Chapter 12

Fourth-order Finite Volume (FV) Methods

Notation 9. We discretize a rectangular problem domain Ω into a collection of rectangular grid cells. Each cell is denoted by a multi-index $\mathbf{i} \in \mathbb{Z}^{\mathrm{D}}$, its region by

$$\mathcal{C}_{\mathbf{i}} = \left[\mathbf{x}_O + \mathbf{i}h,\ \mathbf{x}_O + (\mathbf{i} + \mathbb{1})\, h\right], \tag{12.1}$$

and the region of its higher face in dimension d by

$$\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \left[\mathbf{x}_O + \left(\mathbf{i} + \mathbf{e}^d\right) h,\ \mathbf{x}_O + (\mathbf{i} + \mathbb{1})\, h\right], \tag{12.2}$$

where $\mathbf{x}_O \in \mathbb{R}^{\mathrm{D}}$ is some fixed origin of the coordinates, h the uniform mesh spacing, $\mathbb{1} \in \mathbb{Z}^{\mathrm{D}}$ the multi-index with all its components equal to one, and $\mathbf{e}^d \in \mathbb{Z}^{\mathrm{D}}$ a multi-index with 1 as its d-th component and 0 otherwise.

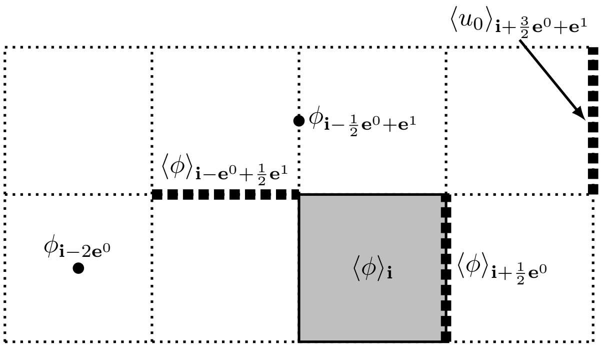
12.1 The FV formulation

Definition 12.1. The *cell average* of a function $\phi : \mathbb{R}^{\mathrm{D}} \to \mathbb{R}$ over the cell $\mathbf{i}$ is a function $\mathbb{Z}^{\mathrm{D}} \to \mathbb{R}$ given by

$$\langle \phi \rangle_{\mathbf{i}} = \frac{1}{h^{\mathrm{D}}} \int_{\mathcal{C}_{\mathbf{i}}} \phi\,(\mathbf{x})\ \mathrm{d}\mathbf{x}. \tag{12.3}$$

Definition 12.2. The *face average* of a function $\phi : \mathbb{R}^{\mathrm{D}} \to \mathbb{R}$ over the face $\mathbf{i} + \frac{1}{2}\mathbf{e}^d$ is a function $\mathbb{Z}^{\mathrm{D}} \to \mathbb{R}$ given by

$$\langle \phi \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \frac{1}{h^{\mathrm{D}-1}} \int_{\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}} \phi\,(\mathbf{x})\ \mathrm{d}\mathbf{x}. \tag{12.4}$$



Notation 10. We strictly distinguishes three different types of quantities, viz. point values, cell averages, and face averages. A symbol without the averaging operator $\langle\cdot\rangle$ denotes a point value; otherwise it denotes either a cell-averaged value if the subscript is an integer multi-index, or a face-averaged value if the subscript is a fractional multi-index. In the above plot, $\phi_{\mathbf{i}-2\mathbf{e}^0}$, and $\phi_{\mathbf{i}-\frac{1}{2}\mathbf{e}^0+\mathbf{e}^1}$ are point values; $\langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^0}, \langle\phi\rangle_{\mathbf{i}-\mathbf{e}^0+\frac{1}{2}\mathbf{e}^1}$, and $\langle u_0\rangle_{\mathbf{i}+\frac{3}{2}\mathbf{e}^0+\mathbf{e}^1}$ are face-averaged values; $\langle\phi\rangle_{\mathbf{i}}$ is a cell-averaged. Horizontal and vertical bold dotted lines represent the averaging processes over a vertical cell face and a horizontal cell face, respectively. Light gray area represents averaging over a cell.

Lemma 12.3. Point values can be converted to face averages and cell averages to the fourth-order accuracy via

$$\langle \phi \rangle_{\mathbf{i}} = \phi_{\mathbf{i}} + \frac{h^2}{24} \sum_{d=1}^{\mathrm{D}} \left.\frac{\partial^2 \phi(\mathbf{x})}{\partial x_d^2}\right|_{\mathbf{i}} + O(h^4), \tag{12.5}$$

$$\langle \phi \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \phi_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{24} \sum_{d' \neq d} \left.\frac{\partial^2 \phi(\mathbf{x})}{\partial x_{d'}^2}\right|_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^4). \tag{12.6}$$

Proof. The above identities follow from Taylor expansions of the integrands in (12.3) and (12.4). □

Theorem 12.4. Cell averages can be converted to face averages to the fourth-order accuracy via

$$\begin{aligned} \langle \phi \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} =& \frac{7}{12}\Big(\langle\phi\rangle_{\mathbf{i}} + \langle\phi\rangle_{\mathbf{i}+\mathbf{e}^d}\Big) \\ & - \frac{1}{12}\Big(\langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d} + \langle\phi\rangle_{\mathbf{i}+2\mathbf{e}^d}\Big) + O(h^4), \end{aligned} \tag{12.7}$$

$$\begin{aligned} \left\langle \frac{\partial \phi}{\partial x_d} \right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} =& \frac{15}{12h}\Big(\langle\phi\rangle_{\mathbf{i}+\mathbf{e}^d} - \langle\phi\rangle_{\mathbf{i}}\Big) \\ & - \frac{1}{12h}\Big(\langle\phi\rangle_{\mathbf{i}+2\mathbf{e}^d} - \langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d}\Big) + O(h^4). \end{aligned} \tag{12.8}$$

