Chapter 5

Explicit prefactorization methods

The development of explicit prefactorization methods, also known as *AGA two-sweep iterative methods* [67, 68, 69, 70, 71, 73, 74], started in 1968 with the first and simplest version, the *EWA algorithm* [66].[1] They have since been applied successfully to problems arising from finite-difference approximations of second-order elliptic partial differential equations, such as the system of neutron diffusion equations, which plays a central role in nuclear reactor physics theory [83]. These methods are convenient to use in practical applications, and when implemented in reactor design codes, they have provided very encouraging results. The double successive overrelaxation process used to accelerate convergence in the HexAGA-II two-dimensional [69] and HexAGA-III three-dimensional [71] production codes has proved to be highly effective, especially in refined-mesh computations [72, 78, 83].

Closely related techniques had been introduced earlier, and independently, by Buleev [12] and Oliphant [41]. These methods remained unnoticed until 1968, when numerical experiments by Stone [58] led to some new developments. However, none of these methods were extensively studied from the viewpoint of practical implementation, and they are not as well documented theoretically as the AGA methods, whose computational efficiency found some theoretical support in comparison theorems, based on an improved theory of regular splittings [67, 68, 74], discussed in detail in chapter 2.

The matrix notation introduced by the author to describe AGA algorithms makes it possible to define many other methods (including the Jacobi and Gauss-Seidel methods and Gaussian elimination) as special cases of the AGA method; their classification was studied in an award-winning paper [73]. The competition for this award was held in the International Topical Meeting on Advances in Reactor Physics, Mathematics and Computation, Paris, April 27-30, 1987.

The explicit prefactorization methods are given in matrix notation in section 5.1. Section 5.2 shows how particular algorithms are implemented to solve systems of two-dimensional difference equations indexed by mesh points for different geometries of mesh structure. The performance of these algorithms is studied in section 5.3, which

[1]Editor's note: The AGA algorithm is also known as *incomplete LU factorization* (*ILU*). Other pioneers in the field include R. Varga, with H. Price, in 1960; H. van der Vorst, with J. Meijerinck, in 1973; and A. Jennings in 1973.

discusses the solution of linear systems arising from the difference approximation of self-adjoint and non-self-adjoint two-dimensional elliptic partial differential equations; numerical experiments are performed for the test problems given in section 3.5. Special attention is paid to determining the optimum relaxation parameters: those providing the maximum rate of convergence.

5.1 Matrix notation

5.1.1 Basic algorithms

Consider the splitting $\mathbf{A} = \mathbf{M} - \mathbf{N}$, where the matrix $\mathbf{A} = \mathbf{K} - \mathbf{L} - \mathbf{U}$ is defined as in (4.31): $\mathbf{K}$ is a nonsingular diagonal matrix, $\mathbf{L}$ is strictly lower triangular, and $\mathbf{U}$ is strictly upper triangular. The idea behind explicit prefactorization methods for solving

$$\mathbf{A}\boldsymbol{\phi} = \mathbf{c} \tag{5.1}$$

iteratively consists of factoring $\mathbf{M}$ as follows:

$$\mathbf{M} = \Big[\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}\Big]\mathbf{D}\Big[\mathbf{I} - \mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\Big],$$

where $\mathbf{H}$ is strictly lower triangular, $\mathbf{Q}$ is strictly upper triangular, and $\mathbf{D}$ is a nonsingular diagonal matrix defined by the implicit relation

$$\mathbf{D} = \mathbf{K} - \operatorname{diag}\Big\{(\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\Big\}.$$

It can be easily verified that

$$\mathbf{N} = \text{off-diag}\Big\{(\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\Big\} - \mathbf{H} - \mathbf{Q}. \tag{5.2}$$

The iteration scheme can be written as

$$\boldsymbol{\phi}^{(t+1)} = \mathcal{F}\boldsymbol{\phi}^{(t)} + \mathbf{M}^{-1}\mathbf{c}, \quad t \geq 0, \tag{5.3}$$

where

$$\mathcal{F} = \mathbf{M}^{-1}\mathbf{N} = \Big[\mathbf{I} - \mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\Big]^{-1}\mathbf{D}^{-1}\Big[\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}\Big]^{-1}\mathbf{N}. \tag{5.4}$$

Since $(\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}$ is strictly lower triangular and $\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})$ is strictly upper triangular, this method can be easily implemented using the well-known *two-sweep* (*forward-backward*) procedure.

