Waves in periodic materials

Nicolás Guarín Z.

September/18/2011

Floquet Theory

Floquet theory is a branch of the theory of ordinary differential equations relating to the class of solutions to linear differential equations of the form

$$\dot{x} = A(t)x\,,$$

with *A(t)* a piecewise continuous periodic function with period *T*.

Blöch Theorem

Let have an equation of the form

$$\mathrm{L}\,u(\mathbf{x}) = -\omega^2 u(\mathbf{x})\,, \tag{1}$$

where L is a differential operator with algebraic wave-like properties.

Blöch Theorem establish that the solution for (1) is

$$u(\mathbf{x}) = w(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}\,, \tag{2}$$

Where $w(\mathbf{x})$ is a function with the same periodicity that $A(\mathbf{x})$.

> *The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave* $\exp(i\mathbf{k}\cdot\mathbf{x})$ *times a functions* $w(\mathbf{x})$ *with the periodicity of the crystal lattice.*

If we write the solution (2) for $\mathbf{x} + \mathbf{a}$, being **a** the *vectorial* periodicity of the lattice, we get

$$u(\mathbf{x}+\mathbf{a}) = w(\mathbf{x}+\mathbf{a})e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{a})}\,,$$

due to the periodicity of $u_{\mathbf{k}}(\mathbf{x})$

$$u(\mathbf{x}+\mathbf{a}) = w(\mathbf{x})e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{a})}\,, \tag{3}$$

and, from (6)

$$w(\mathbf{x}) = u(\mathbf{x}+\mathbf{a})e^{-i\mathbf{k}\cdot\mathbf{x}}\,,$$

replacing it in (7) reads

$$u(\mathbf{x}+\mathbf{a}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}. \tag{4}$$

Blöch Theorem in Elastodynamics

Navier-Cauchy equation, without body forces, is

$$(\lambda+2\mu)\nabla(\nabla\cdot\mathbf{u}) + \mu\nabla\times(\nabla\times\mathbf{u}) = -\omega^2\rho\mathbf{u}$$

Displacement vector could be expressed as $\mathbf{u} = \nabla\phi + \nabla\times\boldsymbol{\psi}$ due to the Helmholtz decomposition theorem and the potentials $\phi, \boldsymbol{\psi}$ verify

$$\begin{aligned}\nabla^2\phi &= -\omega^2 S_1^2\phi \\ \nabla^2\boldsymbol{\psi} &= -\omega^2 S_2^2\boldsymbol{\psi}\end{aligned}, \quad \text{with} \quad \begin{aligned} S_1^2 &= \frac{\rho}{\lambda+2\mu} \\ S_2^2 &= \frac{\rho}{\mu}\end{aligned}.$$

So the Bloch theorem is verified for the wave equation for the potentials and

$$\begin{aligned}\phi(\mathbf{x}) &= \phi(\mathbf{x}+\mathbf{a})e^{i\mathbf{k}\cdot\mathbf{a}}, \\ \boldsymbol{\psi}(\mathbf{x}) &= \boldsymbol{\psi}(\mathbf{x}+\mathbf{a})e^{i\mathbf{k}\cdot\mathbf{a}},\end{aligned}$$

and

$$\begin{aligned}\mathbf{u}(\mathbf{x}) &= \nabla\phi(\mathbf{x}) + \nabla\times\boldsymbol{\psi}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{a}}\nabla\phi(\mathbf{x}+\mathbf{a}) + e^{i\mathbf{k}\cdot\mathbf{a}}\nabla\times\boldsymbol{\psi}(\mathbf{x}+\mathbf{a}) \\ &= e^{i\mathbf{k}\cdot\mathbf{a}}\left[\nabla\phi(\mathbf{x}+\mathbf{a}) + \nabla\times\boldsymbol{\psi}(\mathbf{x}+\mathbf{a})\right] = e^{i\mathbf{k}\cdot\mathbf{a}}\mathbf{u}(\mathbf{x}+\mathbf{a})\end{aligned},$$

So the Blöch theorem for the displacement field is satisfied, i.e.

$$\mathbf{u}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{a}}\mathbf{u}(\mathbf{x}+\mathbf{a}).$$

Boundary Value Problem

Let

$$\mathrm{A}\,u(x) = -\lambda^2 u(x), \tag{5}$$

be an eigenvalue problem where A is a differential operator that satisfies the Blöch Theorem in a domain Ω; which corresponds with a cell of the lattice.