Proof. We prove (12.7) and (12.8) via the first fundamental theorem of calculus (Theorem C.65). Let

$$\Phi(x) = \int_{\xi}^{x} \phi(x')\,\mathrm{d}x' \tag{12.9}$$

denote an indefinite integral with its lower limit ξ fixed. The average of ϕ over the interval $[i-\frac{1}{2}, i+\frac{1}{2}]h$ can be obtained by

$$\begin{aligned} h\langle\phi\rangle_i &= \delta\Phi_i := \Phi_{i+\frac{1}{2}} - \Phi_{i-\frac{1}{2}} \\ &= \Phi\left(\left(i+\frac{1}{2}\right)h\right) - \Phi\left(\left(i-\frac{1}{2}\right)h\right). \end{aligned} \tag{12.10}$$

Then Theorem C.65 yields

$$\phi(x) = \frac{\partial\Phi}{\partial x}. \tag{12.11}$$

Taylor expansions of $\Phi_{i+\frac{3}{2}}$, $\Phi_{i-\frac{1}{2}}$, $\Phi_{i+\frac{5}{2}}$, $\Phi_{i-\frac{3}{2}}$ at $(i+\frac{1}{2})h$ yield

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 2 & 4 & 8 & 16 \\ -2 & 4 & -8 & 16 \end{bmatrix} \begin{bmatrix} h & & & \\ & \frac{h^2}{2} & & \\ & & \frac{h^3}{6} & \\ & & & \frac{h^4}{24} \end{bmatrix} \begin{bmatrix} \frac{\partial\Phi}{\partial x} \\ \frac{\partial^2\Phi}{\partial x^2} \\ \frac{\partial^3\Phi}{\partial x^3} \\ \frac{\partial^4\Phi}{\partial x^4} \end{bmatrix}_{i+\frac{1}{2}}$$

$$= \begin{bmatrix} \delta\Phi_{i+1} \\ -\delta\Phi_i \\ \delta\Phi_{i+1} + \delta\Phi_{i+2} \\ -\delta\Phi_{i-1} - \delta\Phi_i \end{bmatrix} + O(h^5). \tag{12.12}$$

Hence

$$\begin{bmatrix} h\phi \\ h^2\frac{\partial\phi}{\partial x} \\ h^3\frac{\partial^2\phi}{\partial x^2} \\ h^4\frac{\partial^3\phi}{\partial x^3} \end{bmatrix}_{i+\frac{1}{2}} = \mathbf{C} \begin{bmatrix} \delta\Phi_{i+1} \\ -\delta\Phi_i \\ \delta\Phi_{i+1} + \delta\Phi_{i+2} \\ -\delta\Phi_{i-1} - \delta\Phi_i \end{bmatrix} + O(h^5), \tag{12.13}$$

where

$$\mathbf{C} = \begin{bmatrix} \frac{2}{3} & -\frac{2}{3} & -\frac{1}{12} & \frac{1}{12} \\ \frac{4}{3} & \frac{4}{3} & -\frac{1}{12} & -\frac{1}{12} \\ -1 & 1 & \frac{1}{2} & -\frac{1}{2} \\ -4 & -4 & 1 & 1 \end{bmatrix}.$$

Construct an auxiliary matrix

$$\mathbf{M} = \begin{bmatrix} 1 & & & \\ & -1 & & \\ -1 & & 1 & \\ & 1 & & -1 \end{bmatrix}, \tag{12.14}$$

add $\mathbf{M}^{-1}\mathbf{M}$ into the middle of the right-hand side of (12.13), and we have

$$\begin{bmatrix} \phi \\ h\frac{\partial\phi}{\partial x} \\ h^2\frac{\partial^2\phi}{\partial x^2} \\ h^3\frac{\partial^3\phi}{\partial x^3} \end{bmatrix}_{i+\frac{1}{2}} = \mathbf{T}^{(4)} \begin{bmatrix} \langle\phi\rangle_{i+1} \\ \langle\phi\rangle_i \\ \langle\phi\rangle_{i+2} \\ \langle\phi\rangle_{i-1} \end{bmatrix} + O(h^4), \tag{12.15}$$

where the fourth-order interpolation matrix $\mathbf{T}^{(4)}$ is

$$\mathbf{T}^{(4)} = \begin{bmatrix} \frac{7}{12} & \frac{7}{12} & -\frac{1}{12} & -\frac{1}{12} \\ \frac{5}{4} & -\frac{5}{4} & -\frac{1}{12} & \frac{1}{12} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -3 & 3 & 1 & -1 \end{bmatrix}. \tag{12.16}$$

In a multidimensional space, averaging the first row of (12.15) over all other dimensions yields (12.7). The second row of (12.17) and the average of an equation similar to (12.15) yield (12.8). □

Exercise 12.5. Repeat the procedures in the above proof to generate the fifth-order interpolation matrix

$$\mathbf{T}^{(5)} = \begin{bmatrix} \frac{47}{60} & \frac{9}{20} & -\frac{13}{60} & -\frac{1}{20} & \frac{1}{30} \\ \frac{5}{4} & -\frac{5}{4} & -\frac{1}{12} & \frac{1}{12} & 0 \\ -2 & \frac{1}{2} & \frac{3}{2} & \frac{1}{4} & -\frac{1}{4} \\ -3 & 3 & 1 & -1 & 0 \\ 6 & -4 & -4 & 1 & 1 \end{bmatrix}, \tag{12.17}$$

where the additional column is associated with $\langle\phi\rangle_{i+3}$. Explain why the formulas of the fourth order and the fifth order coincide for $\frac{\partial\phi}{\partial x}$.

