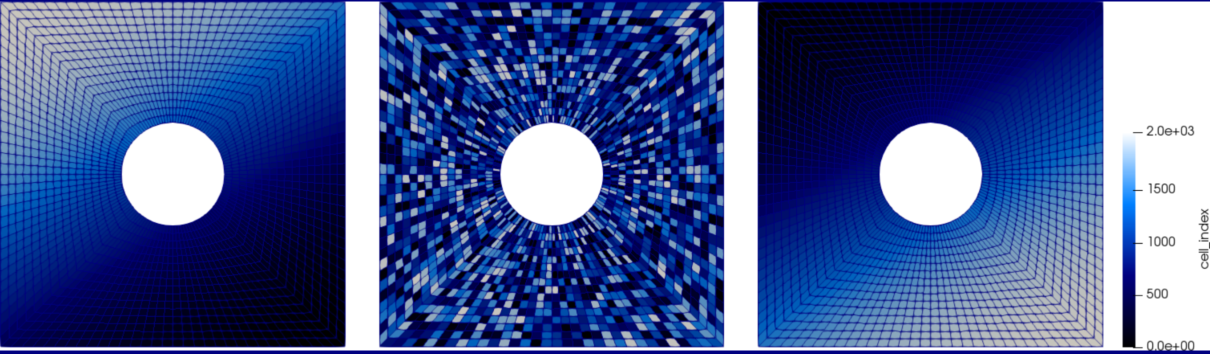
Notes about Thesis Project I



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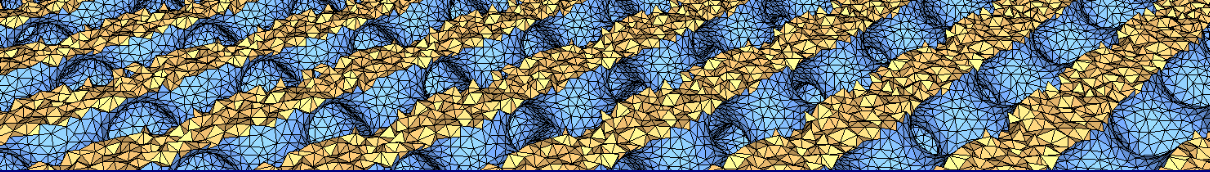


Numerical Quadrature

Numerical Quadrature (Salgado and Wise, p. 397)

Let $f \in C\left([a, b]\right)$. We seek calculate an approximation of

$$I^{(a,b)}\left[f\right] := \int_a^b f\left(x\right)\,\mathrm{d}x.$$

Suppose that $g \in C\left([a, b]\right)$, whose antiderivative is simply obtained, and $\left\|f - g\right\|_\infty < \varepsilon$. Then,

$$\left| \int_a^b f\left(x\right)\,\mathrm{d}x - \int_a^b g\left(x\right)\,\mathrm{d}x \right| \leq \varepsilon\left(b - a\right).$$

Definition (Nodal set)

Let $[a, b] \subset \mathbb{R}$. X is called a *nodal set* of size $n + 1 \in \mathbb{N}$ iff $X = \left\{x_i\right\}_{i=0}^{n} \subset [a, b]$ is a set of distinct elements. The elements of X, x_i are called *nodes*.

Definition (Interpolating polynomial)

Suppose that $X = \left\{x_i\right\}_{i=0}^{n} \subset [a, b]$ is a nodal set and $f\colon\ [a, b] \to \mathbb{R}$ is a function. The function $I\colon\ [a, b] \to \mathbb{R}$ is called an *interpolant of f* subordinate to X iff $\forall i = 0, \ldots, n : I\left(x_i\right) = f\left(x_i\right)$, we write $I\left(X\right) = f\left(X\right)$.

Theorem (existence and uniqueness)

Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a, b]$ is a nodal set and $Y = \{y_i\}_{i=0}^{n} \subset \mathbb{R}$. There is a unique polynomial $p \in \mathbb{P}_n$ with the property that $p(X) = Y$.

