# A geometric frequency-domain wave propagation formulation for fast convergence of iterative solvers

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**The frequency-domain wave propagation problem is notoriously difficult to solve through iterative methods, because it leads to a symmetric but indefinite linear system. For this reason, direct methods are usually employed, at the expense of great memory usage. Convergence of iterative methods however, could be obtained by regularizing the wave equation. We introduce such regularization in Discrete Geometric Approach (DGA) framework on polyhedral grids. Moreover, we extend the regularization to the impedance boundary condition.**

***Index Terms*—Wave propagation, Convergence, Discrete Geometric Approach**

THE time-harmonic wave propagation problem in the spatial domain $\Omega$ is described by the well-known equation

$$\nabla \times \boldsymbol{\nu_r} \nabla \times \boldsymbol{e} - \omega^2 \mu_0 \epsilon_0 \boldsymbol{\epsilon_r} \boldsymbol{e} = -i\omega\mu_0 \boldsymbol{j}, \tag{1}$$

where $\boldsymbol{e}$ and $\boldsymbol{j}$ are complex vector-valued functions of the position, $\omega$ is the angular frequency and $\boldsymbol{\nu}$ and $\boldsymbol{\epsilon}$ are the symmetric positive definite material tensors. Moreover, taking the divergence of (1), it is possible to obtain the so-called continuity equation

$$-i\omega\epsilon_0 \nabla \cdot \boldsymbol{\epsilon_r} \boldsymbol{e} = \nabla \cdot \boldsymbol{j}, \tag{2}$$

which relates the divergence of the electric displacement field $\boldsymbol{d} = \epsilon_0 \boldsymbol{\epsilon_r} \boldsymbol{e}$ with the divergence of the current $\boldsymbol{j}$.

One of the possible settings to discretize (1) and (2) is the Discrete Geometric Approach (DGA) numerical scheme [1], similar to Finite Integration Technique (FIT) [2] but suitable also for polyhedral meshes [3]. In DGA the domain $\Omega$ is discretized with two polyhedral grids $\mathcal{G}, \tilde{\mathcal{G}}$. Grid $\mathcal{G}$ is named *primal grid*, while grid $\tilde{\mathcal{G}}$ is named *dual grid* and is obtained by the standard barycentric subdivision of $\mathcal{G}$. Discrete differential operators are then introduced on both grids. In particular the discrete gradient $\mathbf{G}$, curl $\mathbf{C}$ and divergence $\mathbf{D}$ are respectively the node-edge, edge-face and face-volume incidence matrix on the primal grid. The dual discrete differential operators are then obtained by transposing the primal ones, in particular $\tilde{\mathbf{G}} = \mathbf{D}^T$, $\tilde{\mathbf{C}} = \mathbf{C}^T$ and $\tilde{\mathbf{D}} = -\mathbf{G}^T$. We finally introduce the discrete Hodge operators $\mathbf{M}_{\nu_r}$ (primal face to dual edge), $\mathbf{M}_{\epsilon_r}$ (primal edge to dual face) and $\mathbf{N}^{-1}_{\mu_r \epsilon_r^2}$ (dual volume to primal node) which account for material properties [1]. This setting allows to discretize the equation (1) as

$$\left( \tilde{\mathbf{C}} \mathbf{M}_{\nu_r} \mathbf{C} - \omega^2 \mu_0 \epsilon_0 \mathbf{M}_{\epsilon_r} \right) \mathbf{U} = -i\omega\mu_0 \tilde{\mathbf{I}}, \tag{3}$$

where $\mathbf{U}$ and $\tilde{\mathbf{I}}$ are the arrays of the degrees of freedom corresponding to $\boldsymbol{e}$ and $\boldsymbol{j}$. The entries of $\mathbf{U}$ are the circulations of $\boldsymbol{e}$ on the edges $e_i$ of $\mathcal{G}$

$$U_i = \int_{e_i} \boldsymbol{e} \cdot d\boldsymbol{l}, \tag{4}$$

while the entries of $\tilde{\mathbf{I}}$ are the fluxes of $\boldsymbol{j}$ on the faces $\tilde{f}_i$ of $\tilde{\mathcal{G}}$

$$I_i = \int_{\tilde{f}_i} \boldsymbol{j} \cdot d\boldsymbol{S}, \tag{5}$$

It is well-known, however, that (3) leads to a symmetric indefinite linear system on which iterative solvers fail to converge [4]. For this reason direct solvers are usually employed, but at a great expense of memory resources. This in turn makes the solution of large scale wave propagation problems a quite challenging topic, frequently requiring approaches tailored for the specific problem [5]. In this paper we propose a regularized formulation of (3) that could enable the convergence of iterative solvers on this type of problem. The improvement of our contribution over the existing literature [2], [6], [7] is that support for polyhedral grids is introduced and impedance boundary conditions are correctly handled.

