Chapter 1
Spectral Collocation - By Dorival Pedroso

1.1 Spectral collocation

Let's define the curvilinear coordinates as $a = r^1$, $b = r^2$ and $c = r^3$. Then, given the scalar field $\phi(\boldsymbol{x})$, we compute a Lagrangian approximation as

$$\phi(\boldsymbol{x}) = \phi(a, b, c) \approx \sum_{m=0}^{M} \sum_{n=0}^{N} \sum_{o=0}^{O} \phi^{\star}_{mno}\, \ell_m(a)\, \bar{\ell}_n(b)\, \bar{\bar{\ell}}_o(c) \tag{1.1}$$

where $\phi^{\star}_{mno}$ is the approximation at grid node (m, n, o) such that

$$\phi^{\star}_{mno} = \phi(a_m, b_n, c_o) \tag{1.2}$$

First order derivatives

$$\begin{cases} \dfrac{\partial \phi}{\partial a} = \phi^{\star}_{mno}\, \dfrac{\partial \ell_m}{\partial a}\, \bar{\ell}_n\, \bar{\bar{\ell}}_o \\ \dfrac{\partial \phi}{\partial b} = \phi^{\star}_{mno}\, \ell_m\, \dfrac{\partial \bar{\ell}_n}{\partial b}\, \bar{\bar{\ell}}_o \\ \dfrac{\partial \phi}{\partial c} = \phi^{\star}_{mno}\, \ell_m\, \bar{\ell}_n\, \dfrac{\partial \bar{\bar{\ell}}_o}{\partial c} \end{cases} \tag{1.3}$$

Second order derivatives

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial a^2} = \phi^{\star}_{mno}\, \dfrac{\partial^2 \ell_m}{\partial a^2}\, \bar{\ell}_n\, \bar{\bar{\ell}}_o \\ \dfrac{\partial^2 \phi}{\partial b^2} = \phi^{\star}_{mno}\, \ell_m\, \dfrac{\partial^2 \bar{\ell}_n}{\partial b^2}\, \bar{\bar{\ell}}_o \\ \dfrac{\partial^2 \phi}{\partial c^2} = \phi^{\star}_{mno}\, \ell_m\, \bar{\ell}_n\, \dfrac{\partial^2 \bar{\bar{\ell}}_o}{\partial c^2} \end{cases} \tag{1.4}$$

and

$$\begin{cases} \dfrac{\partial^2\phi}{\partial a\partial b} = \phi^\star_{mno}\,\dfrac{\partial\ell_m}{\partial a}\,\dfrac{\partial\bar{\ell}_n}{\partial b}\,\bar{\bar{\ell}}_o \\ \dfrac{\partial^2\phi}{\partial b\partial c} = \phi^\star_{mno}\,\ell_m\,\dfrac{\partial\bar{\ell}_n}{\partial b}\,\dfrac{\partial\bar{\bar{\ell}}_o}{\partial c} \\ \dfrac{\partial^2\phi}{\partial c\partial a} = \phi^\star_{mno}\,\dfrac{\partial\ell_m}{\partial a}\,\bar{\ell}_n\,\dfrac{\partial\bar{\bar{\ell}}_o}{\partial c} \end{cases} \tag{1.5}$$

Definitions

$$\begin{cases} D_{pm} = \left.\dfrac{\partial\ell_m}{\partial a}\right|_{a_p,b,c} \\ \bar{D}_{qn} = \left.\dfrac{\partial\bar{\ell}_n}{\partial b}\right|_{a,b_q,c} \\ \bar{\bar{D}}_{so} = \left.\dfrac{\partial\bar{\bar{\ell}}_o}{\partial c}\right|_{a,b,c_s} \end{cases} \quad\text{and}\quad \begin{cases} D^2_{pm} = \left.\dfrac{\partial^2\ell_m}{\partial a^2}\right|_{a_p,b,c} \\ \bar{D}^2_{qn} = \left.\dfrac{\partial^2\bar{\ell}_n}{\partial b^2}\right|_{a,b_q,c} \\ \bar{\bar{D}}^2_{so} = \left.\dfrac{\partial^2\bar{\bar{\ell}}_o}{\partial c^2}\right|_{a,b,c_s} \end{cases} \tag{1.6}$$

