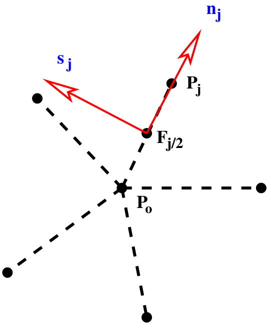
- Point collocation approach
- Least squares approximation at node "0"

$$\frac{\mathrm{d}F_0}{\mathrm{d}t} + v_x \sum_j a_j (F_j - F_0) + v_y \sum_j b_j (F_j - F_0) = 0$$

Leads to unstable scheme; no wave propagation effects

Kinetic Meshless Method

- Upwinding through introduction of a mid-point state (Morinishi, Balakrishnan)



- Kinetic upwind approximation

$$F_{j/2} = \begin{cases} F_0 & \text{if } \vec{v} \cdot \hat{n}_j \geq 0 \\ F_j & \text{if } \vec{v} \cdot \hat{n}_j < 0 \end{cases}$$

Kinetic Meshless Method

- LS using mid-point states

$$\frac{\mathrm{d}F_0}{\mathrm{d}t} + v_x \sum_j a_j (F_{j/2} - F_0) + v_y \sum_j b_j (F_{j/2} - F_0) = 0$$

- Semi-discrete scheme

$$\frac{\mathrm{d}U_0}{\mathrm{d}t} + \sum [a_j (GX_{j/2} - GX_0) + b_j (GY_{j/2} - GY_0)] = 0$$

- No stencil splitting, smaller stencil
- Rotationally invariant
- Nearly positive scheme - good stability properties
- On Cartesian points, KMM reduces to finite volume method
- Edge-based updating possible - speed up of 2

Kinetic Meshless Method

- LS using mid-point states

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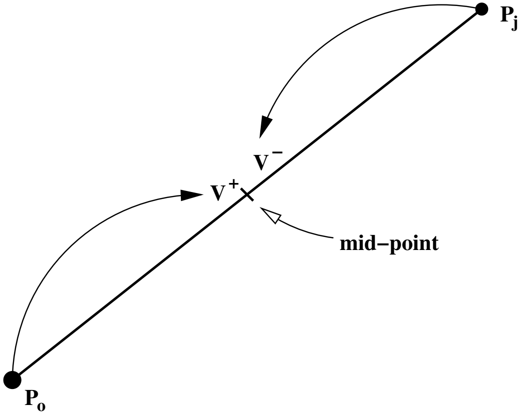
- Edge-based updating possible - speed up of 2

Higher order scheme

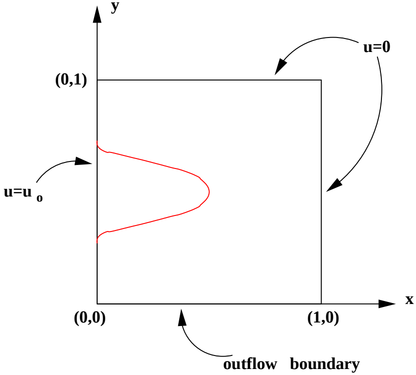
- Define left and right states at each mid-point using linear reconstruction along the ray

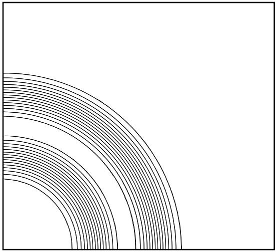
$$V_{j/2}^{+} = V_0 + \frac{1}{2}\Delta\vec{r}_j \cdot \nabla V_0 \quad \text{and} \quad V_{j/2}^{-} = V_j - \frac{1}{2}\Delta\vec{r}_j \cdot \nabla V_j$$



Numerical order of accuracy

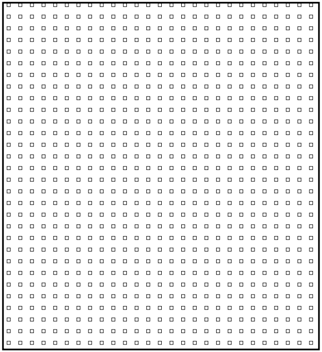
$$\frac{\partial u}{\partial t} + y\frac{\partial u}{\partial x} - x\frac{\partial u}{\partial y} = 0$$

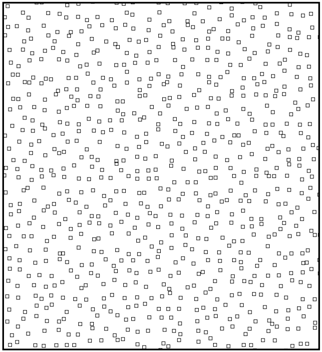




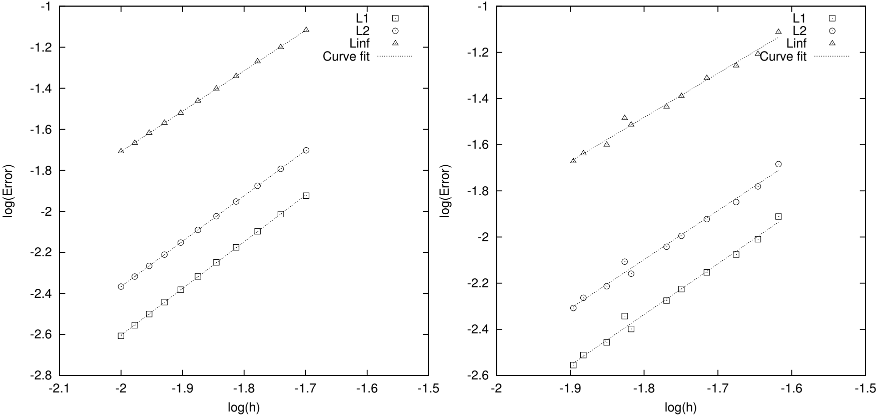
Numerical order of accuracy

Uniform and random point distributions





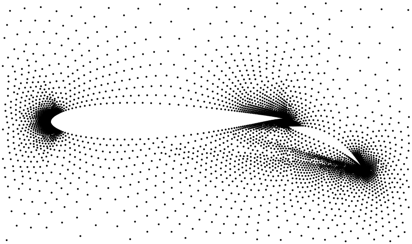
Numerical order of accuracy



Point distribution	L_1	L_2	L_∞
Uniform	2.27	2.21	1.97
Random	2.19	2.12	1.90

Flow over Williams airfoil

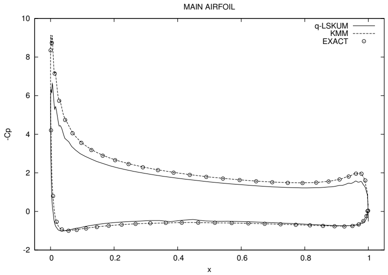
Free-stream Mach number = 0.15
Angle of attack = 0
Number of points = 6415
Points on main airfoil = 234
Points on flap = 117