Definition (Lagrange nodal basis)

Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a, b]$ is a nodal set. The *Lagrange nodal basis* subordinate to X is the set of polynomials $\mathcal{L}_X = \{L_\ell\}_{\ell=0}^{n} \subset \mathbb{P}_n$ defined via

$$L_\ell(x) = \prod_{\substack{i=0 \\ i \neq \ell}}^{n} \frac{x - x_i}{x_\ell - x_i}.$$

Definition (Lagrange interpolating polynomial)

Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a, b]$ is a nodal set, $\mathcal{L}_X = \{L_i\}_{i=0}^{n} \subset \mathbb{P}_n$ is the Lagrange nodal basis subordinate to X, and $f \colon [a, b] \to \mathbb{R}$. The *Lagrange interpolating polynomial* of the function f, subordinate to the nodal set X, is the polynomial

$$p(x) = \sum_{i=0}^{n} f(x_i) L_i(x) \in \mathbb{P}_n.$$

Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a, b]$ is a nodal set and $p \in \mathbb{P}_n$ is the unique Lagrange interpolating polynomial of f subordinate to X. Then

$$\forall i = 0, \ldots, n : f(x_i) = p(x_i)$$

and

$$\forall x \in [a, b] : f(x) = p(x) + E(x),$$

where E is an expression of the interpolation error. Then

$$\int_a^b f(x)\, \mathrm{d}x = \int_a^b p(x)\, \mathrm{d}x + \int_a^b E(x)\, \mathrm{d}x.$$

But

$$\int_a^b p(x)\, \mathrm{d}x = \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x) = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x) = \sum_{i=0}^{n} f(x_i) \beta_i,$$

where $L_i \in \mathbb{P}_n$ is the ith Lagrange nodal basis element and β_i is its definite integral:

$$\beta_i = \int_a^b L_i(x)\, \mathrm{d}x.$$

The expression $\sum_{i=0}^{n} f(x_i) \beta_i$ is a typical numerical integration formula

$$\left| \int_a^b f(x)\, \mathrm{d}x - \sum_{i=0}^{n} f(x_i) \beta_i \right| = \left| \int_a^b E(x)\, \mathrm{d}x \right| \leq \int_a^b |E(x)|\, \mathrm{d}x.$$

The *quadrature weights*, β_i, depends only on the positions of the nodes within $[a, b]$, as well as the interval $[a, b]$ itself. We will consider the approximation of a weight integral

$$I_w^{(a,b)}[f] := \int_a^b f(x)\, w(x)\, \mathrm{d}x.$$

Definition (Quadrature rule)

Suppose that $n, r \in \mathbb{N}_0$, w is a weight function on $[a, b] \subset \mathbb{R}$, $h = b - a > 0$, and $f \in C^r([a, b])$. The expression

$$Q_{w,r}^{(a,b)}[f] = \sum_{i=0}^{r} \sum_{j=0}^{n} \beta_{i,j} f^{(i)}(x_j) = \sum_{j=0}^{n} \left(\beta_{0,j} f(x_j) + \beta_{1,j} f'(x_j) + \cdots + \beta_{r,j} f^{(r)}(x_j) \right),$$

where

$$\forall i \in \{0, \ldots, r\} : \forall j \in \{0, \ldots, n\} : \beta_{i,j} = h^{i+1} \widehat{\beta}_{i,j}$$

and

$$\forall j \in \{0, \ldots, n\} : x_j = a + h \cdot \widehat{x}_j,$$

is called a *quadrature rule of degree* r with *intrinsic nodes* $\widehat{X} = \left\{ \widehat{x}_j \right\} \subset [0, 1]$ and *intrinsic weights* $\{\beta_{i,j}\} \subset \mathbb{R}$ are called the *effective nodes* and *effective weights*, respectively.

A quadrature rule of degree $r = 0$ is called a *simple quadrature rule*, and we simplify the notation by writing $\beta_j = \beta_{0,j}$ and

$$Q_{w,r}^{(a,b)}[f] = \sum_{j=0}^{n} \beta_j f^{(i)}(x_j).$$

The *quadrature rule error* is defined as

$$E_Q[f] = I_w^{(a,b)}[f] - Q_{w,r}^{(a,b)}[f].$$

Definition (consistency)

The quadrature rule is *consistent of order at least* $m \in \mathbb{N}_0$ iff $E_Q[q] = 0$ for all $q \in \mathbb{P}_m$. The quadrature rule is *consistent of order exactly* m iff $E_Q[q] = 0$ for all $q \in \mathbb{P}_m$; however, for some $r \in \mathbb{P}_{m+1}$, $E_Q[r] \neq 0$.