Premultiplying (5.3) by $[\mathbf{I} - \mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})]$ and shifting the term $\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\boldsymbol{\phi}^{(t+1)}$ to the right-hand side of the equation, we have

$$\boldsymbol{\phi}^{(t+1)} = \mathbf{D}^{-1}\Big[(\mathbf{U}+\mathbf{Q})\boldsymbol{\phi}^{(t+1)} + \big[\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}\big]^{-1}\big(\mathbf{N}\boldsymbol{\phi}^{(t)} + \mathbf{c}\big)\Big].$$

Denoting by

$$\boldsymbol{\beta}^{(t+1)} = \Big[\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}\Big]^{-1}\Big[\mathbf{N}\boldsymbol{\phi}^{(t)} + \mathbf{c}\Big]$$

and again premultiplying this expression by $[\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}]^{-1}$, we finally obtain

$$\left.\begin{aligned} \boldsymbol{\beta}^{(t+1)} &= (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}\boldsymbol{\beta}^{(t+1)} + \mathbf{N}\boldsymbol{\phi}^{(t)} + \mathbf{c} \\ \boldsymbol{\phi}^{(t+1)} &= \mathbf{D}^{-1}\Big[(\mathbf{U}+\mathbf{Q})\boldsymbol{\phi}^{(t+1)} + \boldsymbol{\beta}^{(t+1)}\Big], \quad t \geq 0 \end{aligned}\right\}. \tag{5.5}$$