The paper is organized as follows: in Section I the formulation for problems without impedance boundary conditions is presented. In Section II the formulation is extended to work with impedance boundary conditions. Then, some observations about preconditioning are made. Finally, the numerical results are presented.

## I. Regularized formulation

By taking the discrete divergence of (3), the discrete continuity equation is obtained

$$-i\omega\epsilon_0 \tilde{\mathbf{D}} \mathbf{M}_{\epsilon_r} \mathbf{U} = \tilde{\mathbf{D}} \tilde{\mathbf{I}}. \tag{6}$$

By premultiplying both of its sides by $-\mathbf{M}_{\epsilon_r} \mathbf{G} \mathbf{N}^{-1}_{\mu_r \epsilon_r^2} / i\omega\epsilon_0$ and by adding it to (3), the continuity equation can be exploited to enforce the divergence of the electric displacement field [6], [7].

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By setting $\mathbf{K} = \tilde{\mathbf{C}}\mathbf{M}_{\nu_r}\mathbf{C} - \omega^2\mu_0\epsilon_0\mathbf{M}_{\epsilon_r}$, the modified equation reads

$$\left(\mathbf{K} + \mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r}\right)\mathbf{U} = -\frac{1}{i\omega\epsilon_0}\mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\tilde{\mathbf{D}}\tilde{\mathbf{I}} - i\omega\mu_0\tilde{\mathbf{I}}. \tag{7}$$

The premultiplication is justified by the fact that for a vector field $\boldsymbol{f}$ the identity

$$\nabla \times \nabla \times \boldsymbol{f} = \nabla(\nabla \cdot \boldsymbol{f}) = \nabla^2 \boldsymbol{f} \tag{8}$$

holds, and thus what is obtained is a discrete equation having properties similar to the laplacian operator. This, in turn, enables the convergence of the iterative solvers, but it poses some practical problems. The first of them is that $\mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r}$ must be constructed from the *global* terms $\mathbf{M}_{\epsilon_r}$, $\mathbf{G}$ and $\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}$. Then, the term $\mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r}$ has very poor sparsity: explicit computation leads to a matrix which has about 10 times the number of nonzeros of (3). The poor sparsity is due to $\mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r}$ being the product of $\mathbf{R}^T = \mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1/2}_{\mu_r\epsilon_r^2}$ (which has good sparsity) and its transpose. Computing the product $\mathbf{R}^T\mathbf{R}$ and assembling it explicitly produces a fill-in sufficient to make this approach useless. Matrix free techniques, however, allow to keep the product implicit and to keep the memory usage low. In particular, where the computation of a matrix-vector product is required inside the solver, what has to be done is to compute it as $\mathbf{Kv} + \mathbf{R}^T(\mathbf{Rv})$, where $\mathbf{v}$ is the vector that has to be multiplied by the system matrix. In other words, inside the solver it is important to first compute the matrix-vector product $\mathbf{Rv}$, then the resulting vector has to be multiplied by $\mathbf{R}^T$ and finally summed to $\mathbf{Kv}$.

## II. Impedance boundary conditions

The regularization proposed in the previous paragraph has the limitation that it cannot handle an important class of boundary conditions, namely the *impedance boundary conditions*. If impedance boundary conditions [8] are added to (3), the new problem reads

$$\left(\tilde{\mathbf{C}}\mathbf{M}_{\nu_r}\mathbf{C} - \omega^2\mu_0\epsilon_0\mathbf{M}_{\epsilon_r} + i\omega\mathbf{Y}\right)\mathbf{U} = -i\omega\mu_0\tilde{\mathbf{I}}, \tag{9}$$

where $\mathbf{Y}$ is a matrix which has nonzeros only in correspondence of the boundary edges and is computed according to [8]. Taking the divergence of this new expression leads to a different form of the discrete continuity equation which accounts for the impedance boundary:

$$\left(\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r} - \frac{1}{i\omega\epsilon_0}\tilde{\mathbf{D}}\mathbf{Y}\right)\mathbf{U} = -\frac{1}{i\omega\epsilon_0}\tilde{\mathbf{D}}\tilde{\mathbf{I}}. \tag{10}$$