12.2 Discrete operators

Definition 12.6. The *discrete gradient*, the *discrete divergence*, and the *discrete Laplacian* are defined as

$$\mathbf{G}_d\langle\phi\rangle_{\mathbf{i}} = \frac{1}{12h}\Big(-\langle\phi\rangle_{\mathbf{i}+2\mathbf{e}^d} + 8\langle\phi\rangle_{\mathbf{i}+\mathbf{e}^d} - 8\langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d} + \langle\phi\rangle_{\mathbf{i}-2\mathbf{e}^d}\Big), \tag{12.18}$$

$$\begin{aligned} \mathbf{D}\langle\mathbf{u}\rangle_{\mathbf{i}} = \frac{1}{12h}\sum_d \Big(&-\langle u_d\rangle_{\mathbf{i}+2\mathbf{e}^d} + 8\langle u_d\rangle_{\mathbf{i}+\mathbf{e}^d} - 8\langle u_d\rangle_{\mathbf{i}-\mathbf{e}^d} \\ &+ \langle u_d\rangle_{\mathbf{i}-2\mathbf{e}^d}\Big), \end{aligned} \tag{12.19}$$

$$\begin{aligned} \mathbf{L}\langle\phi\rangle_{\mathbf{i}} = \frac{1}{12h^2}\sum_d \Big(&-\langle\phi\rangle_{\mathbf{i}+2\mathbf{e}^d} + 16\langle\phi\rangle_{\mathbf{i}+\mathbf{e}^d} - 30\langle\phi\rangle_{\mathbf{i}} \\ &+ 16\langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d} - \langle\phi\rangle_{\mathbf{i}-2\mathbf{e}^d}\Big). \end{aligned} \tag{12.20}$$

The discrete divergence operator also acts on tensor averages,

$$\mathbf{D}\langle\mathbf{uu}\rangle_{\mathbf{i}} = \frac{1}{h}\sum_d \Big(\mathbf{F}\langle u_d, \mathbf{u}\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} - \mathbf{F}\langle u_d, \mathbf{u}\rangle_{\mathbf{i}-\frac{1}{2}\mathbf{e}^d}\Big), \tag{12.21}$$

where the discrete face average of the product of two scalar functions is

$$\begin{aligned} \mathbf{F}\langle\phi,\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = &\langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \\ &+ \frac{h^2}{12}\sum_{d'\neq d}\left(\mathbf{G}^{\perp}_{d'}\phi\right)_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\left(\mathbf{G}^{\perp}_{d'}\psi\right)_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}, \end{aligned} \tag{12.22}$$

and $\mathbf{G}^{\perp}_{d'}$ is the discrete gradient operator in the transverse directions,

$$\left(\mathbf{G}^{\perp}_{d'}\phi\right)_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \frac{1}{2h}\left(\langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d+\mathbf{e}^{d'}} - \langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d-\mathbf{e}^{d'}}\right). \tag{12.23}$$

Lemma 12.7. The operators in Definition 12.6 are fourth-order accurate, i.e.,

$$\mathbf{G}_d \langle\phi\rangle_{\mathbf{i}} = \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}} \frac{\partial \phi}{\partial x_d} + O(h^4), \tag{12.24a}$$

$$\mathbf{D} \langle\mathbf{u}\rangle_{\mathbf{i}} = \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}} \nabla\cdot\mathbf{u} + O(h^4), \tag{12.24b}$$

$$\mathbf{L} \langle\phi\rangle_{\mathbf{i}} = \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}} \nabla^2\phi + O(h^4), \tag{12.24c}$$

$$\mathbf{D} \langle\mathbf{u}\rangle_{\mathbf{i}} = O(h^4) \;\Rightarrow\; \mathbf{D} \langle\mathbf{uu}\rangle_{\mathbf{i}} = \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}} (\mathbf{u}\cdot\nabla)\mathbf{u} + O(h^4), \tag{12.24d}$$

$$\mathbf{F} \langle\phi,\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \frac{1}{h^{\mathrm{D}-1}}\int_{\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}} \phi\psi + O(h^4). \tag{12.24e}$$

Proof. (12.24a) follows from (12.7), the second fundamental theorem of calculus, and the fact that $\frac{\partial}{\partial x_d}$ commutes with $\langle\cdot\rangle$. (12.24b) follows from the divergence theorem and (12.7). (12.24c) follows from the divergence theorem and (12.8). The rest of the proof concerns (12.24d) and (12.24e).