Definition (interpolatory quadrature rule)

Assume that $n \in \mathbb{N}_0$, w is a weight function on $[a,b] \subset \mathbb{R}$, and $f \in C([a,b])$. Suppose that $X = \{x_i\}_{i=0}^{n} \subset [a,b]$ is a nodal set and $p \in \mathbb{P}_n$ is the unique Lagrange Interpolating polynomial of f subordinate to X, with

$$p(x) = \sum_{j=0}^{n} f(x_j) L_j(x),$$

where $L_j \in \mathbb{P}_n$ is the jth Lagrange nodal basis element.

The expression

$$Q_w^{(a,b)}[f] = \sum_{j=0}^{n} f(x_j) \beta_j,$$

where

$$\beta_j = \int_a^b L_j(x) w(x) \, \mathrm{d}x,$$

is called an *interpolatory quadrature rule subordinate to X of Lagrange type* for approximating $I_w^{(a,b)}[f]$.

Theorem (existence and uniqueness)

Suppose that $X = \{x_i\}_{i=0}^{n} \subset \mathbb{R}$ *is a nodal set. There exists uniqueness weights* $\{\beta_j\}_{j=0}^{n}$ *such that*

$$\forall q \in \mathbb{P}_n : \int\limits_a^b q(x)\, w(x)\; \mathrm{d}x = \sum_{j=0}^{n} \beta_j q(x_j),$$

or, equivalently,

$$\forall q \in \mathbb{P}_n : E_Q[q] = 0.$$

Moreover, these weights are given by

$$\forall j \in \{0, \dots, n\} : \beta_j = \int\limits_a^b L_j(x)\, w(x)\; \mathrm{d}x,$$

where L_j *is the* j*th Lagrange nodal basis polynomial subject to* X*.*

Theorem (consistency)

The last result shows that the simple quadrature rule,

$$Q_w^{(a,b)}[f] = \sum_{j=0}^{n} \beta_i f(x_i),$$

is consistent of order at least n *iff it is a quadrature rule of Lagrange type.*

Theorem (Error estimate)

Suppose that $n \in \mathbb{N}_0$*,* w *is a weight function on* $[a,b] \subset \mathbb{R}$*.* $f \in C^{n+1}([a,b])$*, and* $X = \{x_i\}_{i=0}^{n} \subset [a,b]$ *is a nodal set. Suppose that* $Q_w^{(a,b)}[f]$ *is the interpolatory quadrature rule subordinate to* X *of Lagrange type. Then,*

$$\left|E_Q[f]\right| \leq \frac{M_{n+1}}{(n+1)!} \int_a^b \left|\omega_{n+1}(x)\right| w(x)\,\mathrm{d}x,$$

where

$$\omega_{n+1}(x) = \prod_{j=0}^{n} (x - x_j)$$

and

$$M_{n+1} = \left\| f^{(n+1)} \right\|_{\infty}.$$

Consequently, an interpolatory quadrature rule subordinate to X *of Lagrange type is consistent of order at least* n*.*

Definition (characteristic function)

Suppose that $B \subset \mathbb{R}$. The *characteristic function* of B is the function

$$\chi_B(t) = \begin{cases} 1, & t \in B, \\ 0, & t \in \mathbb{R} \setminus B. \end{cases}$$

Theorem (kernel)

Suppose that $r \in \mathbb{N}_0$ *and* $m \in \mathbb{N}$, *with* $m > r$. *Define the function* $k_m \colon [a,b] \times [a,b] \to \mathbb{R}$ *via*

$$k_m(x,y) = (x-y)^m \xi_{[a,x]}(y) = \begin{cases} (x-y)^m, & a \leq y \leq x \leq b, \\ 0, & a \leq x < y \leq b. \end{cases}$$

Then, for each $i \in \{0, \ldots, r\}$,

$$\frac{\partial^i k_m}{\partial x^i} \in C([a,b] \times [a,b])$$

and

$$\frac{\partial^i k_m(x,y)}{\partial x^i} = \begin{cases} \displaystyle\prod_{k=0}^{i-1} (m-k)(x-y)^{m-i}, & a \leq y \leq x \leq b, \\ 0, & a \leq x < y \leq b. \end{cases}$$

