Weighted Residual Methods

Introductory Course on Multiphysics Modelling

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1 Problem definition

1.1 Boundary-Value Problem

Let $\mathcal{B}$ be a domain with the boundary $\partial\mathcal{B}$, and:

- $\mathcal{L}(.)$ be a (second order) differential operator defined on functions $u(\boldsymbol{x})$, $\boldsymbol{x} \in \mathcal{B}$,
- $f = f(\boldsymbol{x})$ be a known source term in $\mathcal{B}$,
- $\boldsymbol{n} = \boldsymbol{n}(\boldsymbol{x})$ be the unit vector normal to the boundary $\partial\mathcal{B}$.

Boundary-Value Problem: Find $u = u(\boldsymbol{x}) =?$ satisfying **PDE**

$$\mathcal{L}(u) = f \quad \text{in } \mathcal{B} \tag{1}$$

and subject to (at least one of) the following **boundary conditions**

$$u = \hat{u} \quad \text{on } \partial\mathcal{B}_1\,, \qquad \frac{\partial u}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} = \hat{\gamma} \quad \text{on } \partial\mathcal{B}_2\,, \qquad \frac{\partial u}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} + \hat{\alpha}\, u = \hat{\beta} \quad \text{on } \partial\mathcal{B}_3\,. \tag{2}$$

where $\hat{u} = \hat{u}(\boldsymbol{x})$, $\hat{\gamma} = \hat{\gamma}(\boldsymbol{x})$, $\hat{\alpha} = \hat{\alpha}(\boldsymbol{x})$, and $\hat{\beta} = \hat{\beta}(\boldsymbol{x})$ are fields prescribed on adequate parts of the boundary $\partial\mathcal{B} = \partial\mathcal{B}_1 \cup \partial\mathcal{B}_2 \cup \partial\mathcal{B}_3$.

Remarks:

- the boundary parts are mutually disjoint, i.e., $\partial\mathcal{B}_1 \cap \partial\mathcal{B}_2 = \emptyset$, $\partial\mathcal{B}_1 \cap \partial\mathcal{B}_3 = \emptyset$, and $\partial\mathcal{B}_2 \cap \partial\mathcal{B}_3 = \emptyset$,
- for $f \equiv 0$ the PDE is called *homogeneous*.

1.2 Boundary conditions

There are three **kinds of boundary conditions**:

1. the first kind (or **Dirichlet** b.c)

$$u = \hat{u} \quad \text{on } \partial\mathcal{B}_1\,, \tag{3}$$

2. the second kind (or **Neumann** b.c)

$$\frac{\partial u}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} = \hat{\gamma} \quad \text{on } \partial\mathcal{B}_2\,, \tag{4}$$

3. the third kind (or **Robin** b.c.)

$$\frac{\partial u}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} + \hat{\alpha}\, u = \hat{\beta} \quad \text{on } \partial\mathcal{B}_3\,, \tag{5a}$$

sometimes termed also the **generalized Neumann** b.c., it can be presented as

$$\frac{\partial u}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} = \hat{\gamma} + \hat{\alpha}\big(\hat{u} - u\big) \quad \text{on } \partial\mathcal{B}_3\,. \tag{5b}$$

Indeed, this form is obtained for $\hat{\beta} = \hat{\gamma} + \hat{\alpha}\,\hat{u}$. Now, one can easily notice that the third kind is just a linear combination of the first two kinds. However, in this case the fields $\hat{u}$ and $\hat{\gamma}$ are prescribed simultaneously on *the same* fragment of boundary, and their effect is controlled by another known boundary value, $\hat{\alpha}$, which usually can be interpreted as an essential property of the surrounding medium. Finally, notice that the Dirichlet condition is obtained for the limit $\hat{\alpha} \to \infty$, while the Neumann condition for $\hat{\alpha} = 0$.

2 Weighted Residual Method

2.1 General idea

Weighted Residual Method (WRM) assumes that a solution can be approximated analytically or piecewise analytically. In general,

- a solution to a PDE can be expressed as a linear combination of a base set of functions where the coefficients are determined by a chosen method, and
- the method attempts to minimize the approximation error (for instance, finite differences try to minimize the error specifically at the chosen grid points).

In fact, WRM represents a particular group of methods where an integral error is minimized in a certain way. Depending on this way the WRM can generate:

- the finite volume method,
- finite element methods,
- spectral methods, and also
- finite difference methods.