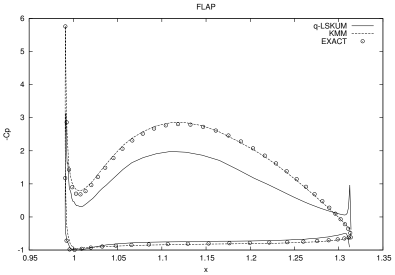


n	KMM	q-LSKUM
3	0.19	-
4	4.86	0.02
5	6.84	0.12
6	80.45	71.36
7	6.50	27.79
8	0.16	0.69
9	-	0.02

William's airfoil

Pressure coefficient



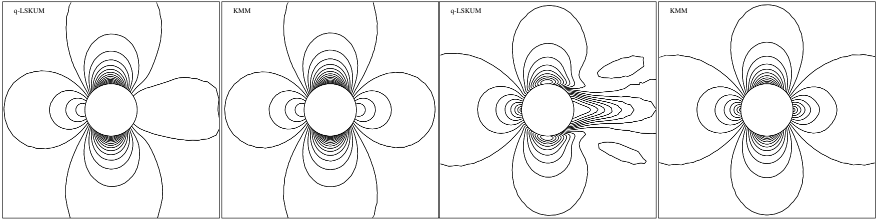


Scheme	C_l	C_d	$S_{\min}$	$S_{\max}$
q-LSKUM	3.0927	0.0197	-1.535×10^{-3}	1.031×10^{-2}
KMM	3.7608	0.0069	-4.99×10^{-4}	7.246×10^{-3}
Potential	3.736	0	0	0

Flow over cylinder

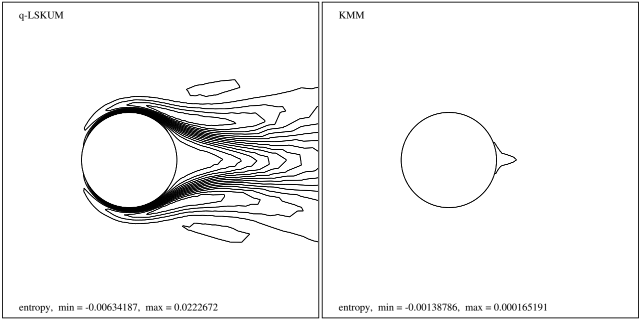
$M_\infty = 0.38$ and $\alpha = 0$
No of points = 4111
Points on cylinder = 250

n	4	5	6	7	8	9
KMM	6.67	5.50	83.12	4.72	-	-
LSKUM	-	0.19	82.56	16.78	0.44	0.02



Pressure Mach

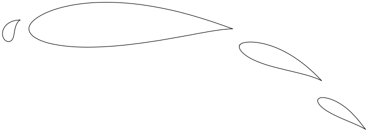
Subsonic flow over cylinder



q-LSKUM KMM

Scheme	C_l	C_d	$S_{\min}$	$S_{\max}$
q-LSKUM	0.0237	0.0324	-0.00634	0.022267
KMM	0.0006	0.0012	-0.00138	0.000165

Suddhoo-Hall airfoil

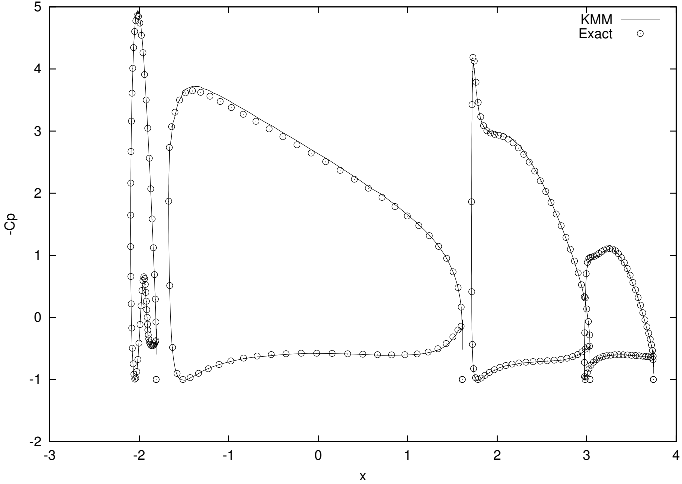


- Number of points = 14091
- On airfoils = 229, 196, 217, 157
- Mach = 0.2 and $\alpha = 0$

	1	2	3	4
KMM	0.5387	4.8095	2.0925	0.7065
Exact	0.5215	4.7157	2.0794	0.7216
% Error	3.3	1.9	0.6	-2.0