The boundary conditions are Blöch-periodicity conditions, i.e.

$$\begin{aligned} &u(\mathbf{x}+\mathbf{a}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}, \\ &\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}. \end{aligned} \tag{6}$$

The BVP can also be formulated in terms of the Blöch function *w*, and the original problem is rewritten as

$$\mathrm{B}\,w(x) = -\lambda^2 w(x), \tag{7}$$

and B is a differential operator that not coincide with A. The boundary conditions for this case are transformed to periodicity conditions

$$\begin{aligned} &w(\mathbf{x}+\mathbf{a}) = w(\mathbf{x}), \\ &\frac{\partial w}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial w}{\partial \mathbf{n}}(\mathbf{x}). \end{aligned} \tag{8}$$

Example 1: Laplacian operator

If A is the Laplacian operator the BVP is

$$\begin{aligned} &\nabla^2 u(\mathbf{x}) = -\lambda^2 u(\mathbf{x}), \\ &u(\mathbf{x}+\mathbf{a}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}, \\ &\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}. \end{aligned}$$

The Laplacian is self-adjoint under the Blöch-periodicity conditions, so the eigenvalues λ^2 are all real and the discrete version should be a Hermitian or real-Symmetric matrix.

The BVP for the Blöch function is then

$$
\begin{aligned}
&\left[\nabla^2 + 2i\nabla\cdot\mathbf{k}\ \right]w(\mathbf{x}) = -\left(\lambda^2 - \|\mathbf{k}\|^2\right)w(\mathbf{x}),\\
&w(\mathbf{x}+\mathbf{a}) = w(\mathbf{x}),\\
&\frac{\partial w}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}).
\end{aligned}
$$

Where the operator $\mathrm{B} = \left[\nabla^2 + 2i\nabla\cdot\mathbf{k}\ \right] = \left[\nabla^2 + 2i\mathbf{k}\cdot\nabla\ \right]$ since $\mathbf{k}$ doesn't depend on $\mathbf{x}$. And the boundary conditions don't imply Blöch-periodicity but periodicity, they don't have the phase shift factor $e^{i\mathbf{k}\cdot\mathbf{a}}$. B is also a self-adjoint operator.

Example 2: Hamiltonian operator

If A is the Hamiltonian operator, in quantum mechanics, the BVP is

$$
\begin{aligned}
&\mathrm{H}u(\mathbf{x}) = Eu(\mathbf{x}),\\
&\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]u(\mathbf{x}) = Eu(\mathbf{x}),\\
&u(\mathbf{x}+\mathbf{a}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}},\\
&\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}.
\end{aligned}
$$

The Hamiltonian is self-adjoint under the Blöch-periodicity conditions, so the eigenvalues E are all real and the discrete version should be a Hermitian or real-Symmetric matrix.

The BVP for the Blöch function is then

$$
\begin{aligned}
&\left[-\frac{\hbar^2}{2m}\nabla^2 - 2i\mathbf{k}\cdot\nabla - \|\mathbf{k}\|^2 + V(\mathbf{x})\right]w(\mathbf{x}) = Ew(\mathbf{x}),\\
&w(\mathbf{x}+\mathbf{a}) = w(\mathbf{x}),\\
&\frac{\partial w}{\partial \mathbf{n}}(\mathbf{x}+\mathbf{a}) = \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}).
\end{aligned}
$$

Where the operator $\mathrm{B} = \left[-\hbar^2/2m\nabla^2 - 2i\nabla\cdot\mathbf{k} - \|\mathbf{k}\|^2 + V(\mathbf{x})\right] = \left[-\hbar^2/2m\nabla^2 - 2i\mathbf{k}\cdot\nabla - \|\mathbf{k}\|^2 + V(\mathbf{x})\ \right]$ since $\mathbf{k}$ doesn't depend on $\mathbf{x}$. And the boundary conditions don't imply Blöch-periodicity but periodicity, they don't have the phase shift factor $e^{i\mathbf{k}\cdot\mathbf{a}}$. B is also a self-adjoint operator.