2.2 Approximation

Assumption: the exact solution, u, can be approximated by a linear combination of N (linearly-independent) analytical functions, that is,

$$u(\boldsymbol{x}) \approx \tilde{u}(\boldsymbol{x}) = \sum_{s=1}^{N} U_s \, \phi_s(\boldsymbol{x}) \tag{6}$$

where $\tilde{u}$ is an approximated solution, and

- U_s are unknown coefficients, the so-called **degrees of freedom**,
- $\phi_s = \phi_s(\boldsymbol{x})$ form a base set of selected functions (often called as **trial functions** or **shape functions**). This set of functions generates the space of approximated solutions.

Here, $s = 1, \ldots N$ where N is the number of degrees of freedom.

2.3 Error functions

In general, an approximated solution, $\tilde{u}$, does not satisfy exactly the PDE and/or some (or all) boundary conditions. The generated errors can be described by the following **error functions**:

0. the **PDE residuum**

$$\mathcal{R}_0(\tilde{u}) = \mathcal{L}(\tilde{u}) - f \,, \tag{7}$$

1. the **Dirichlet condition residuum**

$$\mathcal{R}_1(\tilde{u}) = \tilde{u} - \hat{u}\,, \tag{8}$$

2. the **Neumann condition residuum**

$$\mathcal{R}_2(\tilde{u}) = \frac{\partial \tilde{u}}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} - \hat{\gamma}\,, \tag{9}$$

3. the **Robin condition residuum**

$$\mathcal{R}_3(\tilde{u}) = \frac{\partial \tilde{u}}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} + \hat{\alpha}\tilde{u} - \hat{\beta}\,. \tag{10}$$

2.4 Minimization of errors

Demand: Minimize the errors in a weighted integral sense

$$\int_{\mathcal{B}} \mathcal{R}_0(\tilde{u})\overset{0}{\psi}_r + \int_{\partial\mathcal{B}_1} \mathcal{R}_1(\tilde{u})\overset{1}{\psi}_r + \int_{\partial\mathcal{B}_2} \mathcal{R}_2(\tilde{u})\overset{2}{\psi}_r + \int_{\partial\mathcal{B}_3} \mathcal{R}_3(\tilde{u})\overset{3}{\psi}_r = 0\,. \tag{11}$$

Here, $\{\overset{0}{\psi}_r\}$, $\{\overset{1}{\psi}_r\}$, $\{\overset{2}{\psi}_r\}$, and $\{\overset{3}{\psi}_r\}$ $(r = 1,\ldots M)$ are sets of **weight functions**.

Note that M weight functions yield M conditions (or equations) from which to determine the N coefficients U_s. To determine these N coefficients uniquely we need N independent conditions (equations).

Now, using the formulae for residua results in

$$\begin{aligned}\int_{\mathcal{B}} \mathcal{L}(\tilde{u})\overset{0}{\psi}_r + \int_{\partial\mathcal{B}_1} \tilde{u}\overset{1}{\psi}_r + \int_{\partial\mathcal{B}_2} \frac{\partial \tilde{u}}{\partial \boldsymbol{x}} \cdot \boldsymbol{n}\overset{2}{\psi}_r + \int_{\partial\mathcal{B}_3} \Big(\frac{\partial \tilde{u}}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} + \hat{\alpha}\,\tilde{u}\Big)\overset{3}{\psi}_r \\ = \int_{\mathcal{B}} f\overset{0}{\psi}_r + \int_{\partial\mathcal{B}_1} \hat{u}\overset{1}{\psi}_r + \int_{\partial\mathcal{B}_2} \hat{\gamma}\overset{2}{\psi}_r + \int_{\partial\mathcal{B}_3} \hat{\beta}\overset{3}{\psi}_r\,.\end{aligned} \tag{12}$$

2.5 System of algebraic equations

Applying the approximation $\tilde{u} = \sum_{s=1}^{N} U_s\phi_s$, and using the linearity of operators,

$$\mathcal{L}(\tilde{u}) = \sum_{s=1}^{N} U_s\,\mathcal{L}(\phi_s), \qquad \frac{\partial \tilde{u}}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} = \sum_{s=1}^{N} U_s\,\frac{\partial \phi_s}{\partial \boldsymbol{x}} \cdot \boldsymbol{n}\,, \tag{13}$$

leads to the the following system of algebraic equations

$$\boxed{\sum_{s=1}^{N} A_{rs}U_s = B_r} \tag{14}$$

where

$$A_{rs} = \int_{\mathcal{B}} \mathcal{L}(\phi_s)\overset{0}{\psi}_r + \int_{\partial\mathcal{B}_1} \phi_s\overset{1}{\psi}_r + \int_{\partial\mathcal{B}_2} \frac{\partial \phi_s}{\partial \boldsymbol{x}} \cdot \boldsymbol{n}\overset{2}{\psi}_r + \int_{\partial\mathcal{B}_3} \left(\frac{\partial \phi_s}{\partial \boldsymbol{x}} \cdot \boldsymbol{n} + \hat{\alpha}\,\phi_s\right)\overset{3}{\psi}_r \tag{15}$$

and

$$B_r = \int_{\mathcal{B}} f\overset{0}{\psi}_r + \int_{\partial\mathcal{B}_1} \hat{u}\overset{1}{\psi}_r + \int_{\partial\mathcal{B}_2} \hat{\gamma}\overset{2}{\psi}_r + \int_{\partial\mathcal{B}_3} \hat{\beta}\overset{3}{\psi}_r\,. \tag{16}$$