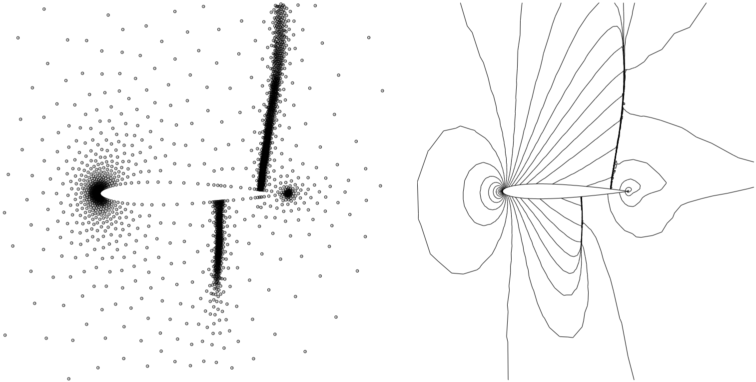
Circulation around different elements

Suddhoo-Hall airfoil



NACA-0012 airfoil

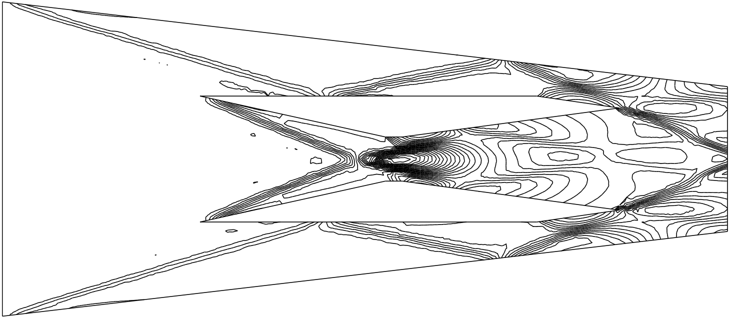
$M_\infty = 0.85, \alpha = 1^o$



Adapted points, 3777 | Mach contours

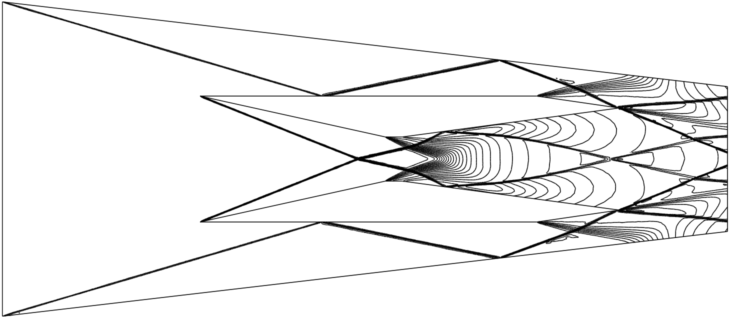
Scramjet Intake - initial solution

Inlet Mach number = 5



Scramjet Intake - adapted solution

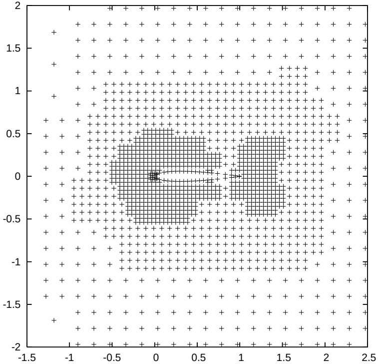
Inlet Mach number = 5



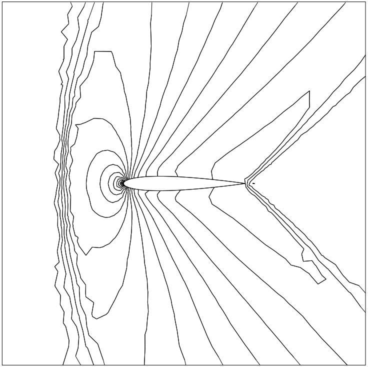
Cartesian Points

NACA-0012 - coarse

$M_\infty = 1.2$, $\alpha = 0^o$



Points



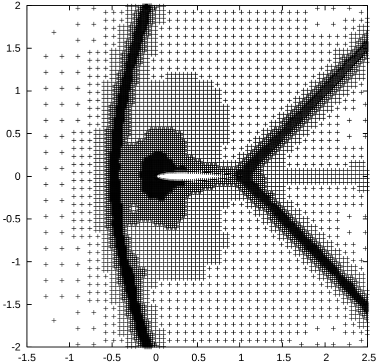
Mach number

(Mohan Varma)

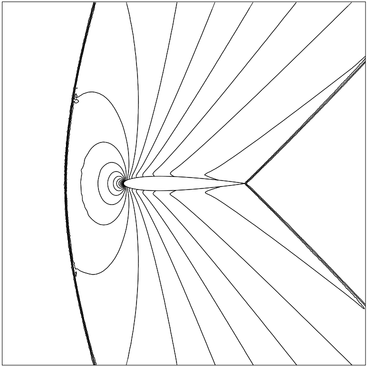
Cartesian Points

NACA-0012 - adapted

$M_\infty = 1.2,\ \alpha = 0^o$



Points



Mach number

(Mohan Varma)

Finite Point Method

Morinishi, Lohner, etc.

Conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0$$

Meshless finite difference using mid-point fluxes

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} + \sum_j \alpha_{ij}(f_{ij} - f_i) + \sum_j \beta_{ij}(g_{ij} - g_i) = 0$$

Define vector $\ell_{ij} = (\alpha_{ij}, \beta_{ij})$

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} + \sum_j [\underbrace{(\alpha_{ij} f_{ij} + \beta_{ij} g_{ij})}_{\text{flux along } \ell_{ij}} - (\alpha_{ij} f_i + \beta_{ij} g_i)] = 0$$

Use your favourite numerical flux function (Roe, KFVS, etc.) H

$$\alpha_{ij} f_{ij} + \beta_{ij} g_{ij} = H(u_i, u_j; \ell_{ij})$$

What is the direction of ℓ_{ij} ?

A positive meshless method

FM Report 2004-FM-16

Semi-discrete scheme

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \sum_j c_{ij}(u_j - u_i)$$

if

$$c_{ij} \ge 0$$

then maxima do not increase and minima do not decrease.
Under a CFL-condition this leads to a `positive` update scheme

$$u_i^{n+1} = \sum_j k_{ij} u_j^n, \qquad k_{ij} \ge 0 \tag{1}$$

is stable in maximum norm

$$\min_j u_j^n \le u_i^{n+1} \le \max_j u_j^n$$

Conservation law

$$\frac{\partial u}{\partial t} + \text{div } \vec{Q}(u) = 0, \quad \vec{Q}(u) = \vec{a}u, \quad \vec{a} = (a_x, a_y)$$

Least squares approximation of derivatives

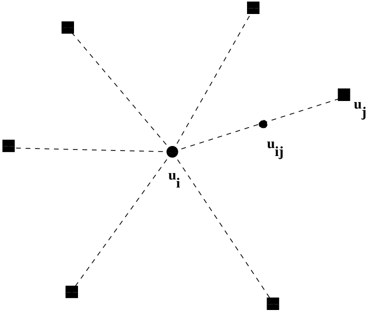
$$\left.\frac{\partial u}{\partial x}\right|_i = \sum_{j \in C_i} \alpha_{ij}(u_j - u_i), \quad \left.\frac{\partial u}{\partial y}\right|_i = \sum_{j \in C_i} \beta_{ij}(u_j - u_i)$$

Central difference scheme

$$\text{div } \vec{Q}(u)_i = a_x \sum_j \alpha_{ij}(u_j - u_i) + a_y \sum_j \beta_{ij}(u_j - u_i)$$

is unstable since it does not account for wave propagation effects.

Upwind scheme I



$$\text{div } \vec{Q}(u)_i = 2a_x \sum_j \alpha_{ij}(u_{ij} - u_i) + 2a_y \sum_j \beta_{ij}(u_{ij} - u_i)$$

Now let θ_{ij} be the angle between $\overrightarrow{N_iN_j}$ and the positive x-axis, $\hat{n}_{ij} = (\cos\theta_{ij}, \sin\theta_{ij})$ be the unit vector along $\overrightarrow{N_iN_j}$ and

Upwind scheme II

$\hat{s}_{ij} = (-\sin\theta_{ij}, \cos\theta_{ij})$ be the unit vector normal to $\hat{n}_{ij}$ so that $(\hat{n}_{ij}, \hat{s}_{ij})$ form a right-handed coordinate system. The wave vector $\vec{a}$ can be written in terms of this coordinate system after a rotational transformation

$$\begin{aligned} a_x &= (\vec{a}\cdot\hat{n}_{ij})\cos\theta_{ij} - (\vec{a}\cdot\hat{s}_{ij})\sin\theta_{ij} \\ a_y &= (\vec{a}\cdot\hat{n}_{ij})\sin\theta_{ij} + (\vec{a}\cdot\hat{s}_{ij})\cos\theta_{ij} \end{aligned}$$