Denote the cell center of $\mathcal{C}_{\mathbf{i}}$ by $\mathbf{x}_{\mathbf{i}} = \left(\mathbf{i}+\frac{1}{2}\mathbb{1}\right)h$, and the face centers by $\mathbf{x}_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} = \mathbf{x}_{\mathbf{i}} \pm \frac{h}{2}\mathbf{e}^d$. Let $\mathbf{x}_c = \mathbf{x}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$ be the center of $\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$. Then the Taylor series of a function ϕ about $\mathbf{x}_c$ can be expressed in multi-index notation as

$$\begin{aligned}\phi(\mathbf{x}) &= \sum_{|\mathbf{j}|\le 3}\frac{1}{\mathbf{j}!}(\mathbf{x}-\mathbf{x}_c)^{\mathbf{j}}\phi^{(\mathbf{j})}(\mathbf{x}_c) + O(h^4)\\ &= \sum_{|\mathbf{j}|\le 3}\frac{1}{\mathbf{j}!}\boldsymbol{\eta}^{\mathbf{j}}\phi^{(\mathbf{j})}(\mathbf{x}_c) + O(h^4),\end{aligned} \tag{12.25}$$

where $\boldsymbol{\eta} = \mathbf{x}-\mathbf{x}_c$, so that $\eta_d = 0$ and $|\boldsymbol{\eta}| \approx O(h)$ on $\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$.

Then the product of two functions $\phi,\psi : \mathbb{R}^{\mathrm{D}} \to \mathbb{R}$ is

$$\begin{aligned}\phi(\mathbf{x})\psi(\mathbf{x}) &= \left(\sum_{|\mathbf{j}|\le 3}\frac{1}{\mathbf{j}!}\boldsymbol{\eta}^{\mathbf{j}}\phi^{(\mathbf{j})}(\mathbf{x}_c)\right)\left(\sum_{|\mathbf{k}|\le 3}\frac{1}{\mathbf{k}!}\boldsymbol{\eta}^{\mathbf{k}}\psi^{(\mathbf{k})}(\mathbf{x}_c)\right)\\ &\quad + O(h^4)\\ &= \sum_{\mathbf{k}:|\mathbf{k}|\le 3}\frac{1}{\mathbf{k}!}\boldsymbol{\eta}^{\mathbf{k}}\sum_{\mathbf{j}:\mathbf{j}\le\mathbf{k}}\binom{\mathbf{k}}{\mathbf{j}}\phi^{(\mathbf{j})}(\mathbf{x}_c)\psi^{(\mathbf{k}-\mathbf{j})}(\mathbf{x}_c)\\ &\quad + O(h^4),\end{aligned}$$

where the second step follows from a variable substitution. Then the average over $\mathcal{F}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$ (dropping indices on $\mathcal{F}$ and evaluation at $\mathbf{x}_c$) is

$$\begin{aligned}&\frac{1}{h^{\mathrm{D}-1}}\int_{\mathcal{F}}\phi\psi\,\mathrm{d}\mathbf{x}\\ =&\frac{1}{h^{\mathrm{D}-1}}\int_{\mathcal{F}}\sum_{\mathbf{k}:|\mathbf{k}|\le 3}\frac{1}{\mathbf{k}!}\boldsymbol{\eta}^{\mathbf{k}}\sum_{\mathbf{j}:\mathbf{j}\le\mathbf{k}}\binom{\mathbf{k}}{\mathbf{j}}\phi^{(\mathbf{j})}\psi^{(\mathbf{k}-\mathbf{j})}\,\mathrm{d}\mathbf{x} + O(h^4)\\ =& \sum_{\mathbf{k}:|\mathbf{k}|\le 3}\frac{1}{\mathbf{k}!}\left(\frac{1}{h^{\mathrm{D}-1}}\int_{\mathcal{F}}\boldsymbol{\eta}^{\mathbf{k}}\,\mathrm{d}\mathbf{x}\right)\sum_{\mathbf{j}:\mathbf{j}\le\mathbf{k}}\binom{\mathbf{k}}{\mathbf{j}}\phi^{(\mathbf{j})}\psi^{(\mathbf{k}-\mathbf{j})} + O(h^4).\end{aligned}$$

If $k_d \neq 0$ or $\mathbf{k}$ is odd in any component, then $\int_{\mathcal{F}}\boldsymbol{\eta}^{\mathbf{k}}\,\mathrm{d}\mathbf{x} = 0$. Hence, the only nonzero terms come from the two cases $\mathbf{k}=\mathbf{0}$, $\mathbf{j}=\mathbf{0}$ and $\mathbf{k}=2\mathbf{e}^{d'}$, $\mathbf{j}=\mathbf{0},\mathbf{e}^{d'},2\mathbf{e}^{d'}$ with $d'\neq d$. Thus,

$$\begin{aligned}&\frac{1}{h^{\mathrm{D}-1}}\int_{\mathcal{F}}\phi\psi\,\mathrm{d}\mathbf{x}\\ =&\phi\psi + \frac{h^2}{24}\sum_{d'\neq d}\left(\phi^{\left(2\mathbf{e}^{d'}\right)}\psi + \psi^{\left(2\mathbf{e}^{d'}\right)}\phi\right)\\ &+ \frac{h^2}{12}\sum_{d'\neq d}\left(\phi^{\left(\mathbf{e}^{d'}\right)}\psi^{\left(\mathbf{e}^{d'}\right)}\right) + O(h^4)\\ =&\left(\phi + \frac{h^2}{24}\sum_{d'\neq d}\phi^{\left(2\mathbf{e}^{d'}\right)}\right)\left(\psi + \frac{h^2}{24}\sum_{d'\neq d}\psi^{\left(2\mathbf{e}^{d'}\right)}\right)\\ &+ \frac{h^2}{12}\sum_{d'\neq d}\left(\phi^{\left(\mathbf{e}^{d'}\right)}\psi^{\left(\mathbf{e}^{d'}\right)}\right) + O(h^4)\\ =&\langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{12}\sum_{d'\neq d}\left(\phi^{\left(\mathbf{e}^{d'}\right)}\psi^{\left(\mathbf{e}^{d'}\right)}\right) + O(h^4),\end{aligned}$$