2.6 Categories of WRM

Assume that the boundary conditions are met and approximated must be only the PDE in the domain. The error of this approximation is minimized by zeroing an integral of weighted residuum. There are four main categories of weight functions which generate the following categories of WRM:

Subdomain method Here the domain is divided in M subdomains $\Delta\mathcal{B}_r$ where

$$\overset{0}{\psi}_r(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in \Delta\mathcal{B}_r, \\ 0 & \text{outside}, \end{cases} \tag{17}$$

such that this method minimizes the residual error in each of the chosen subdomains. Note that the choice of the subdomains is free. In many cases an equal division of the total domain is likely the best choice. However, if higher resolution (and a corresponding smaller error) in a particular area is desired, a non-uniform choice may be more appropriate.

Collocation method In this method the weight functions are chosen to be Dirac delta functions

$$\overset{0}{\psi}_r(\boldsymbol{x}) = \delta(\boldsymbol{x} - \boldsymbol{x}_r). \tag{18}$$

such that the error is zero at the chosen nodes $\boldsymbol{x}_r$.

Least squares method This method uses derivatives of the residual itself as weight functions in the form

$$\overset{0}{\psi}_r(\boldsymbol{x}) = \frac{\partial \mathcal{R}_0(\tilde{u}(\boldsymbol{x}))}{\partial U_r}. \tag{19}$$

The motivation for this choice is to minimize $\int_{\mathcal{B}} \mathcal{R}_0^2$ of the computational domain. Note that (if the boundary conditions are satisfied) this choice of the weight function implies

$$\frac{\partial}{\partial U_r}\left(\int_{\mathcal{B}} \mathcal{R}_0^2\right) = 0 \tag{20}$$

for all values of U_r.

Galerkin method In this method the weight functions are chosen to be identical to the base functions.

$$\overset{0}{\psi}_r(\boldsymbol{x}) = \phi_r(\boldsymbol{x}). \tag{21}$$

In particular, if the base function set is orthogonal (i.e., $\int_{\mathcal{B}} \phi_r \phi_s = 0$ if $r \neq s$), this choice of weight functions implies that the residual $\mathcal{R}_0$ is rendered orthogonal with the minimization condition

$$\int_{\mathcal{B}} \mathcal{R}_0 \overset{0}{\psi}_r = 0 \tag{22}$$

for all base functions.

3 ODE example

3.1 A simple BVP approached by WRM

Boundary Value Problem (for an ODE): Find $u = u(x) =?$ satisfying

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} - \frac{\mathrm{d}u}{\mathrm{d}x} = 0 \quad \text{in } \mathcal{B} = [a,b], \tag{23}$$

subject to boundary conditions on $\partial\mathcal{B} = \partial\mathcal{B}_1 \cup \partial\mathcal{B}_2 = \{a\} \cup \{b\}$:

$$u\big|_{x=a} = \hat{u} \quad \text{(Dirichlet)}, \qquad \left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=b} = \hat{\gamma} \quad \text{(Neumann)}. \tag{24}$$

WRM approach

- Residua for an approximated solution $\tilde{u}$

$$\mathcal{R}_0(\tilde{u}) = \frac{\mathrm{d}^2\tilde{u}}{\mathrm{d}x^2} - \frac{\mathrm{d}\tilde{u}}{\mathrm{d}x}, \qquad \mathcal{R}_1(\tilde{u}) = \tilde{u}\big|_{x=a} - \hat{u}, \qquad \mathcal{R}_2(\tilde{u}) = \left.\frac{\mathrm{d}\tilde{u}}{\mathrm{d}x}\right|_{x=b} - \hat{\gamma}. \tag{25}$$

- Minimization of weighted residual error (for weight functions $\overset{0}{\psi}_r(x)$, $\overset{1}{\psi}_r(x)$, and $\overset{2}{\psi}_r(x)$, $r = 1,\ldots N$)

$$\int_a^b \left(\frac{\mathrm{d}^2\tilde{u}}{\mathrm{d}x^2} - \frac{\mathrm{d}\tilde{u}}{\mathrm{d}x}\right)\overset{0}{\psi}_r + \left[\left(\tilde{u} - \hat{u}\right)\overset{1}{\psi}_r\right]_{x=a} + \left[\left(\frac{\mathrm{d}\tilde{u}}{\mathrm{d}x} - \hat{\gamma}\right)\overset{2}{\psi}_r\right]_{x=b} = 0. \tag{26}$$