Thus

$$\begin{cases} \left.\dfrac{\partial\phi}{\partial a}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,D_{pm}\,\delta_{qn}\,\delta_{so} \\ \left.\dfrac{\partial\phi}{\partial b}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,\delta_{pm}\,\bar{D}_{qn}\,\delta_{so} \\ \left.\dfrac{\partial\phi}{\partial c}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,\delta_{pm}\,\delta_{qn}\,\bar{\bar{D}}_{so} \end{cases} \tag{1.7}$$

and

$$\begin{cases} \left.\dfrac{\partial^2\phi}{\partial a^2}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,D^2_{pm}\,\delta_{qn}\,\delta_{so} \\ \left.\dfrac{\partial^2\phi}{\partial b^2}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,\delta_{pm}\,\bar{D}^2_{qn}\,\delta_{so} \\ \left.\dfrac{\partial^2\phi}{\partial c^2}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,\delta_{pm}\,\delta_{qn}\,\bar{\bar{D}}^2_{so} \end{cases} \tag{1.8}$$

and

$$\begin{cases} \left.\dfrac{\partial^2\phi}{\partial a\partial b}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,D_{pm}\,\bar{D}_{qn}\,\delta_{so} \\ \left.\dfrac{\partial^2\phi}{\partial b\partial c}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,\delta_{pm}\,\bar{D}_{qn}\,\bar{\bar{D}}_{so} \\ \left.\dfrac{\partial^2\phi}{\partial c\partial a}\right|_{a_p,b_q,c_s} = \phi^\star_{mno}\,D_{pm}\,\delta_{qn}\,\bar{\bar{D}}_{so} \end{cases} \tag{1.9}$$

1.2 Gradients in 2D

The gradient is given by

$$\underset{\cdot}{\boldsymbol{\nabla}}\,\phi = \frac{\partial \phi}{\partial a}\,\underset{\cdot}{\boldsymbol{g}}^1 + \frac{\partial \phi}{\partial b}\,\underset{\cdot}{\boldsymbol{g}}^2 \tag{1.10}$$

Thus, at a grid node (a_p, b_q),

$$\underset{\cdot}{\boldsymbol{\nabla}}\,\phi\big|_{a_p,b_q} = \left(D_{pm}\,\delta_{qn}\;\underset{\cdot}{\boldsymbol{g}}^1\Big|_{a_p,b_q} + \delta_{pm}\,\bar{D}_{qn}\;\underset{\cdot}{\boldsymbol{g}}^2\Big|_{a_p,b_q} \right)\phi^\star_{mn} \tag{1.11}$$

The flux at grid node (a_p, b_q) is

$$\underset{\cdot}{\boldsymbol{\nabla}}\,\phi \boldsymbol{\cdot} \underset{\cdot}{\hat{\boldsymbol{n}}}\big|_{a_p,b_q} = \bar{G}_{pqmn}\,\phi^\star_{mn} \tag{1.12}$$

where

$$\bar{G}_{pqmn} = D_{pm}\,\delta_{qn}\,\alpha + \delta_{pm}\,\bar{D}_{qn}\,\beta \tag{1.13}$$

and

$$\alpha = \underset{\cdot}{\hat{\boldsymbol{n}}} \boldsymbol{\cdot} \underset{\cdot}{\boldsymbol{g}}^1\Big|_{a_p,b_q} \qquad \text{and} \qquad \beta = \underset{\cdot}{\hat{\boldsymbol{n}}} \boldsymbol{\cdot} \underset{\cdot}{\boldsymbol{g}}^2\Big|_{a_p,b_q} \tag{1.14}$$

1.3 Laplacian in 2D

In curvilinear coordinates, the 2D Laplacian is given by

$$\nabla^2\phi = \frac{\partial^2 \phi}{\partial a^2}\,g^{11} + \frac{\partial^2 \phi}{\partial b^2}\,g^{22} + \frac{\partial^2 \phi}{\partial a \partial b}\,2g^{12} - \frac{\partial \phi}{\partial a}\,L^1 - \frac{\partial \phi}{\partial b}\,L^2 \tag{1.15}$$

Thus, at a grid node (a_p, b_q),

$$\nabla^2\phi\big|_{a_p,b_q} = \bar{K}_{pqmn}\,\phi^\star_{mn} \tag{1.16}$$

where

$$\begin{aligned}\bar{K}_{pqmn} = {} & D^2_{pm}\,\delta_{qn}\;\; g^{11}\big|_{a_p,b_q} \\ & + \delta_{pm}\,\bar{D}^2_{qn}\;\; g^{22}\big|_{a_p,b_q} \\ & + D_{pm}\,\bar{D}_{qn}\,2\;g^{12}\big|_{a_p,b_q} \\ & - D_{pm}\,\delta_{qn}\;\; L_1\big|_{a_p,b_q} \\ & - \delta_{pm}\,\bar{D}_{qn}\;\; L_2\big|_{a_p,b_q}\end{aligned} \tag{1.17}$$