After some rearrangement we obtain

$$\text{div } \vec{Q}(u)_i = 2\sum_j \{\bar{\alpha}_{ij}(\vec{a}\cdot\hat{n}_{ij})(u_{ij}-u_i) + \bar{\beta}_{ij}(\vec{a}\cdot\hat{s}_{ij})(u_{ij}-u_i)\} \tag{2}$$

where we have defined

$$\begin{bmatrix} \bar{\alpha}_{ij} \\ \bar{\beta}_{ij} \end{bmatrix} = \begin{bmatrix} \cos\theta_{ij} & \sin\theta_{ij} \\ -\sin\theta_{ij} & \cos\theta_{ij} \end{bmatrix} \begin{bmatrix} \alpha_{ij} \\ \beta_{ij} \end{bmatrix} \tag{3}$$

Upwind scheme III

Flux along $\hat{n}_{ij}$

$$(\vec{a} \cdot \hat{n}_{ij}) u_{ij} = \frac{\vec{a} \cdot \hat{n}_{ij} + |\vec{a} \cdot \hat{n}_{ij}|}{2} u_i + \frac{\vec{a} \cdot \hat{n}_{ij} - |\vec{a} \cdot \hat{n}_{ij}|}{2} u_j \tag{4}$$

The semi-discrete scheme can be written as

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = -2 \sum_{j \in C_i} \left\{ \bar{\alpha}_{ij} (\vec{a} \cdot \hat{n}_{ij})^- + \bar{\beta}_{ij} (\vec{a} \cdot \hat{s}_{ij}) \frac{(u_{ij} - u_i)}{(u_j - u_i)} \right\} (u_j - u_i) \tag{5}$$

We can show that

$$\bar{\alpha}_{ij} > 0$$

Flux along $\hat{s}_{ij}$

$$(\vec{a} \cdot \hat{s}_{ij}) u_{ij} = (\vec{a} \cdot \hat{s}_{ij}) \frac{u_i + u_j}{2} - \lambda_{ij} (u_j - u_i) \tag{6}$$

where λ_{ij} is a dissipation coefficient which has to be determined.

Upwind scheme IV

If we take

$$\lambda_{ij} = \text{sign}(\bar{\beta}_{ij}) \frac{|\vec{a} \cdot \hat{s}_{ij}|}{2} \tag{7}$$

then the second term becomes

$$\bar{\beta}_{ij}(\vec{a} \cdot \hat{s}_{ij}) \frac{(u_{ij} - u_i)}{(u_j - u_i)} = \frac{\bar{\beta}_{ij}(\vec{a} \cdot \hat{s}_{ij}) - |\bar{\beta}_{ij}(\vec{a} \cdot \hat{s}_{ij})|}{2} \le 0$$

With the choice (6), (7) the semi-discrete scheme can be written as

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \sum_{j \in C_i} c_{ij}(u_j - u_i) \tag{8}$$

where the coefficients are given by

$$c_{ij} = -\bar{\alpha}_{ij}(\vec{a} \cdot \hat{n}_{ij})^- - \bar{\beta}_{ij}\left(\frac{\vec{a} \cdot \hat{s}_{ij}}{2} - \lambda_{ij}\right) \ge 0 \tag{9}$$

Extension to non-linear equations and systems I

Let the flux function $\vec{Q}(u) = (F(u), G(u))$ be nonlinear. Then the semi-discrete scheme can be written as

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = -\sum_{j \in C_i} \{\alpha_{ij}(F_{ij} - F_i) + \beta_{ij}(G_{ij} - G_i)\} \tag{10}$$

where the mid-point fluxes (F_{ij}, G_{ij}) are given by

$$\begin{bmatrix} F_{ij} \\ G_{ij} \end{bmatrix} = R^{-1}(\theta_{ij}) \begin{bmatrix} F(u_i, u_j, \hat{n}_{ij}) \\ G(u_i, u_j, \hat{s}_{ij}) \end{bmatrix} \tag{11}$$

The flux along $\hat{n}_{ij}$ is obtained by an upwind formula

$$F(u_i, u_j, \hat{n}_{ij}) = \frac{\vec{Q}(u_i) + \vec{Q}(u_j)}{2} \cdot \hat{n}_{ij} - \frac{1}{2} |\vec{a}_{ij} \cdot \hat{n}_{ij}| (u_j - u_i) \tag{12}$$

Extension to non-linear equations and systems II

and

$$\vec{a}_{ij} = \begin{cases} \frac{\vec{Q}(u_j) - \vec{Q}(u_i)}{u_j - u_i} & \text{if } u_j \neq u_i \\ \\ \frac{\mathrm{d}}{\mathrm{d}u} \vec{Q}(u_i) & \text{if } u_j = u_i \end{cases} \tag{13}$$

while the flux along $\hat{s}_{ij}$ is given by

$$G(u_i, u_j, \hat{s}_{ij}) = \frac{\vec{Q}(u_i) + \vec{Q}(u_j)}{2} \cdot \hat{s}_{ij} - \mathrm{sign}(\bar{\beta}_{ij}) \frac{|\vec{a}_{ij} \cdot \hat{s}_{ij}|}{2} (u_j - u_i) \tag{14}$$

On the coefficients α, β I

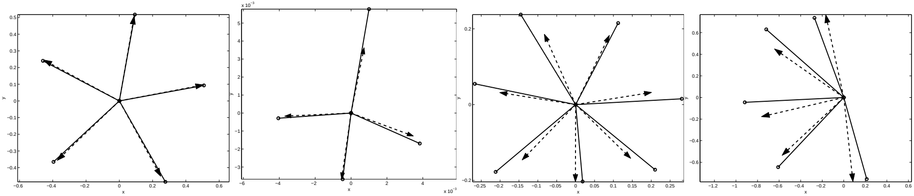
In some special situations the connectivity is such that

$$\sum_{j \in C_i} \Delta x_{ij}^2 = \sum_{j \in C_i} \Delta y_{ij}^2, \quad \sum_{j \in C_i} \Delta x_{ij} \Delta y_{ij} = 0 \tag{15}$$

then

$$\alpha_{ij} = \frac{\Delta x_{ij}}{\sum_k \Delta x_{ik}^2}, \quad \beta_{ij} = \frac{\Delta y_{ij}}{\sum_k \Delta y_{ik}^2} \quad \Longrightarrow \quad \frac{\alpha_{ij}}{\beta_{ij}} = \frac{\Delta x_{ij}}{\Delta y_{ij}}$$

and the vector $(\alpha_{ij}, \beta_{ij})$ is parallel to $(\Delta x_{ij}, \Delta y_{ij})$ so that $\bar{\beta}_{ij} = 0$.