$\mathbf{H}$	$\mathbf{Q}$	$\mathbf{M} = [\mathbf{I} - (\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}]\mathbf{D}[\mathbf{I} - \mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})]$ $\mathbf{D} = \mathbf{K} - \text{diag}\{(\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\}$	$\mathbf{N} = \text{off-diag}\{(\mathbf{L}+\mathbf{H})\mathbf{D}^{-1}(\mathbf{U}+\mathbf{Q})\} - \mathbf{H} - \mathbf{Q}$	Name
$-\mathbf{L}$	$-\mathbf{U}$	$\mathbf{M}_J = \mathbf{K}$ $\mathbf{D}_J = \mathbf{K}$	$\mathbf{N}_J = \mathbf{L} + \mathbf{U}$	Jacobi (see page 136)
$\mathbf{O}$	$-\mathbf{U}$	$\mathbf{M}_{fG} = \mathbf{K}[\mathbf{I} - \mathbf{K}^{-1}\mathbf{L}]$ $\mathbf{D}_{fG} = \mathbf{K}$	$\mathbf{N}_{fG} = \mathbf{U}$	forward Gauss-Seidel (see page 136)
$-\mathbf{L}$	$\mathbf{O}$	$\mathbf{M}_{bG} = \mathbf{K}[\mathbf{I} - \mathbf{K}^{-1}\mathbf{U}]$ $\mathbf{D}_{bG} = \mathbf{K}$	$\mathbf{N}_{bG} = \mathbf{L}$	backward Gauss-Seidel (see page 136)
$\mathbf{O}$	$\mathbf{O}$	$\mathbf{M}_E = [\mathbf{I} - \mathbf{L}\mathbf{D}_E^{-1}]\mathbf{D}_E[\mathbf{I} - \mathbf{D}_E^{-1}\mathbf{U}]$ $\mathbf{D}_E = \mathbf{K} - \text{diag}\{\mathbf{L}\mathbf{D}_E^{-1}\mathbf{U}\}$	$\mathbf{N}_E = \text{off-diag}\{\mathbf{L}\mathbf{D}_E^{-1}\mathbf{U}\}$	EWA - Woźnicki (1968, [66])
$\mathbf{O}$	$\mathbf{O}$	$\mathbf{M}_V = [\mathbf{I} - \mathbf{U}^T\mathbf{D}_V^{-1}]\mathbf{D}_V[\mathbf{I} - \mathbf{D}_V^{-1}\mathbf{U}]$ $\mathbf{D}_V = \mathbf{K} - \text{diag}\{\mathbf{U}^T\mathbf{D}_V^{-1}\mathbf{U}\}$	$\mathbf{N}_V = \text{off-diag}\{\mathbf{U}^T\mathbf{D}_V^{-1}\mathbf{U}\}$ $(\mathbf{L} = \mathbf{U}^T)$	Varga (1960, [60])
$\mathbf{O}$	$\mathbf{O}$	$\mathbf{M}_B = [\mathbf{I} - \mathbf{L}\mathbf{D}_B^{-1}]\mathbf{D}_B[\mathbf{I} - \mathbf{D}_B^{-1}\mathbf{U}]$ $\mathbf{D}_B = \mathbf{K} - \text{diag}\{\mathbf{L}\mathbf{D}_B^{-1}\mathbf{U}\} + e\mathbf{K}$	$\mathbf{N}_E = \text{off-diag}\{\mathbf{L}\mathbf{D}_B^{-1}\mathbf{U}\} + e\mathbf{K}$ $(e = 0,\ \mathbf{M}_B = \mathbf{M}_E,\ \mathbf{N}_B = \mathbf{N}_E)$	Buleev (1960, [12])
$(g-1)\mathbf{L}$	$\mathbf{O}$	$\mathbf{M}_O = [\mathbf{I} - \mathbf{g}\mathbf{L}\mathbf{D}_O^{-1}]\mathbf{D}_O[\mathbf{I} - \mathbf{D}_O^{-1}\mathbf{U}]$ $\mathbf{D}_O = \mathbf{K} - \text{diag}\{g\mathbf{L}\mathbf{D}_O^{-1}\mathbf{U}\}$	$\mathbf{N}_O = \text{off-diag}\{g\mathbf{L}\mathbf{D}_O^{-1}\mathbf{U}\} - (g-1)\mathbf{L}$ $(g = 0,\ \mathbf{M}_O = \mathbf{M}_{fG},\ \mathbf{N}_O = \mathbf{N}_{fG};$ $g = 1,\ \mathbf{M}_O = \mathbf{M}_E,\ \mathbf{N}_O = \mathbf{N}_E)$	Oliphant (1962 [41])
$a\overline{\mathbf{L}}$	$a\overline{\mathbf{U}}$	$\mathbf{M}_S = [\mathbf{I} - (\mathbf{L}+a\overline{\mathbf{L}})\mathbf{D}_S^{-1}]\mathbf{D}_S[\mathbf{I} - \mathbf{D}_S^{-1}(\mathbf{U}+a\overline{\mathbf{U}})]$ $\mathbf{D}_S = \mathbf{K} - \text{diag}\{(\mathbf{L}+a\overline{\mathbf{L}})\mathbf{D}_S^{-1}(\mathbf{U}+a\overline{\mathbf{U}})\}$	$\mathbf{N}_S = \text{off-diag}\{(\mathbf{L}+a\overline{\mathbf{L}})\mathbf{D}_S^{-1}(\mathbf{U}+a\overline{\mathbf{U}})\} - a\overline{\mathbf{L}} - a\overline{\mathbf{U}}$ $(a = 0,\ \mathbf{M}_S = \mathbf{M}_E,\ \mathbf{N}_S = \mathbf{N}_E)$	Stone (1968, [58])
$\mathbf{H}_A$	$\mathbf{Q}_A$	$\mathbf{M}_A = [\mathbf{I} - (\mathbf{L}+\mathbf{H}_A)\mathbf{D}_A^{-1}]\mathbf{D}_A[\mathbf{I} - \mathbf{D}_A^{-1}(\mathbf{U}+\mathbf{Q}_A)]$ $\mathbf{D}_A = \mathbf{K} - \text{diag}\{(\mathbf{L}+\mathbf{H}_A)\mathbf{D}_A^{-1}(\mathbf{U}+\mathbf{Q}_A)\}$	$\mathbf{N}_A = \text{off-diag}\{(\mathbf{L}+\mathbf{H}_A)\mathbf{D}_A^{-1}(\mathbf{U}+\mathbf{Q}_A)\} - \mathbf{H}_A - \mathbf{Q}_A$	AGA - Woźnicki (1970, [67])
$\mathbf{H}_D$	$\mathbf{Q}_D$	$\mathbf{M}_D = [\mathbf{I} - (\mathbf{L}+\mathbf{H}_D)\mathbf{D}_D^{-1}]\mathbf{D}_D[\mathbf{I} - \mathbf{D}_D^{-1}(\mathbf{U}+\mathbf{Q}_D)]$ $\mathbf{D}_D = \mathbf{K} - \text{diag}\{(\mathbf{L}+\mathbf{H}_D)\mathbf{D}_D^{-1}(\mathbf{U}+\mathbf{Q}_D)\}$	$\mathbf{N}_D = \mathbf{O}$ $(\text{off-diag}\{(\mathbf{L}+\mathbf{H}_D)\mathbf{D}_D^{-1}(\mathbf{U}+\mathbf{Q}_D)\} = \mathbf{H}_D - \mathbf{Q}_D)$	AGA - direct method Woźnicki (1970, [67])

TABLE 5.1.1. The classification of prefactorization splittings of $\mathbf{A} = \mathbf{M} - \mathbf{N} = \mathbf{K} - \mathbf{L} - \mathbf{U}$.