where we have used (12.6) to convert the first two terms in parentheses to face averages. The last term representing the product of transverse gradients can be approximated with

$$\begin{aligned}\mathbf{G}^{\perp}_{d'}\phi\big|_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} &= \frac{1}{2h}\left(\langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d+\mathbf{e}^{d'}} - \langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d-\mathbf{e}^{d'}}\right)\\ &= \frac{\partial\phi}{\partial x_{d'}}\bigg|_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^2),\end{aligned}$$

leading to $O(h^4)$ overall for the average flux formula:

$$\begin{aligned}\langle\phi\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} &= \langle\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\\ &\quad + \frac{h^2}{12}\sum_{d'\neq d}\left(\mathbf{G}^{\perp}_{d'}\phi\big|_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\,\mathbf{G}^{\perp}_{d'}\psi\big|_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\right)\\ &\quad + C_4(\mathbf{x}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d})h^4 + O(h^5).\end{aligned} \tag{12.26}$$

Furthermore,

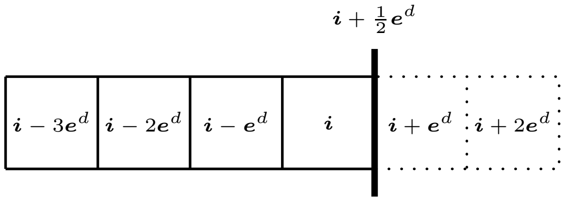
$$\begin{aligned}\frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}}(\mathbf{u}\cdot\nabla)\mathbf{u} &= \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}}\nabla\cdot(\mathbf{uu}) - \frac{1}{h^{\mathrm{D}}}\int_{\mathcal{C}_{\mathbf{i}}}(\nabla\cdot\mathbf{u})\mathbf{u}\\ &= \frac{1}{h}\sum_d \mathbf{e}^d\cdot\left(\langle\mathbf{uu}\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} - \langle\mathbf{uu}\rangle_{\mathbf{i}-\frac{1}{2}\mathbf{e}^d}\right) + O(h^4),\end{aligned}$$

where we have applied the chain rule, the divergence theorem, (12.24b), and the given condition $\mathbf{D}\langle\mathbf{u}\rangle_{\mathbf{i}} = O(h^4)$. Then (12.24d) follows from (12.21) and (12.24e). Another necessary condition is the cancellation from the symmetry of the difference stencils, i.e.,

$$C_4(\mathbf{x}_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}) - C_4(\mathbf{x}_{\mathbf{i}-\frac{1}{2}\mathbf{e}^d}) = O(h). \qquad \square$$

12.3 Ghost cells

Definition 12.8. *Ghost cells* are convenience devices for evaluating FD or FV discrete operators at cells near non-periodic domain boundaries.



Example 12.9. Two layers of ghost cells are used to enforce boundary conditions for fourth-order FV methods. We set the values of ghost cells by extrapolating those of the interior cells, with the boundary conditions incorporated in the extrapolation formulas. Referring to the above plot, different boundary conditions entail different cell-averaged values for the cells $\mathbf{i}+\mathbf{e}^d$ and $\mathbf{i}+2\mathbf{e}^d$. In particular, Dirichlet boundary conditions g are fulfilled to fourth-order accuracy by filling ghost cells with the following formulas:

$$\begin{aligned}\langle\phi\rangle_{\mathbf{i}+\mathbf{e}^d} =& \frac{1}{3}\left(-13\langle\phi\rangle_{\mathbf{i}} + 5\langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d} - \langle\phi\rangle_{\mathbf{i}-2\mathbf{e}^d}\right)\\ &+ 4\langle g\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^4); \qquad (12.27a)\\ \langle\phi\rangle_{\mathbf{i}+2\mathbf{e}^d} =& \frac{1}{3}\left(-70\langle\phi\rangle_{\mathbf{i}} + 32\langle\phi\rangle_{\mathbf{i}-\mathbf{e}^d} - 7\langle\phi\rangle_{\mathbf{i}-2\mathbf{e}^d}\right)\\ &+ 12\langle g\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^4). \qquad (12.27b)\end{aligned}$$

Neumann boundary conditions are fulfilled to the fifth order by

$$\begin{aligned}\langle\psi\rangle_{\mathbf{i}+\mathbf{e}^d} =& \frac{1}{10}\left(5\langle\psi\rangle_{\mathbf{i}} + 9\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} - 5\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d} + \langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d}\right)\\ &+ \frac{6}{5}h\left\langle\frac{\partial\psi}{\partial n}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^5), \qquad (12.28a)\\ \langle\psi\rangle_{\mathbf{i}+2\mathbf{e}^d} =& \frac{1}{10}\left(-75\langle\psi\rangle_{\mathbf{i}} + 145\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} - 75\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d} + 15\langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d}\right)\\ &+ 6h\left\langle\frac{\partial\psi}{\partial n}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^5), \qquad (12.28b)\end{aligned}$$

where $\left\langle\frac{\partial\psi}{\partial n}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$ is the Neumann condition for ψ.