Higher order scheme

$$u_{ij}^{+} = u_i + \frac{1}{2}\Delta\vec{r}_{ij}\cdot\nabla u_i, \quad u_{ij}^{-} = u_j - \frac{1}{2}\Delta\vec{r}_{ij}\cdot\nabla u_j \tag{16}$$

and calculate the mid-point fluxes as

$$\begin{bmatrix} F_{ij} \\ G_{ij} \end{bmatrix} = R^{-1}(\theta_{ij}) \begin{bmatrix} F(u_{ij}^{+}, u_{ij}^{-}, \hat{n}_{ij}) \\ G(u_{ij}^{+}, u_{ij}^{-}, \hat{s}_{ij}) \end{bmatrix} \tag{17}$$

$$\begin{aligned} u_{ij}^{+} &= u_i + \tfrac{s_i}{4}[(1 - ks_i)\Delta_{ij}^{-} + (1 + ks_i)(u_j - u_i)] \\ u_{ij}^{-} &= u_j - \tfrac{s_j}{4}[(1 - ks_j)\Delta_{ij}^{+} + (1 + ks_j)(u_j - u_i)] \end{aligned} \tag{18}$$

where

$$\Delta_{ij}^{-} = 2\Delta\vec{r}_{ij}\cdot\nabla u_i - (u_j - u_i), \qquad \Delta_{ij}^{+} = 2\Delta\vec{r}_{ij}\cdot\nabla u_j - (u_j - u_i) \tag{19}$$

and

$$s_i = \max\left[0, \frac{2\Delta_{ij}^{-}(u_j - u_i) + \epsilon}{(\Delta_{ij}^{-})^2 + (u_j - u_i)^2 + \epsilon}\right]$$

$$s_j = \max\left[0, \frac{2\Delta_{ij}^{+}(u_j - u_i) + \epsilon}{(\Delta_{ij}^{+})^2 + (u_j - u_i)^2 + \epsilon}\right]$$

Higher order scheme

$$u_{ij}^+ = u_i + \frac{1}{2}\Delta\vec{r}_{ij} \cdot \nabla u_i, \quad u_{ij}^- = u_j - \frac{1}{2}\Delta\vec{r}_{ij} \cdot \nabla u_j \tag{16}$$

and calculate the mid-point fluxes as

$$\begin{bmatrix} F_{ij} \\ G_{ij} \end{bmatrix} = R^{-1}(\theta_{ij}) \begin{bmatrix} F(u_{ij}^+, u_{ij}^-, \hat{n}_{ij}) \\ G(u_{ij}^+, u_{ij}^-, \hat{s}_{ij}) \end{bmatrix} \tag{17}$$

$$\begin{aligned} u_{ij}^+ &= u_i + \tfrac{s_i}{4}[(1 - ks_i)\Delta_{ij}^- + (1 + ks_i)(u_j - u_i)] \\ u_{ij}^- &= u_j - \tfrac{s_j}{4}[(1 - ks_j)\Delta_{ij}^+ + (1 + ks_j)(u_j - u_i)] \end{aligned} \tag{18}$$

where

$$\Delta_{ij}^- = 2\Delta\vec{r}_{ij} \cdot \nabla u_i - (u_j - u_i), \qquad \Delta_{ij}^+ = 2\Delta\vec{r}_{ij} \cdot \nabla u_j - (u_j - u_i) \tag{19}$$

and

$$s_i = \max\left[0, \frac{2\Delta_{ij}^-(u_j - u_i) + \epsilon}{(\Delta_{ij}^-)^2 + (u_j - u_i)^2 + \epsilon}\right]$$

$$s_j = \max\left[0, \frac{2\Delta_{ij}^+(u_j - u_i) + \epsilon}{(\Delta_{ij}^+)^2 + (u_j - u_i)^2 + \epsilon}\right]$$

NACA 0012 Test case

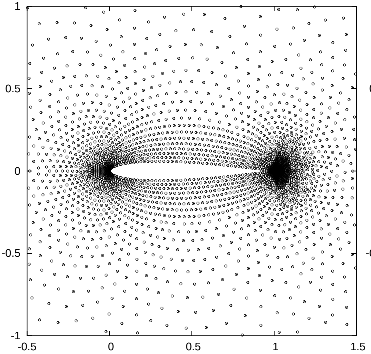
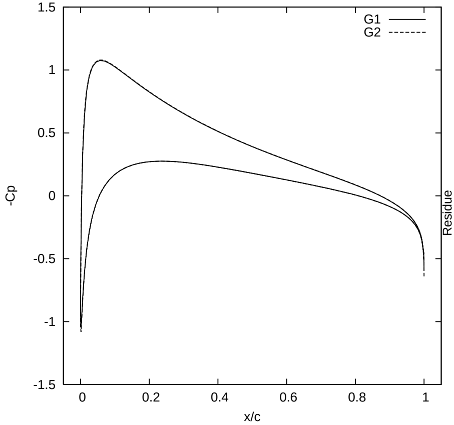


Figure: Point distributions for NACA-0012 with 4733 (G_1) and 4385 (G_2) points

Subsonic case $M_\infty = 0.63$, $\alpha = 2$ deg.



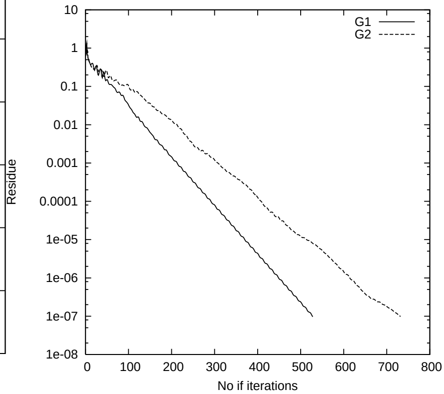
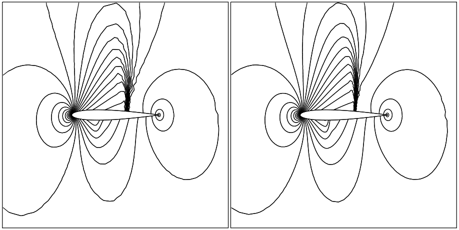


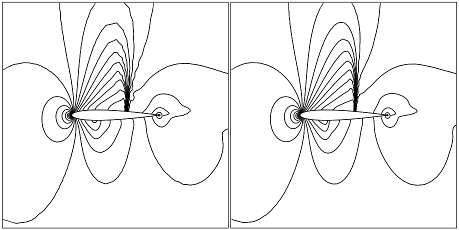
Figure: Pressure coefficient and convergence history for subsonic flow over NACA-0012

Transonic case $M_\infty = 0.80$, $\alpha = 1.25$ deg.