Example 3: Navier-Cauchy equation

If one takes the time independent Navier-Cauchy equation the BVP is

$$
\begin{aligned}
&(\lambda+2\mu)\nabla(\nabla\cdot\mathbf{u}(\mathbf{x}))-\mu\nabla\times(\nabla\times\mathbf{u}(\mathbf{x}))=-\rho\omega^{2}\mathbf{u}(\mathbf{x}),\\
&\mathbf{u}(\mathbf{x}+\mathbf{a})=\mathbf{u}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}},\\
&\frac{\partial\mathbf{u}}{\partial\mathbf{n}}(\mathbf{x}+\mathbf{a})=\frac{\partial\mathbf{u}}{\partial\mathbf{n}}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{a}}.
\end{aligned}
$$

In this case the author thinks that is not a good idea to establish the problem in terms of the Blöch function, since it’s cumbersome.

$$
\begin{aligned}
&\mathrm{B}\,\mathbf{w}(x)=-\rho\omega^{2}\mathbf{w}(\mathbf{x}),\\
&\mathbf{w}(\mathbf{x}+\mathbf{a})=\mathbf{w}(\mathbf{x}),\\
&\frac{\partial\mathbf{w}}{\partial\mathbf{n}}(\mathbf{x}+\mathbf{a})=\frac{\partial\mathbf{w}}{\partial\mathbf{n}}(\mathbf{x}).
\end{aligned}
$$

Where $\mathrm{B}=(\lambda+\mu)\left[\nabla\nabla\cdot+i\{\mathbf{k}\nabla\cdot\ +\mathbf{k}\cdot\nabla+\mathbf{k}\times\nabla\times\ \}\right](\,)-\mu\left[\nabla^{2}+2i\mathbf{k}\cdot\nabla-\|\mathbf{k}\|^{2}\right](\,)$.

Periodicity in FEM

Periodicity in one dimension

Let have the following Stiffness matrix

$$\begin{bmatrix} K_{II} & K_{IC} & K_{IF} \\ K_{CI} & K_{CC} & K_{CF} \\ K_{FI} & K_{FC} & K_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} = \begin{Bmatrix} b_I \\ b_C \\ b_F \end{Bmatrix},$$

where the subscripts *I*,*C* and *F* refers to Initial, Central and Final nodes, respectively.

Then the initial row is added to the final one

$$\begin{bmatrix} K_{II} & K_{IC} & K_{IF} \\ K_{CI} & K_{CC} & K_{CF} \\ K_{FI} + K_{II} & K_{FC} + K_{IC} & K_{FF} + K_{IF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} = \begin{Bmatrix} b_I \\ b_C \\ b_F + b_I \end{Bmatrix},$$

And the periodicity condition is imposed, i.e. $u_I = u_F$,

$$\begin{bmatrix} I & 0 & -I \\ K_{CI} & K_{CC} & K_{CF} \\ K_{FI} + K_{II} & K_{FC} + K_{IC} & K_{FF} + K_{IF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} = \begin{Bmatrix} 0 \\ b_C \\ b_F + b_I \end{Bmatrix}.$$

And the matrix is rearranged; the initial column is added to the final one,

$$\begin{bmatrix} K_{CC} & K_{CF} + K_{CI} \\ K_{FC} + K_{IC} & K_{FF} + K_{IF} + K_{FI} + K_{II} \end{bmatrix} \begin{Bmatrix} u_C \\ u_F \end{Bmatrix} = \begin{Bmatrix} b_C \\ b_F + b_I \end{Bmatrix}.$$

If the initial stiffness matrix was symmetric then the final one is symmetric too.

Blöch-periodicity in one dimension

Let have the following system

$$\begin{bmatrix} K_{II} & K_{IC} & K_{IF} \\ K_{CI} & K_{CC} & K_{CF} \\ K_{FI} & K_{FC} & K_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} - \lambda \begin{bmatrix} M_{II} & M_{IC} & M_{IF} \\ M_{CI} & M_{CC} & M_{CF} \\ M_{FI} & M_{FC} & M_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} = 0,$$

where the subscripts *I*,*C* and *F* refers to Initial, Central and Final nodes, respectively.

Then, the rows corresponding to boundary nodes are multiplied by $e^{-i\mathbf{k}\cdot\mathbf{x}}$, where $\mathbf{x}$ is the position vector for each node. The columns corresponding to boundary nodes are multiplied by $e^{i\mathbf{k}\cdot\mathbf{x}}$.

$$\begin{bmatrix} K_{II} & e^{-ikx_I} K_{IC} & e^{-ikx_I} e^{ikx_F} K_{IF} \\ e^{ikx_I} K_{CI} & K_{CC} & e^{ikx_F} K_{CF} \\ e^{ikx_I} e^{-ikx_F} K_{FI} & e^{-ikx_F} K_{FC} & K_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} = \lambda \begin{bmatrix} M_{II} & e^{-ikx_I} M_{IC} & e^{-ikx_I} e^{ikx_F} K_{IF} \\ e^{ikx_I} M_{CI} & M_{CC} & e^{ikx_F} M_{CF} \\ e^{ikx_I} e^{-ikx_F} M_{FI} & e^{-ikx_F} M_{FC} & M_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix}$$