Exercise 12.10. When no boundary conditions are known, a scalar ψ can be smoothly extended to fill a ghost cell abutting the boundary. Derive the following formulas

$$\begin{aligned}\langle\psi\rangle_{\mathbf{i}+\mathbf{e}^d} =& 5\langle\psi\rangle_{\mathbf{i}} - 10\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} + 10\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d} - 5\langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d}\\ &+ \langle\psi\rangle_{\mathbf{i}-4\mathbf{e}^d} + O(h^5); \qquad (12.29)\end{aligned}$$

and those for its faced-averaged value at the boundary,

$$\begin{aligned}\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} =& \frac{1}{60}\left(137\langle\psi\rangle_{\mathbf{i}} - 163\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} + 137\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d}\right.\\ &\left.-63\langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d} + 12\langle\psi\rangle_{\mathbf{i}-4\mathbf{e}^d}\right) + O(h^5). \qquad (12.30)\end{aligned}$$

Lemma 12.11. Face-averaged derivatives can be calculated from known boundary conditions and interior cell averages:

$$\begin{aligned}\left\langle\frac{\partial\psi}{\partial n}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} =& \frac{1}{72h}\left(-415\langle\psi\rangle_{\mathbf{i}} + 161\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} - 55\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d}\right.\\ &\left.+9\langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d} + 300\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\right) + O(h^4), \qquad (12.31a)\\ \left\langle\frac{\partial^2\psi}{\partial^2 n}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} =& \frac{1}{48h^2}\left(-755\langle\psi\rangle_{\mathbf{i}} + 493\langle\psi\rangle_{\mathbf{i}-\mathbf{e}^d} - 191\langle\psi\rangle_{\mathbf{i}-2\mathbf{e}^d}\right.\\ &\left.+33\langle\psi\rangle_{\mathbf{i}-3\mathbf{e}^d} + 420\langle\psi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}\right) + O(h^3). \qquad (12.31b)\end{aligned}$$

Algorithm 12.12. The discrete convection $\mathbf{D}\langle\mathbf{uu}\rangle$ are evaluated as follows:

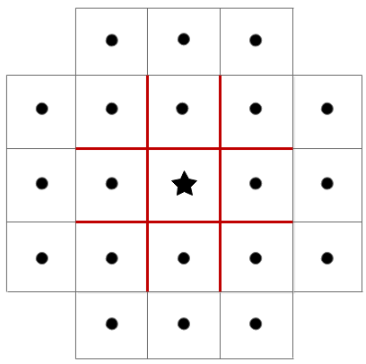
(Cnv-1) fill the ghost cells of cell-averaged velocity $\langle\mathbf{u}\rangle_{\mathbf{i}}$ using (12.27),

(Cnv-2) convert $\langle\mathbf{u}\rangle_{\mathbf{i}}$ to face-averaged *normal* velocity $\langle u_d\rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d}$ for each dimension d using (12.7),

(Cnv-3) convert $\langle\mathbf{u}\rangle_{\mathbf{i}}$ to face-averaged velocity $\langle\mathbf{u}\rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d}$ for *each* component of the velocity and each dimension d using (12.7).

(Cnv-4) calculate the discrete velocity product $\mathbf{F}(u_d,\mathbf{u})$ using (12.22) and (12.23).

(Cnv-5) compute $\mathbf{D}\langle\mathbf{uu}\rangle$ using (12.21).



12.4 FV-MOL algorithms for the advection-diffusion equation

Definition 12.13. The *advection-diffusion equation* is a PDE of the form

$$\frac{\partial\phi}{\partial t} = -\nabla\cdot(\mathbf{u}\phi) + \nu\Delta\phi + f, \qquad (12.32)$$

where the constant diffusivity ν, the velocity field $\mathbf{u} : \mathbb{R}^{\mathrm{D}}\times\mathbb{R}\to\mathbb{R}^{\mathrm{D}}$, and the forcing term $f : \mathbb{R}^{\mathrm{D}}\times\mathbb{R}\to\mathbb{R}$ are known *a priori*.

Example 12.14. To generate a semi-discrete system of the advection-diffusion equation in the FV formulation, we average (12.32) over a control volume $\mathcal{C}_{\mathbf{i}}$ and apply the divergence theorem to obtain a system of ODEs:

$$\frac{\mathrm{d}\,\langle\phi\rangle_{\mathbf{i}}}{\mathrm{d}t} = L_{\mathrm{adv}}(\langle\phi\rangle, t)_{\mathbf{i}} + L_{\mathrm{diff}}(\langle\phi\rangle)_{\mathbf{i}} + \langle f\rangle_{\mathbf{i}}, \tag{12.33}$$

where

$$\begin{aligned} L_{\mathrm{adv}}(\langle\phi\rangle, t)_{\mathbf{i}} &= -\frac{1}{h}\sum_{d=1}^{D}\left(\langle u_d\phi\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} - \langle u_d\phi\rangle_{\mathbf{i}-\frac{1}{2}\mathbf{e}^d}\right), \\ L_{\mathrm{diff}}(\langle\phi\rangle)_{\mathbf{i}} &= \nu\,\langle\Delta\phi\rangle_{\mathbf{i}} \\ &= \frac{\nu}{h}\sum_{d=1}^{D}\left(\left\langle\frac{\partial\phi}{\partial x_d}\right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} - \left\langle\frac{\partial\phi}{\partial x_d}\right\rangle_{\mathbf{i}-\frac{1}{2}\mathbf{e}^d}\right). \end{aligned}$$