Theorem (Peano Kernel Theorem)

Suppose that $r \in \mathbb{N}_0$, $m \in \mathbb{N}$, with $m > n$, w is a weight function on $[a, b] \subset \mathbb{R}$, and $f \in C^{m+1}([a, b])$. Assume that $Q_{w,r}^{(a,b)}[f]$ is a quadrature rule of degree r, that is consistent of order at least m. Let the function $k_m \colon [a, b] \times [a, b] \to \mathbb{R}$. Set

$$K_m(y) = E_Q[k_m(\cdot, y)] = \int_a^b k_m(x, y)\, w(x)\, \mathrm{d}x - \sum_{j=0}^{n} \sum_{i=0}^{r} \beta_{i,j} \frac{\partial^i k_m(x_j, y)}{\partial x^i}.$$

Then the quadrature error satisfies

$$E_Q[f] = \frac{1}{m!} \int_a^b f^{(m+1)}(y)\, K_m(y)\, \mathrm{d}y.$$

The function $K_m(y)$ is called the Peano Kernel.

Theorem (quadrature error stability)

We have

$$\left| E_Q[f] \right| \le \frac{1}{m!} \left\| f^{(m+1)} \right\|_\infty \|K_m\|_1.$$

Since $\|K_m\|_1 < \infty$, there is a constant $C > 0$ that may depend on the size of the interval but is independent of f such that

$$\left| E_Q[f] \right| \le C \left\| f^{(m+1)} \right\|_\infty.$$

Theorem (constant sign)

If K_m does not change sign in $[a, b]$, then

$$E_Q[f] = \frac{f^{(m+1)(\xi)}}{m!} \int_a^b K_m \, \mathrm{d}y$$

for some $\xi \in [a, b]$. Furthermore, we have the simple representation for the error

$$E_Q[f] = \frac{E_Q\left[x^{m+1}\right]}{(m+1)!} f^{(m+1)}(\xi)$$

for some $\xi \in [a, b]$, where $E_Q\left[x^{m+1}\right]$ is the quadrature error for the function $x \mapsto x^{m+1}$.

Definition (Peano Kernel)

Let $M_1 = \chi_{[a,b]}$. For $k \in \mathbb{N}$ with $k \geq 2$, set

$$M_k(x) = \int_{\mathbb{R}} M_{k-1}(x-y) M_1(y) \, \mathrm{d}y.$$

For $k \in \mathbb{N}$ and $h > 0$, we define

$$M_k(x, h) = \frac{1}{h} M_k\left(\frac{x}{h}\right).$$

Definition (Closed Newton-Cotes quadrature rule)

Suppose that w is a weight function on $[a,b] \subset \mathbb{R}$ and $n \in \mathbb{N}$. Set $h = b - a > 0$ and $\hbar = \frac{h}{n}$. Suppose that, for the simple quadrature rule, the nodal set $X = \{x_i\}_{i=0}^{n} \subset [a,b]$ is defined by

$$x_j = a + j\hbar, \quad j \in \{0, \ldots, n\}.$$

The resulting method, denoting $Q_n[f]$, is called a *closed Newton-Cotes quadrature rule of order* n.

Example (Newton-Cotes quadrature rules of order $n = 1, 2$ and weight function $w \equiv 1$ on $[a,b]$)

$$x_j = a + h\widehat{x}_j, \quad \beta_j = h\widehat{\beta}_j, \quad h = b - a.$$

n	rule	$\widehat{x}_j$	$\widehat{\beta}_j$	Error Formula
1	Trapezoidal	$0, 1$	$\frac{1}{2}, \frac{1}{2}$	$-\frac{1}{12}\hbar^3 f^{(2)}(\xi)$
2	Simpson's	$0, \frac{1}{2}, 1$	$\frac{1}{6}, \frac{4}{6}, \frac{1}{6}$	$-\frac{1}{90}\hbar^5 f^{(4)}(\xi)$