Then, the initial row is added to the final one

$$\begin{bmatrix} K_{II} & e^{-ikx_I} K_{IC} & e^{-ikx_I} e^{ikx_F} K_{IF} \\ e^{ikx_I} K_{CI} & K_{CC} & e^{ikx_F} K_{CF} \\ K_{II} + e^{ikx_I} e^{-ikx_F} K_{FI} & e^{-ikx_I} K_{IC} + e^{-ikx_F} K_{FC} & e^{-ikx_I} e^{ikx_F} K_{IF} + K_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} =$$

$$\begin{bmatrix} M_{II} & e^{-ikx_I} M_{IC} & e^{-ikx_I} e^{ikx_F} M_{IF} \\ e^{ikx_I} M_{CI} & M_{CC} & e^{ikx_F} M_{CF} \\ M_{II} + e^{ikx_I} e^{-ikx_F} M_{FI} & e^{-ikx_I} M_{IC} + e^{-ikx_F} M_{FC} & e^{-ikx_I} e^{ikx_F} M_{IF} + M_{FF} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix},$$

The initial column is added to the final one

$$\begin{bmatrix} K_{II} & e^{-ikx_I} K_{IC} & e^{-ikx_I} e^{ikx_F} K_{IF} + K_{II} \\ e^{ikx_I} K_{CI} & K_{CC} & e^{ikx_F} K_{CF} + e^{ikx_I} K_{CI} \\ K_{II} + e^{ikx_I} e^{-ikx_F} K_{FI} & e^{-ikx_I} K_{IC} + e^{-ikx_F} K_{FC} & e^{-ikx_I} e^{ikx_F} K_{IF} + K_{FF} + K_{II} + e^{ikx_I} e^{-ikx_F} K_{FI} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix} =$$

$$\lambda \begin{bmatrix} M_{II} & e^{-ikx_I} M_{IC} & e^{-ikx_I} e^{ikx_F} M_{IF} + M_{II} \\ e^{ikx_I} M_{CI} & M_{CC} & e^{ikx_F} M_{CF} + e^{ikx_I} M_{CI} \\ M_{II} + e^{ikx_I} e^{-ikx_F} M_{FI} & e^{-ikx_I} M_{IC} + e^{-ikx_F} M_{FC} & e^{-ikx_I} e^{ikx_F} M_{IF} + M_{FF} + M_{II} + e^{ikx_I} e^{-ikx_F} M_{FI} \end{bmatrix} \begin{Bmatrix} u_I \\ u_C \\ u_F \end{Bmatrix}$$

And the matrix is rearranged,

$$\begin{bmatrix} K_{CC} & e^{ikx_F} K_{CF} + e^{ikx_I} K_{CI} \\ e^{-ikx_F} K_{FC} + e^{-ikx_I} K_{IC} & K_{II} + K_{FF} + e^{ikx_I} e^{ikx_F} (K_{IF} + K_{FI}) \end{bmatrix} \begin{Bmatrix} u_C \\ u_F \end{Bmatrix} =$$

$$\lambda \begin{bmatrix} M_{CC} & e^{ikx_F} M_{CF} + e^{ikx_I} M_{CI} \\ e^{-ikx_F} M_{FC} + e^{-ikx_I} M_{IC} & M_{II} + M_{FF} + e^{ikx_I} e^{ikx_F} (e^{-2ikx_I} M_{IF} + e^{-2ikx_F} M_{FI}) \end{bmatrix} \begin{Bmatrix} u_C \\ u_F \end{Bmatrix}.$$

If the initial stiffness and mass matrices were symmetric then the final ones are Hermitian.

Implementation in a FEM code

The implementation of both Pediodicity and Blöch-Periodicity BC could be done with two different approaches:

- Modify mesh connectivity, and so the interpolation functions (see Figure 1), or
- Make row and column operations over the resulting matrices.