Definition 12.15. An *ERK-ESDIRK IMplicit-EXplicit (IMEX) Runge-Kutta scheme* for solving an ODE

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = \mathbf{X}^{[\mathrm{E}]}(\phi, t) + \mathbf{X}^{[\mathrm{I}]}(\phi) \tag{12.34}$$

consists of steps as follows:

$$\begin{aligned} \phi^{(1)} &= \phi^n \approx \phi(t^n), && (12.35\mathrm{a}) \\ \forall s &= 2, 3, \ldots, n_{\mathrm{s}}, \\ \left(I - k\gamma\mathbf{X}^{[\mathrm{I}]}\right)\phi^{(s)} &= \phi^n + k\sum_{j=1}^{s-1} a_{s,j}^{[E]}\mathbf{X}^{[\mathrm{E}]}\left(\phi^{(j)}, t^{(j)}\right) && (12.35\mathrm{b}) \\ &\quad + k\sum_{j=1}^{s-1} a_{s,j}^{[I]}\mathbf{X}^{[\mathrm{I}]}\phi^{(j)}, \\ \phi^{n+1} &= \phi^n + k\sum_{s=1}^{n_{\mathrm{s}}} b_s^{[E]}\mathbf{X}^{[\mathrm{E}]}\left(\phi^{(s)}, t^{(s)}\right) && (12.35\mathrm{c}) \\ &\quad + k\sum_{s=1}^{n_{\mathrm{s}}} b_s^{[I]}\mathbf{X}^{[\mathrm{I}]}\phi^{(s)}, \end{aligned}$$

where the superscript $^{(s)}$ denotes an intermediate stage, $t^{(s)} = t^n + c_s k$ the time of that stage, n_{s} the number of stages, and $A, \mathbf{b}, \mathbf{c}$ standard coefficients of the Butcher tableau.

Algorithm 12.16. A *fourth-order FV method for solving the advection-diffusion equation on periodic domains* is obtained by directly applying the ERK-ESDIRK IMEX algorithm (12.35) to the ODE system (12.33) with

$$\mathbf{X}^{[\mathrm{E}]} = L_{\mathrm{adv}} + \langle f\rangle, \qquad \mathbf{X}^{[\mathrm{I}]} = L_{\mathrm{diff}}. \tag{12.36}$$

Example 12.17. Kennedy and Carpenter [2003] studied a group of implicit-explicit Runge-Kutta schemes from third- to fifth-order accurate with the following form:

$$\begin{array}{c|c} \mathbf{c}^{[E]} & A^{[E]} \\ \hline & \left(\mathbf{b}^{[E]}\right)^T \\ \hline & \left(\hat{\mathbf{b}}^{[E]}\right)^T \end{array} = \begin{array}{c|cccccc} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 2\gamma & 2\gamma & 0 & 0 & \cdots & 0 & 0 \\ c_3 & a_{31}^{[E]} & a_{32}^{[E]} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{s-1} & a_{s-1,1}^{[E]} & a_{s-1,2}^{[E]} & a_{s-1,3}^{[E]} & \cdots & 0 & 0 \\ 1 & a_{s,1}^{[E]} & a_{s,2}^{[E]} & a_{s,3}^{[E]} & \cdots & a_{s,s-1}^{[E]} & 0 \\ \hline & b_1 & b_2 & b_3 & \cdots & b_{s-1} & \gamma \\ \hline & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_{s-1} & \hat{b}_s \end{array}, \tag{12.37}$$

$$\begin{array}{c|c} \mathbf{c}^{[I]} & A^{[I]} \\ \hline & \left(\mathbf{b}^{[I]}\right)^T \\ \hline & \left(\hat{\mathbf{b}}^{[I]}\right)^T \end{array} = \begin{array}{c|cccccc} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 2\gamma & \gamma & \gamma & 0 & \cdots & 0 & 0 \\ c_3 & a_{31}^{[I]} & a_{32}^{[I]} & \gamma & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{s-1} & a_{s-1,1}^{[I]} & a_{s-1,2}^{[I]} & a_{s-1,3}^{[I]} & \cdots & \gamma & 0 \\ 1 & b_1 & b_2 & b_3 & \cdots & b_{s-1} & \gamma \\ \hline & b_1 & b_2 & b_3 & \cdots & b_{s-1} & \gamma \\ \hline & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_{s-1} & \hat{b}_s \end{array}, \tag{12.38}$$

where coefficients in $\hat{\mathbf{b}}$ are useful for error estimation.

The coefficients of `ARK4(3)6L[2]SA`, a particular IMEX scheme, are, in decimal form, $\gamma = 0.25$, $\mathbf{c}^{[E]} = \mathbf{c}^{[I]} = \mathbf{c}$, $\mathbf{b}^{[E]} = \mathbf{b}^{[I]} = \mathbf{b}$ where

$$\mathbf{c} = (0.0,\ 0.5,\ 0.332,\ 0.62,\ 0.85,\ 1.0)^T$$

$$\begin{aligned} b_1 &= 0.15791629516167136, \\ b_2 &= 0., \\ b_3 &= 0.18675894052400077, \\ b_4 &= 0.6805652953093346, \\ b_5 &= -0.27524053099500667, \end{aligned}$$