For $n = 2$, we observe the phenomenon of super-convergence, i.e., a higher than expected convergence.
For example, consider the case $n = 3$, Simpson's $\frac{3}{8}$ rule, on the reference interval $[0, 1]$. The second Lagrange nodal basis element is

$$\widehat{L}_1(x) = \frac{x\left(x - \frac{2}{3}\right)(x - 1)}{\frac{1}{3}\left(\frac{1}{3} - \frac{2}{3}\right)\left(\frac{1}{3} - 1\right)} = \frac{27}{2}\left(x^3 - \frac{5}{3}x^2 + \frac{2}{3}x\right).$$

Then,

$$\widehat{\beta}_1 = \int_0^1 \widehat{L}_1(x)\,\mathrm{d}x = \frac{27}{2}\left(\frac{1}{4}x^4 - \frac{5}{9}x^3 + \frac{1}{3}x^2\right)\Big|_{x=0}^{x=1} = \frac{3}{8}.$$

Theorem (Error estimate)

Let $[a, b] \subset \mathbb{R}$. Suppose that $Q_n^{(a,b)}[f]$ is a closed Newton-Cotes quadrature rule of order $n \in \mathbb{N}$. Then, the order of quadrature rule is consistent of order at least n. Moreover, if $f \in C^{n+1}([a, b])$, then

$$\left|E_{Q_n}[f]\right| \leq C h^{n+2} \left\| f^{(n+1)} \right\|_{\infty},$$

where $h = b - a$ and $C > 0$ is independent of h and f.

Theorem (Integral Mean Value Theorem)

Suppose that $-\infty < a < b < \infty$, $f \in C([a, b])$, and $g \in \mathcal{R}(a, b)$. Furthermore, suppose that $\forall x \in [a, b] : g(x) \geq 0$. Then there exists a point $\xi \in [a, b]$ such that

$$\int_a^b f(x) g(x) \, \mathrm{d}x = f(\xi) \int_a^b g(x) \, \mathrm{d}x.$$

Thus, if $\forall x \in [a, b] : g(x) = 1$, there exists a point $\xi \in [a, b]$ such that

$$f(\xi) = \frac{1}{b - a} \int_a^b f(x) \, \mathrm{d}x.$$

Heuristic derivation of Advection Differential Equation

Definition (Average concentration)

Let $h > 0$, $h \ll 1$. We define the *average concentration* $\overline{u}(x,t)$ in a space-time cell $\left[x - \frac{1}{2}h, +x\frac{1}{2}h\right] \times [0,T]$.

$$\overline{u}(x,t) = \frac{1}{h}\int\limits_{x-\frac{1}{2}h}^{x+\frac{1}{2}h} u(s,t)\,\mathrm{d}s.$$

Definition (Mass flux)

The mass flux is the product of

$$J_x = cv_x.$$

- J_x is the mass flux in x-direction.
- c is the concentration of the substance.
- v_x is the velocity of the substance in the x-direction.

Theorem (Conservation law)

If the species is carried along by a flowing medium with velocity $a(x,t)$, then the mass conservation law implies that the change of $\overline{u}(x,t)$ per unit of time is the net balance of inflow and outflow over the cell boundaries,

$$\frac{\partial\overline{u}(x,t)}{\partial t} = \frac{1}{h}\left[a\left(x - \frac{1}{2}h, t\right)u\left(x - \frac{1}{2}h, t\right) - a\left(x + \frac{1}{2}h, t\right)u\left(x + \frac{1}{2}h, t\right)\right].$$

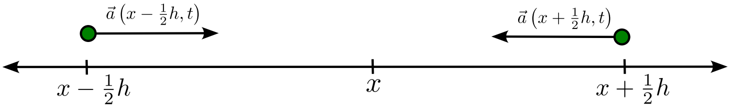
Numerical Quadrature (Hundsdorfer and Verwer, p. 9)

Definition (Advection equation)

$$\frac{\partial u\left(x,t\right)}{\partial t}+\frac{\partial a\left(x,t\right)u\left(x,t\right)}{\partial x}=0.$$

Definition (Diffusion equation)

$$\frac{\partial u\left(x,t\right)}{\partial t}=\frac{\partial}{\partial x}\left(d\left(x,t\right)\frac{\partial u\left(x,t\right)}{\partial x}\right).$$



Theorem (Mass conservation law)