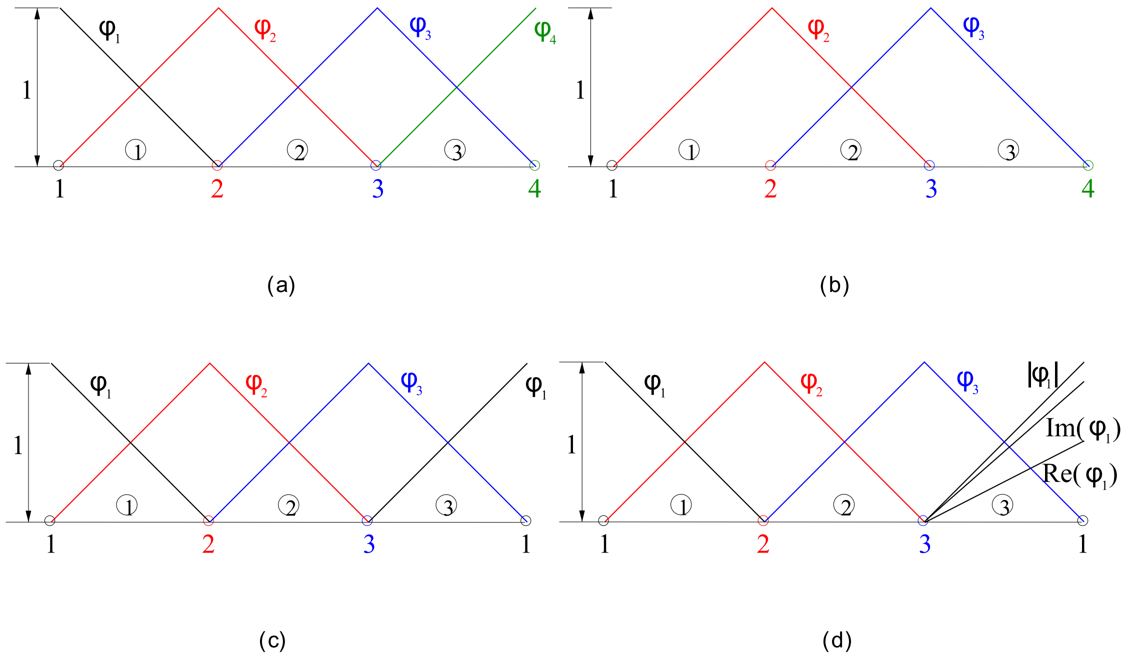

Figure 1. Linear finite element bases. (a) Neumann; (b) Dirichlet; (c) Periodic; and (d) Blöch-periodic. The real and imaginary parts of ϕ_1 are illustrated for the Blöch basis in (d) for phase shift $ka = \pi/3$ ($\Omega=[0,a]$). The modulus of ϕ_1 is the same at x=0 and x=a. (Taken from *N. Sukumar and J.E. Pask, 2009*).

The modification over the mesh is well illustrated in Figure 1, where the continuity is granted for Periodicity and a phase shift appears in the Blöch-Periodicity case.

Let call the nodes in a side of the cell *reference nodes* and the corresponding nodes in the opposite side *image nodes*. The procedure to obtain the equivalent stiffness and mass matrices is:

- Multiply all A_{kl} associated with boundary nodes by $f_k{}^*f_l$.
- To each row i of A associated with a reference node, add all rows k associated with corresponding image nodes; then to each column j associated with a reference node, add all columns l associated with corresponding image nodes.
- Delete all rows k and columns l associated with image nodes.

The multiplying factor is defined as $f_j = e^{i\mathbf{k}\cdot\mathbf{x}_j}$, and * denotes complex conjugate.

References

[1] Arfken, George, Weber, Hans and Harris, Frank (2005). *Mathematical Methods for Physicists*. Academic Press; 6 edition, 2005.

[2] Brillouin, León (1960). *Wave Propagation and Group Velocity*. Academic Press, 1960.

[3] Shoichi Fujima, Yasuji Fukasawa and Masahisa Tabata (1993). Finite Element Formulation of Periodic Conditions and Numerical Observation of Three-Dimensional Behavior in a Flow. *RIMS Kôkyûroku Bessatsu*, 836,113-119, 1993.

[4] Mark S. Gockenach (2002). *Partial Differential Equations: Analytical and Numerical Methods*. SIAM, Philadelphia, 2002.

[5] Charles Kittel (1996). *Introduction to Solid State Physics*. Wiley; 7 edition, 1996.

[6] N. Sukumar and J.E. Pask (2009). Classical and enriched finite element formulations for Bloch-periodic boundary conditions. *Int. J. Numer. Meth. Engng.* 7, 8, 1121-1138, 2009.