$$
\begin{aligned}
a_{31}^{[E]} &= 0.221776,\\
a_{32}^{[E]} &= 0.110224,\\
a_{41}^{[E]} &= -0.04884659515311857,\\
a_{42}^{[E]} &= -0.17772065232640102,\\
a_{43}^{[E]} &= 0.8465672474795197,\\
a_{51}^{[E]} &= -0.15541685842491548,\\
a_{52}^{[E]} &= -0.3567050098221991,\\
a_{53}^{[E]} &= 1.0587258798684427,\\
a_{54}^{[E]} &= 0.30339598837867193,\\
a_{61}^{[E]} &= 0.2014243506726763,\\
a_{62}^{[E]} &= 0.008742057842904185,\\
a_{63}^{[E]} &= 0.15993995707168115,\\
a_{64}^{[E]} &= 0.4038290605220775,\\
a_{65}^{[E]} &= 0.22606457389066084
\end{aligned}
$$

$$
\begin{aligned}
a_{31}^{[I]} &= 0.137776,\\
a_{32}^{[I]} &= -0.055776,\\
a_{41}^{[I]} &= 0.14463686602698217,\\
a_{42}^{[I]} &= -0.22393190761334475,\\
a_{43}^{[I]} &= 0.4492950415863626,\\
a_{51}^{[I]} &= 0.09825878328356477,\\
a_{52}^{[I]} &= -0.5915442428196704,\\
a_{53}^{[I]} &= 0.8101210538282996,\\
a_{54}^{[I]} &= 0.283164405707806,
\end{aligned}
$$

Lemma 12.18. The *stability function* of the IMEX Runge-Kutta methods in Definition 12.15 is

$$R\left(\bar{\lambda}^d + \mathtt{i}\bar{\lambda}^a\right) = \frac{\det\left(I - \bar{\lambda}^d A^{[I]} - \mathtt{i}\bar{\lambda}^a A^{[E]} + (\bar{\lambda}^d + \mathtt{i}\bar{\lambda}^a)\,\mathbb{1}\otimes \mathbf{b}^T\right)}{\det\left(I - \bar{\lambda}^d A^{[I]} - \mathtt{i}\bar{\lambda}^a A^{[E]}\right)}, \tag{12.39}$$

where $\bar{\lambda}^d = \lambda^d k$, $\bar{\lambda}^a = \lambda^a k$. The vector $\mathbf{b}$ and the matrices $A^{[E]}$ and $A^{[I]}$ are the coefficients in (12.37) and (12.38).

Proof. See Calvo et al. [2001]. □

Lemma 12.19. For a periodic domain, the ODE system (12.33) with constant velocity $\mathbf{u}$ and $\langle f\rangle = 0$ can be converted to a system of decoupled ODEs of the form

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \lambda y = \left(\lambda^d + \mathtt{i}\lambda^a\right) y, \tag{12.40}$$

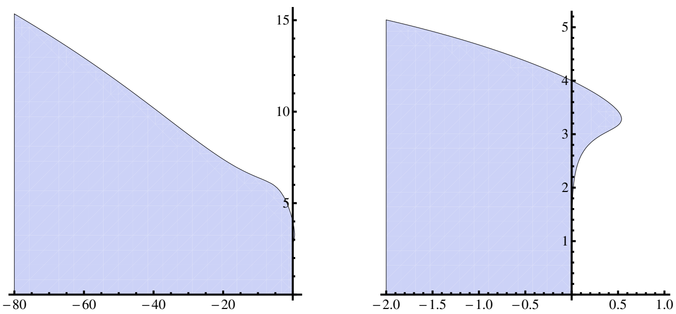
where $\lambda^d, \mathtt{i}\lambda^a$ are the eigenvalues of the diffusion and advection operators:

$$
\begin{aligned}
\lambda^d &= -4\frac{\nu}{h^2}\sum_{d=1}^{\mathrm{D}} \sin^2\frac{\theta_d}{2}\left(1+\frac{1}{3}\sin^2\frac{\theta_d}{2}\right),\\
\lambda^a &= -\frac{|u_{d,\max}|}{h}\sum_{d=1}^{\mathrm{D}} \sin\theta_d\left(1+\frac{2}{3}\sin^2\frac{\theta_d}{2}\right),
\end{aligned}
\tag{12.41}
$$

with $\theta_d = \xi_d h_d \in (0,\pi)$. Here ξ_d and h_d are the wave number and grid size in the dth dimension; we assume that a single Fourier mode of the cell average $\langle\phi\rangle_{\mathbf{i}}$ is of the form $y(t)e^{i\boldsymbol{\xi}\cdot\mathbf{x}_{\mathbf{i}}}$.

Exercise 12.20. Prove Lemma 12.19.

Exercise 12.21. Reproduce the following stability region $|R(z)| < 1$ in the complex plane for the fourth-order advection-diffusion solver that discretizes (12.32) with operators in Definition 12.6 and adopts `ARK4(3)6L[2]SA` to solve the resulting ODE system (12.33).



The first plot shows the stability region in the range $(\bar{\lambda}_d, \bar{\lambda}_a) \in [-80, 0] \times [0, 15]$ and the second is a zoom-in of the first near the origin. It is clear from these plots that

- the maximum stable Courant number increases as diffusion becomes stronger,
- in the absence of diffusion the scaled advection eigenvalue should be less than 4.

Deduce from the second plot and (12.41) that the range of stable Courant numbers for `ARK4(3)6L[2]SA` is

$$\mu \le \frac{2.91}{\mathrm{D}}. \tag{12.42}$$

Theorem 12.22. The FV method in Algorithm 12.16 is convergent with fourth-order accuracy.

Proof. This follows from Lemma 12.7, Lemma 12.19, and Theorem 10.22. □