If $u(x,t)$ is a concentration and

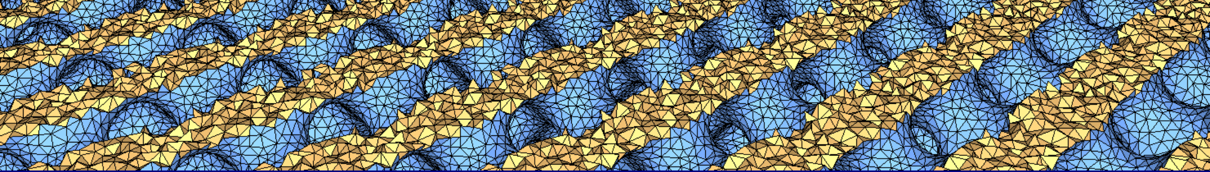
$$M(t) := \int_0^1 u(x,t)\,\mathrm{d}x$$

represents the mass in $[0,1]$ at time t, then M is a conserved quantity.

Proof.

$$\begin{aligned}\frac{\mathrm{d}M(t)}{\mathrm{d}t} &= \int_0^1 u_t(x,t)\,\mathrm{d}x = \int_0^1 \left(-au_x(x,t) + du_{xx}(x,t)\right)\mathrm{d}x \\ &= -a\left(u(1,t) - u(0,t)\right) + d\left(u_x(1,t) - u_x(0,t)\right) = 0.\end{aligned}$$

$\square$



The Advection Problem in One Dimension

Definition (space-time grid)

Let $d \in \mathbb{N}$, $\Omega = (0,1)^d$, and $T > 0$. For $K, N \in \mathbb{N}$, we set $\tau = \frac{T}{K}$ and $h = \frac{1}{N+1}$. We define the *space-time grid domain*

$$\overline{\mathcal{C}}_h^\tau = \overline{\Omega}_h \times [0,T]_\tau = \left\{ (\mathbf{x}, t_k) \mid \mathbf{x} \in \overline{\Omega}_h, t_k = k\tau, k \in \{0, \ldots, K\} \right\},$$

where we recall that $\overline{\Omega}_h = \overline{\Omega} \cap \mathbb{Z}_h^d$. We define the *discrete interior* of $\overline{C}_h^\tau$ to be

$$\mathcal{C}_h^\tau = \Omega_h \times (0,T)_\tau .$$

Definition (space-time grid functions)

Let $\mathcal{C}_h^\tau$ be a space-time grid domain. We denote by

$$\mathcal{V}\left(\overline{\mathcal{C}}_h^\tau\right) = \left\{ v \mid \overline{C}_h^\tau \to \mathbb{R} \right\}$$

be the space of *space-time grid functions*. The spaces

$$\mathcal{V}\left(\mathcal{C}_h^\tau\right), \mathcal{V}\left(\partial_L \mathcal{C}_h^\tau\right)$$

Definition (space-time discrete norms)

Let $d \in \{1, 2\}$, $p \in [1, \infty]$, and $q \in [1, \infty)$. We define the *space-time* norm

$$\|v\|_{L_\tau^q\left(L_h^p\right)} = \left(\tau \sum_{k=1}^{K} \left\|v^k\right\|_{L_h^p}^q\right)^{\frac{1}{q}}$$

and

$$\|v\|_{L_\tau^\infty\left(L_h^p\right)} = \max_{k=0}^{K} \left\|v^k\right\|_{L_h^p}$$

Definition (Péclet number)

Consider the simple constant-coefficient advection-diffusion equation

$$u_t + au_x = du_{xx}, \quad t > 0, \quad 0 < x < L,$$

with the given initial profile $u(x, 0)$. If $d > 0$ we need boundary conditions at $x = 0$ and $x = L$, such as Dirichlet conditions. On the other hand, for the pure advection problem we need only to prescribe the solution at the *inflow* boundary, that is, at $x = 0$ if $a > 0$ and $x = L$ if $a < 0$. If $d > 0$ but $d \approx 0$, or more precisely if the *Péclet number*

$$|a| \frac{L}{d}$$

is large, the Dirichlet condition at the outflow boundary will give rise to a *boundary layer*.
If the Péclet number $\left|a\frac{L}{d}\right|$ is large, the problem is called *singularity perturbed*.

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