Pressure - G_1 and G_2

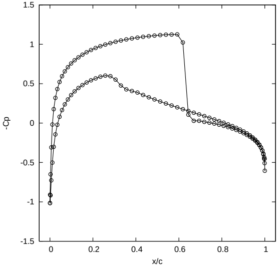


Mach number - G_1 and G_2

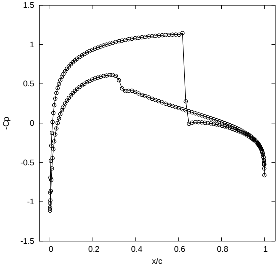


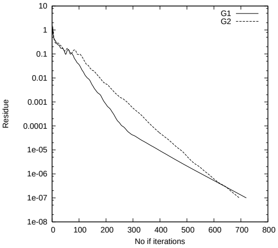
Transonic case $M_\infty = 0.80$, $\alpha = 1.25$ deg.

G_1



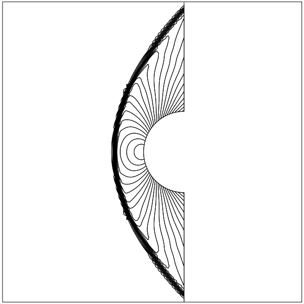
G_2



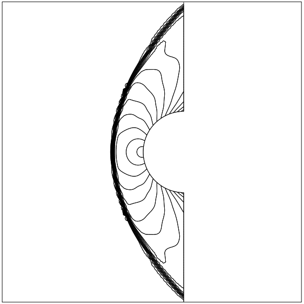


Mach 3 flow over semi-cylinder

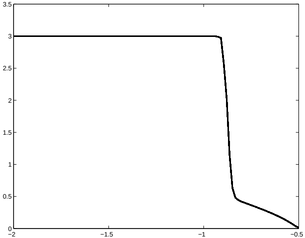
Pressure



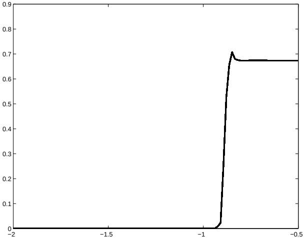
Mach



Mach number



$(p_{o1} - p_{o2})/p_{o1}$



Alternate least squares: 1-D case I

FM Report 2004-FM-16

We start by assuming a formula of the form

$$\left.\frac{\partial u}{\partial x}\right|_i = \sum_{j \in C_i} \alpha_{ij}(u_j - u_i) \tag{20}$$

and this is consistent to first order if

$$\sum_{j \in C_i} \alpha_{ij}(x_j - x_i) = 1 \tag{21}$$

Undertermined case, solve a minimization problem:

$$\min \frac{1}{2} \sum_{j \in C_i} \frac{\alpha_{ij}^2}{w_{ij}}, \quad \text{wrt} \quad \{\alpha_{ij}\} \tag{22}$$

Alternate least squares: 1-D case II

FM Report 2004-FM-16

Unconstrained minimization:

$$\min \frac{1}{2} \sum_{j \in C_i} \frac{\alpha_{ij}^2}{w_{ij}} + \lambda \left[\sum_{j \in C_i} \alpha_{ij}(x_j - x_i) - 1 \right], \quad \text{wrt} \quad \{\alpha_{ij}\}, \lambda \tag{23}$$

leads to

$$\lambda = -\frac{1}{\sum_{j \in C_i} w_{ij}(x_j - x_i)^2}, \quad \alpha_{ij} = \frac{w_{ij}(x_j - x_i)}{\sum_{k \in C_i} w_{ik}(x_k - x_i)^2}$$

which is precisely the standard least squares formula for the derivative.

Alternate LS: 2-D case

$$\left.\frac{\partial u}{\partial x}\right|_i = \sum_{j \in C_i} \alpha_{ij}(u_j - u_i), \qquad \left.\frac{\partial u}{\partial y}\right|_i = \sum_{j \in C_i} \beta_{ij}(u_j - u_i)$$

First order consistency conditions:

$$\begin{array}{ll} \sum_{j \in C_i} \alpha_{ij}(x_j - x_i) = 1, & \sum_{j \in C_i} \beta_{ij}(y_j - y_i) = 1 \\ \sum_{j \in C_i} \alpha_{ij}(y_j - y_i) = 0, & \sum_{j \in C_i} \beta_{ij}(x_j - x_i) = 0 \end{array}$$

Constrained minimization:

$$\min \frac{1}{2} \sum_{j \in C_i} \frac{\alpha_{ij}^2 + \beta_{ij}^2}{w_{ij}} \quad \text{wrt} \quad \{\alpha_{ij}\}, \{\beta_{ij}\}$$

leads to the usual formulae for derivatives. In this case $\{\alpha_{ij}\}$ and $\{\beta_{ij}\}$ are decoupled.

LS formulae leading to positive scheme

Conservation law

$$\frac{\partial u}{\partial t} + \vec{a} \cdot \nabla u = 0$$

Assume

$$\nabla u_i = \sum_{j \in C_i} c_{ij} (u_j - u_i) \hat{n}_{ij}, \quad c_{ij} \ge 0$$

and

$$\vec{a} \cdot \nabla u_i = 2 \sum_{j \in C_i} c_{ij} (\vec{a} \cdot \hat{n}_{ij})(u_{ij} - u_i)$$

Upwind flux

$$(\vec{a} \cdot \hat{n}_{ij}) u_{ij} = \frac{\vec{a} \cdot \hat{n}_{ij} + |\vec{a} \cdot \hat{n}_{ij}|}{2} u_i + \frac{\vec{a} \cdot \hat{n}_{ij} - |\vec{a} \cdot \hat{n}_{ij}|}{2} u_j$$

Semi-discrete scheme

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = -2 \sum_{j \in C_i} c_{ij} (\vec{a} \cdot \hat{n}_{ij})^{-} (u_j - u_i)$$

satisfies LED condition.