At a first sight it could appear reasonable to apply to this new equation the same approach we used with (6). We found, however, that using the same approach used for the problem without impedance boundary conditions does not lead to improved convergence of iterative solvers. In particular, COCG (Conjugated Orthogonal Conjugated Gradient) fails to converge, while QMR (Quasi-Minimal Residuals) stagnates at very high values of relative residual. The technique we propose to overcome this difficulty is introducing a scaling matrix $\boldsymbol{\alpha}$ and not considering $\mathbf{Y}$ in the premultiplication term:

$$\boldsymbol{\beta}^T\left(\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r} - \frac{1}{i\omega\epsilon_0}\tilde{\mathbf{D}}\mathbf{Y}\right)\mathbf{U} = -\frac{1}{i\omega\epsilon_0}\boldsymbol{\beta}^T\tilde{\mathbf{D}}\tilde{\mathbf{I}}, \tag{11}$$

where $\boldsymbol{\beta}^T = \mathbf{M}_{\epsilon_r}\mathbf{G}\mathbf{N}^{-1}_{\mu_r\epsilon_r^2}\boldsymbol{\alpha}$. The scaling matrix $\boldsymbol{\alpha}$ is a diagonal matrix where all the entries are equal to one, except the entries corresponding to the nodes on the impedance boundary. Those entries are set to the value $\alpha$. The new formulation reads

$$\left(\mathbf{K} + \boldsymbol{\beta}^T\mathbf{P}\right)\mathbf{U} = -i\omega\mu_0\tilde{\mathbf{I}} - \frac{1}{i\omega\epsilon_0}\boldsymbol{\beta}^T\tilde{\mathbf{D}}\tilde{\mathbf{I}} \tag{12}$$

This new regularization has again poor sparsity, but it also leads to a non-symmetric matrix, which require the use of appropriate solvers like QMR. Regarding the matrix-free solver, in this last case the matrix-vector products are computed as $\mathbf{Kv} + \boldsymbol{\beta}^T(\mathbf{Pv})$ where $\mathbf{P} = \left(\tilde{\mathbf{D}}\mathbf{M}_{\epsilon_r} - \frac{1}{i\omega\epsilon_0}\tilde{\mathbf{D}}\mathbf{Y}\right)$.

## III. Preconditioning

We investigated ways to precondition the solvers, and we found a very simple but effective way to precondition COCG for the solution of problem (7). By taking $M = diag(\mathbf{K})$, we observed that the number of iterations required for convergence is more than halved. Taking the inverse of the diagonal of the whole matrix (and thus using a simple Jacobi preconditioner) is not as efficient, since the number of iterations required to reach convergence is slightly higher. The same preconditioner unfortunately is not effective with QMR, neither in the case with only PEC and PMC boundary conditions nor in the case with impedance boundary conditions.

## IV. Numerical results


Fig. 1. Picture of the structure used in simulations. The structure resebles a coax-waveguide transition, with the source applied to the pin inside the waveguide ($TE_{10}$ cutoff frequency fc = 8.33 GHz).

The proposed regularizations were tested by simulating a structure resembling a coax to waveguide transition (Figure 1) excited at f = 10 GHz. Simulations were made on tetrahedral grids, however polyhedral grids are supported by the method [3]. The solutions obtained were compared against the solutions computed by a direct solver on the same problem but without regularization; the difference was always comparable with the tolerance of the iterative solver. Three meshes were used, a coarser one with 21k elements, a medium one with 181k elements and a finer one with 300k elements. The iterative solvers were implemented inside EMT, a DGA workbench written in C++14, using the Eigen linear algebra library version 3.2.9. As direct solver we used Intel MKL PARDISO.

### A. *Problem with only PEC boundary conditions*

In the first experiment we simulated our waveguide-like structure only in presence of Perfect Electrical Conductor (PEC) boundary conditions, and we obtained the convergence behaviours depicted in the Figures (2), (3) and (4). In those figures it is possible to see how COCG greatly benefits of the preconditioning described in Section III.

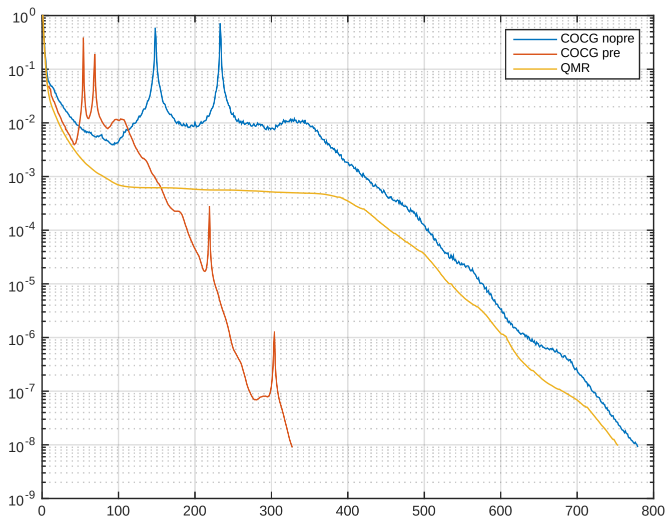


Fig. 2. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem without impedance boundary conditions. 21k elements.