- System of algebraic equations (for the approximation $\tilde{u}(x) = \sum_{s=1}^{N} U_s \phi_s(x)$)

$$\sum_{s=1}^{N} A_{rs} U_s = B_r \tag{27}$$

$$\text{where} \quad A_{rs} = \int_a^b \left(\frac{\mathrm{d}^2\phi_s}{\mathrm{d}x^2} - \frac{\mathrm{d}\phi_s}{\mathrm{d}x}\right)\overset{0}{\psi}_r + \left[\phi_s \overset{1}{\psi}_r\right]_{x=a} + \left[\frac{\mathrm{d}\phi_s}{\mathrm{d}x}\overset{2}{\psi}_r\right]_{x=b}, \tag{28}$$

$$B_r = \left[\hat{u}\overset{1}{\psi}_r\right]_{x=a} + \left[\hat{\gamma}\overset{2}{\psi}_r\right]_{x=b}. \tag{29}$$

3.2 Numerical solution

- Boundary limits and values:

$$a = 0, \quad \hat{u} = 1, \qquad b = 1, \quad \hat{\gamma} = 2.$$

- Shape functions ($s = 1,2$):

$$\{\phi_s\} = \{1, \mathrm{e}^x\}.$$

- Weight functions ($r = 1,2$):

$$\{\overset{0}{\psi}_r\} = \{\overset{1}{\psi}_r\} = \{\overset{2}{\psi}_r\} = \{1, x\}.$$

- System of equations:

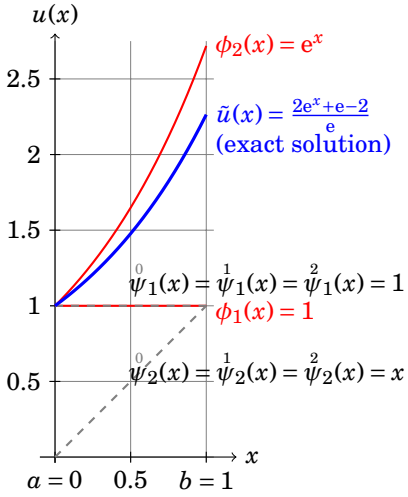
$$\begin{bmatrix} 1 & (1+\mathrm{e}) \\ 0 & \mathrm{e} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}.$$

- Coefficients:

$$U_1 = 1 - \frac{2}{\mathrm{e}}, \quad U_2 = \frac{2}{\mathrm{e}}.$$

- Approximated solution:

$$\tilde{u} = U_1 + U_2\,\mathrm{e}^x = \frac{2\mathrm{e}^x + \mathrm{e} - 2}{\mathrm{e}}.$$



One can check that this approximation is in fact the exact solution. Such result is obtained thanks to the choice of shape functions (the simple subspace generated by the shape functions happens to contain the exact solution).

3.3 Another numerical solution

- Boundary limits and values:

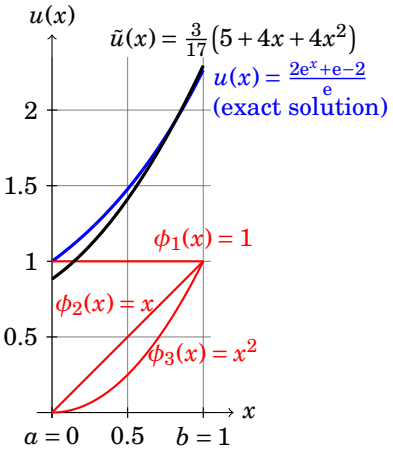
$$a = 0, \quad \hat{u} = 1, \qquad b = 1, \quad \hat{\gamma} = 2.$$

- Shape and weight functions ($s = 1,2,3$):

$$\{\phi_s\} = \{\overset{0}{\psi}_s\} = \{\overset{1}{\psi}_s\} = \{\overset{2}{\psi}_s\} = \{1, x, x^2\}.$$

- System of equations:

$$\begin{bmatrix} 1 & 0 & 3 \\ 0 & \frac{1}{2} & \frac{7}{3} \\ 0 & \frac{2}{3} & \frac{13}{6} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ 2 \end{bmatrix}.$$



- Coefficients:

$$U_1 = \frac{15}{17}, \quad U_2 = \frac{12}{17}, \quad U_3 = \frac{12}{17}.$$

- Approximated solution:

$$\tilde{u} = U_1 + U_2 x + U_3 x^2 = \frac{3}{17}\left(5 + 4x + 4x^2\right).$$