LS approximation

$$\min \frac{1}{2} \sum_{j \in C_i} \frac{c_{ij}^2}{w_{ij}}, \qquad \text{wrt} \quad \{c_{ij}\}_{j \in C_i}$$

subject to first order consistency conditions

$$\begin{aligned}
\sum_{j \in C_i} c_{ij} \frac{\Delta x_{ij}^2}{\Delta r_{ij}} &= 1 \\
\sum_{j \in C_i} c_{ij} \frac{\Delta y_{ij}^2}{\Delta r_{ij}} &= 1 \\
\sum_{j \in C_i} c_{ij} \frac{\Delta x_{ij} \Delta y_{ij}}{\Delta r_{ij}} &= 0
\end{aligned}$$

and positivity conditions

$$c_{ij} \ge 0$$

A second approach I

If

$$\sum_j w_j \Delta x_j \Delta y_j = 0, \qquad \sum_j w_j (\Delta x_j^2 - \Delta y_j^2) = 0 \tag{24}$$

Let $w_j = \omega_j w_g(\Delta r_j)$, and define

$$p_j = w_g(\Delta r_j)\Delta x_j \Delta y_j, \quad q_j = w_g(\Delta r_j)(\Delta x_j^2 - \Delta y_j^2)$$

Find ω_j from

$$\min \frac{1}{2}\sum_j (\omega_j - 1)^2 + \lambda_1 \sum_j \omega_j p_j + \lambda_2 \sum_j \omega_j q_j \quad \text{wrt} \quad \{\omega_j\}, \lambda_1, \lambda_2 \tag{25}$$

Optimality condition:

$$\begin{bmatrix} I & M \\ M^\top & 0 \end{bmatrix} \begin{bmatrix} \{\omega\} \\ \{\lambda\} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

A second approach II

where I is an $N \times N$ identity matrix and

$$M = \begin{bmatrix} p_1 & p_2 & \dots & p_N \\ q_1 & q_2 & \dots & q_N \end{bmatrix}^\top$$

Solution:

$$\begin{bmatrix} \sum p_j^2 & \sum p_j q_j \\ \sum p_j q_j & \sum q_j^2 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} \sum p_j \\ \sum q_j \end{bmatrix}$$

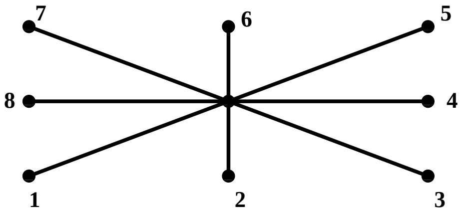
and

$$\omega_j = 1 - \lambda_1 p_j - \lambda_2 q_j$$

Does not in general guarantee that $\omega_j \geq 0$. This can be achieved by numerically solving the constrained minimization problem, and enforcing the constraint $\omega_j \geq 0$.

A second approach III

Behaviour on Cartesian stencil:



$\Delta x/\Delta y$	1,3,5,7	4,8	2,6
1	1	1	1
2	0.73529	0.55882	1.4412
10	0.51000	0.50010	1.4999
100	0.50010	0.50000	1.5000
1000	0.50000	0.50000	1.5000

Other works using alternate LS

- Positive, minimal stencil, meshfree discretization for Laplace operator
  - Seibold, 2008
- Conservative meshless discretization for conservation laws
  - Wang, Chiu, Jameson, Hu (2010)

Third order least squares scheme I

Steady solution to a conservation law

$$r = f_x + g_y = 0$$

Finite difference approximation for the residual r

$$\tilde{r} = \delta_x f + \delta_y g \tag{26}$$

Motivated by residual-based scheme of Lerat and Corre. Try to develop such a scheme for arbitrary grids.
To approximate the derivatives at node "0", we choose a stencil of neighbouring points P_j, $j = 1, \ldots, N$ and write the approximations as

$$\delta_x f = \sum_j a_j (f_j - f_0), \quad \delta_y g = \sum_j b_j (g_j - g_0)$$

Third order least squares scheme II

where the coefficients (a_j, b_j) have to be determined to satisfy some accuracy requirements. Expanding in Taylor's series we have

$$
\begin{aligned}
& \sum_j a_j (f_j - f_0) \\
= \quad & f_x \sum_j a_j \Delta x_j + f_y \sum_j a_j \Delta y_j \\
+ \quad & f_{xx} \tfrac{1}{2} \sum_j a_j \Delta x_j^2 + f_{xy} \sum_j a_j \Delta x_j \Delta y_j + f_{yy} \tfrac{1}{2} \sum_j a_j \Delta y_j^2 \\
+ \quad & f_{xxx} \frac{1}{6} \sum_j a_j \Delta x_j^3 + f_{xxy} \tfrac{1}{2} \sum_j a_j \Delta x_j^2 \Delta y_j + f_{xyy} \tfrac{1}{2} \sum_j a_j \Delta x_j \Delta y_j^2 + f_{yyy} \frac{1}{6} \sum_j a_j \Delta y_j^3 \\
+ \quad & O(h^3)
\end{aligned}
$$

Third order least squares scheme III

and

$$
\begin{aligned}
& \sum_j b_j (g_j - g_0) \\
= \quad & g_x \sum_j b_j \Delta x_j + g_y \sum_j b_j \Delta y_j \\
+ \quad & g_{xx} \tfrac{1}{2} \sum_j b_j \Delta x_j^2 + g_{xy} \sum_j b_j \Delta x_j \Delta y_j + g_{yy} \tfrac{1}{2} \sum_j b_j \Delta y_j^2 \\
+ \quad & g_{xxx} \frac{1}{6} \sum_j b_j \Delta x_j^3 + g_{xxy} \tfrac{1}{2} \sum_j b_j \Delta x_j^2 \Delta y_j + g_{xyy} \tfrac{1}{2} \sum_j b_j \Delta x_j \Delta y_j^2 + g_{yyy} \frac{1}{6} \sum_j b_j \Delta y_j^3 \\
+ \quad & O(h^3)
\end{aligned}
$$

Third order least squares scheme IV

For first order accuracy, we require

$$\sum_j a_j \Delta x_j = 1 \qquad (f_x) \tag{27}$$

$$\sum_j a_j \Delta y_j = 0 \qquad (f_y) \tag{28}$$

$$\sum_j b_j \Delta x_j = 0 \qquad (g_x) \tag{29}$$

$$\sum_j b_j \Delta y_j = 1 \qquad (g_y) \tag{30}$$

In order to maximise the accuracy of $\tilde{r}$ we will next choose conditions on (a_j, b_j) so that we can write the remaining truncation terms in terms of derivatives of r.

Third order least squares scheme V

For the second order terms, we will choose

$$\frac{1}{2}\sum_j a_j \Delta x_j^2 - \sum_j b_j \Delta x_j \Delta y_j = 0 \qquad (f_{xx}, g_{xy}) \tag{31}$$

$$\sum_j a_j \Delta x_j \Delta y_j - \frac{1}{2}\sum_j b_j \Delta y_j^2 = 0 \qquad (f_{xy}, g_{yy}) \tag{32}$$

$$\sum_j a_j \Delta y_j^2 = 0 \qquad (f_{yy}) \tag{33}$$

$$\sum_j b_j \Delta x_j^2 = 0 \qquad (g_{xx}) \tag{34}$$

For convenience, let us define the following lengths

$$h_1 = \frac{1}{2}\sum_j a_j \Delta x_j^2 \qquad h_2 = \frac{1}{2}\sum_j b_j \Delta y_j^2 \tag{35}$$

Third order least squares scheme VI

Under the conditions (27)-(34), we get

$$\begin{aligned}\tilde{r} &= f_x + g_y + h_1(f_x + g_y)_x + h_2(f_x + g_y)_y + O(h^2) \\ &= r + h_1 r_x + h_2 r_y + O(h^2) \\ &= O(h^2)\end{aligned}$$

which is second order accurate in general.