Assuming a *lexicographic* ordering of nodes, each pair of grid indices (m, n) is mapped into a unique identifier using the following function

$$\iota(m,n) = m + n\, N_1 \tag{1.18}$$

where N_1 is the number of points along the 1-direction. For a known identifier I, the inverse mapping allows the computation of the grid indices as follows

$$\begin{cases} m = I \,\%\, N_1 \\ n = I \,/\, N_1 \end{cases} \tag{1.19}$$

where the symbol "%" represents the remainder (modulo) operator. Now we can write the discretised Laplacian in matrix notation as follows

$$\{\nabla^2 \phi\} = \boldsymbol{K}\, \boldsymbol{u} \tag{1.20}$$

where the components of the matrix $\boldsymbol{K}$ are given by

$$K_{\iota(p,q)\ \iota(m,n)} = \bar{K}_{pqmn} \tag{1.21}$$

and the components of the vector $\boldsymbol{u}$ are

$$u_{\iota(m,n)} = \phi^{\star}_{mn} \tag{1.22}$$

1.4 Laplacian in 3D

In curvilinear coordinates, the 3D Laplacian is given by

$$\begin{aligned} \nabla^2\phi = & \frac{\partial^2\phi}{\partial a\partial a}\, g^{11} + \frac{\partial^2\phi}{\partial b\partial b}\, g^{22} + \frac{\partial^2\phi}{\partial c\partial c}\, g^{33} \\ & + \frac{\partial^2\phi}{\partial a\partial b}\, 2g^{12} + \frac{\partial^2\phi}{\partial b\partial c}\, 2g^{23} + \frac{\partial^2\phi}{\partial c\partial a}\, 2g^{31} \\ & - \frac{\partial\phi}{\partial a}\, L^1 - \frac{\partial\phi}{\partial b}\, L^2 - \frac{\partial\phi}{\partial c}\, L^3 \end{aligned} \tag{1.23}$$

Thus, at a grid node (a_p, b_q, c_o),

$$\nabla^2\phi\big|_{a_p,b_q,c_o} = \bar{K}_{pqsmno}\, \phi^{\star}_{mno} \tag{1.24}$$

where

$$\begin{aligned}
\bar{K}_{pqsmno} = {} & D^2_{pm}\,\delta_{qn}\,\delta_{so}\;\; g^{11}\big|_{a_p,b_q,c_o} \\
& + \delta_{pm}\,\bar{D}^2_{qn}\,\delta_{so}\;\; g^{22}\big|_{a_p,b_q,c_o} \\
& + \delta_{pm}\,\delta_{qn}\,\bar{\bar{D}}^2_{so}\;\; g^{33}\big|_{a_p,b_q,c_o} \\
& + D_{pm}\,\bar{D}_{qn}\,\delta_{so}\,2\;g^{12}\big|_{a_p,b_q,c_o} \\
& + \delta_{pm}\,\bar{D}_{qn}\,\bar{\bar{D}}_{so}\,2\;g^{23}\big|_{a_p,b_q,c_o} \\
& + D_{pm}\,\delta_{qn}\,\bar{\bar{D}}_{so}\,2\;g^{31}\big|_{a_p,b_q,c_o} \\
& + D_{pm}\,\delta_{qn}\,\delta_{so}\;\; L^1\big|_{a_p,b_q,c_o} \\
& + \delta_{pm}\,\bar{D}_{qn}\,\delta_{so}\;\; L^2\big|_{a_p,b_q,c_o} \\
& + \delta_{pm}\,\delta_{qn}\,\bar{\bar{D}}_{so}\;\; L^3\big|_{a_p,b_q,c_o}
\end{aligned} \tag{1.25}$$

Assuming a *lexicographic* ordering of nodes, each triple of grid indices (m, n, o) is mapped into a unique identifier using the following function

$$\iota(m, n, o) = m + n\,N_1 + o\,N_1\,N_2 \tag{1.26}$$

where N_1 is the number of points along the 1-direction and N_2 is the number of points along the 2-direction. For a known identifier I, the inverse mapping allows the computation of the grid indices as follows

$$\begin{cases} m = [I \,\%\, (N_1 N_2)] \,\%\, N_1 \\ n = [I \,\%\, (N_1 N_2)] \,/\, N_1 \\ o = I \,/\, (N_1 N_2) \end{cases} \tag{1.27}$$

Now we can write the discretised Laplacian in matrix notation as follows

$$\{\nabla^2 \phi\} = \boldsymbol{K}\,\boldsymbol{u} \tag{1.28}$$

where the components of the matrix $\boldsymbol{K}$ are given by

$$K_{\iota(p,q,s)\ \iota(m,n,o)} = \bar{K}_{pqsmno} \tag{1.29}$$

and the components of the vector $\boldsymbol{u}$ are

$$u_{\iota(m,n,o)} = \phi^{\star}_{mno} \tag{1.30}$$