Third order least squares scheme VII

To obtain a third order accurate approximation, we require the following additional conditions

$$\frac{1}{6}\sum_j a_j \Delta x_j^3 - \frac{1}{2}\sum_j b_j \Delta x_j^2 \Delta y_j = 0 \qquad (f_{xxx}, g_{xxy}) \tag{36}$$

$$\frac{1}{2}\sum_j a_j \Delta x_j^2 \Delta y_j - \frac{1}{2}\sum_j b_j \Delta x_j \Delta y_j^2 = 0 \qquad (f_{xxy}, g_{xyy}) \tag{37}$$

$$\frac{1}{2}\sum_j a_j \Delta x_j \Delta y_j^2 - \frac{1}{6}\sum_j b_j \Delta y_j^3 = 0 \qquad (f_{xyy}, g_{yyy}) \tag{38}$$

$$\sum_j a_j \Delta y_j^3 = 0 \qquad (f_{yyy}) \tag{39}$$

$$\sum_j b_j \Delta x_j^3 = 0 \qquad (g_{xxx}) \tag{40}$$

We define the following quantities

$$h_{11} = \frac{1}{6}\sum_j a_j \Delta x_j^3, \quad h_{12} = \frac{1}{2}\sum_j a_j \Delta x_j^2 \Delta y_j, \quad h_{22} = \frac{1}{6}\sum_j b_j \Delta y_j^3 \tag{41}$$

Third order least squares scheme VIII

Under the conditions (27)-(34), (36)-(40) the approximation becomes

$$
\begin{aligned}
\tilde{r} &= r + h_1 r_x + h_2 r_y + h_{11}(f_x + g_y)_{xx} + h_{12}(f_x + g_y)_{xy} + h_{22}(f_x + g_y)_{yy} \\
&\quad + O(h^3) \\
&= r + h_1 r_x + h_2 r_y + h_{11} r_{xx} + h_{12} r_{xy} + h_{22} r_{yy} + O(h^3) \\
&= O(h^3)
\end{aligned}
$$

There are $2N$ coefficients (a_j, b_j), $j = 1, \ldots, N$ to be determined. Let us set

$$
c = [a_1, \ldots, a_N, b_1, \ldots, b_N]^\top \tag{42}
$$

Then the constraints on the coefficients can be written in matrix form

$$
Ac = d \tag{43}
$$

For the second order approximation, we have 8 constraints and hence we need $N \geq 4$ while for the third order approximation we have 13

Third order least squares scheme IX

constraints which requires $N \geq 7$. When the number of coefficients is more than the number of constraints, then we determine the coefficients from the following minimization problem

$$\min_{(a_j, b_j)} \frac{1}{2} \sum_j \frac{a_j^2 + b_j^2}{w_j^2} \qquad \text{such that} \qquad Ac = b \tag{44}$$

where the weights w_j are taken to be

$$w_j = \frac{1}{(\Delta x_j^2 + \Delta y_j^2)^{p/2}}, \quad p = 0 \text{ or } 1 \tag{45}$$

The function to be minimised is convex and we have linear constraints; hence the problem is convex. If a solution exists, then it is unique. This problem has a solution if there is atleast one vector c which satisfies the constraints.

Third order least squares scheme X

Under what geometrical conditions of the stencil, the above problem is solvable ?

In the numerical examples, we choose a 9 point stencil $(N = 8)$ on Cartesian-type grids for which we are able to solve the minimization problem to determine the coefficients (a_j, b_j) for both the second order and third order schemes.

Third order least squares scheme XI

Numerical order of accuracy

We apply the finite difference scheme to an analytical divergence-free field in the unit square $[0,1] \times [0,1]$

$$f(x,y) = -\cos(2\pi x)\sin(2\pi y), \quad g(x,y) = \sin(2\pi x)\cos(2\pi y)$$

which is divergence-free

$$f_x + g_y = 0$$

Third order least squares scheme XII

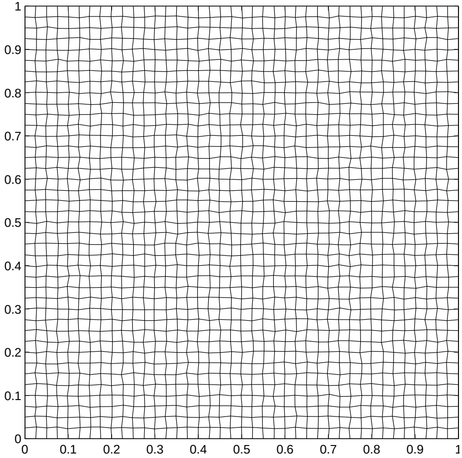


Figure: Grid of size 41×41 perturbed randomly

Third order least squares scheme XIII

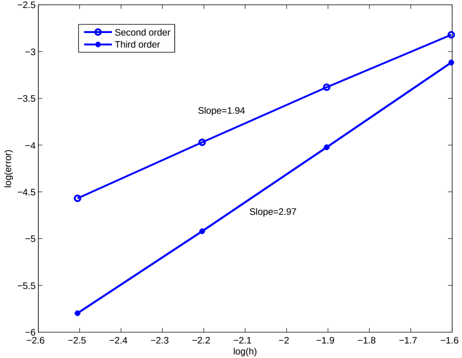


Figure: Convergence of error in divergence

Third order least squares scheme XIV

Application to conservation laws

The approximation of the divergence derived here cannot be used to solve convection dominated problems like hyperbolic conservation laws. It is necessary to add some dissipation to stabilize the numerical scheme. Lerat and Corre suggest using a dissipation that depends on the residual; hence they solve

$$w_t + f_x + g_y = \frac{\delta x}{2}(\Phi_1 r)_x + \frac{\delta y}{2}(\Phi_2 r)_y \tag{46}$$

where $\Phi_1, \Phi_2 = O(1)$. At steady state, the residual vanishes and the dissipation is of much lower order. The Φ_1, Φ_2 are chosen so that the above equation is dissipative. We have to construct an approximation to the above modified equation of the form

$$\frac{\mathrm{d}w}{\mathrm{d}t} + \delta_x f + \delta_y g = \frac{\delta x}{2}\Delta_x(\Phi_1 \bar{r}) + \frac{\delta y}{2}\Delta_y(\Phi_2 \bar{r}) \tag{47}$$

Third order least squares scheme XV

- For second order accuracy, we require $\bar{r} = O(h)$
- For third order accuracy we need $\bar{r} = O(h^2)$
- The operators Δ_x, Δ_y can be first order accurate.

Thank You