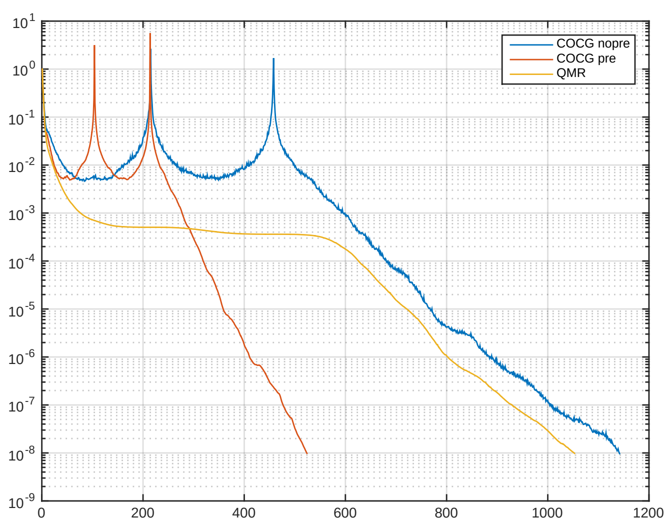


Fig. 3. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem without impedance boundary conditions. 181k elements.

### B. *Problem with PEC and PMC boundary conditions*

In the second numerical experiment we replaced two of the six boundary conditions with a Perfect Magnetic Conductor (PMC) condition. In particular, referring to Figure (1), the PMC walls were the one in the front and the one in the back. The solvers in this case showed slower and less smooth

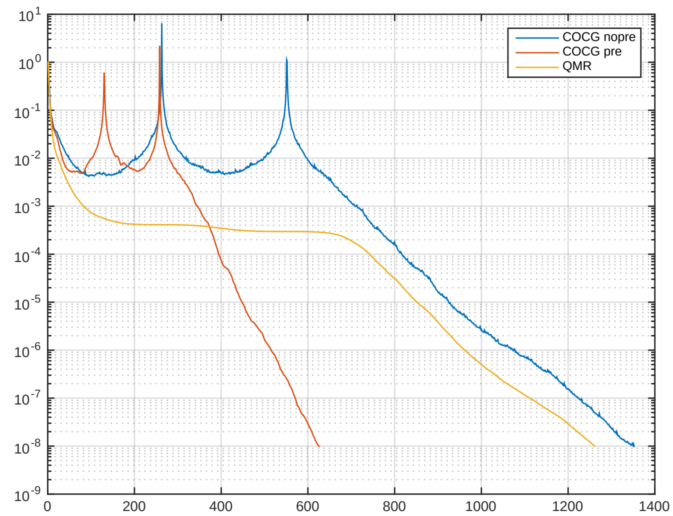


Fig. 4. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem without impedance boundary conditions. 300k elements.

convergence (Figures 5, 6 and 7), however the modified regularization remains equally useful. The preconditioner improved greatly the convergence of COCG also in this case.

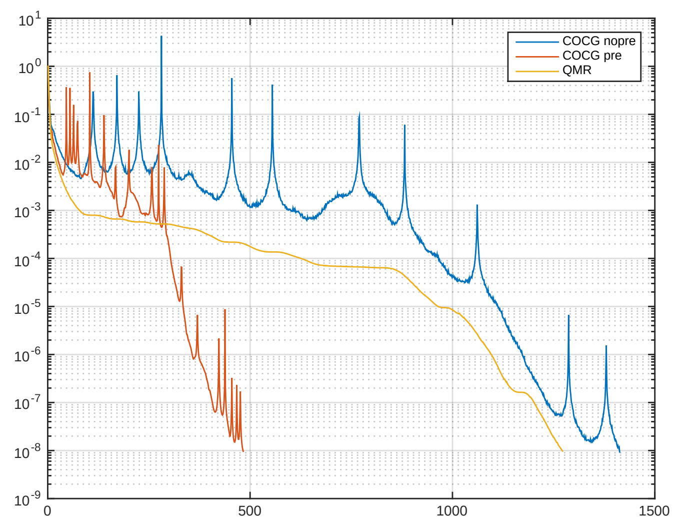


Fig. 5. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem with only PEC and PMC boundary conditions, 21k elements.

### C. *Problem with impedance boundary conditions*

The problem we ran in this case had PEC boundaries everywhere, except in the rightmost wall of the waveguide (Figure 1). When impedance boundary conditions are used, the only solver that correctly handles the (nonsymmetric) problem is QMR. We observed that, in general, impedance boundary conditions slow down the convergence significatively (Figure 8). Moreover, we found that a good value for the scaling parameter is $\alpha = 0.001$.

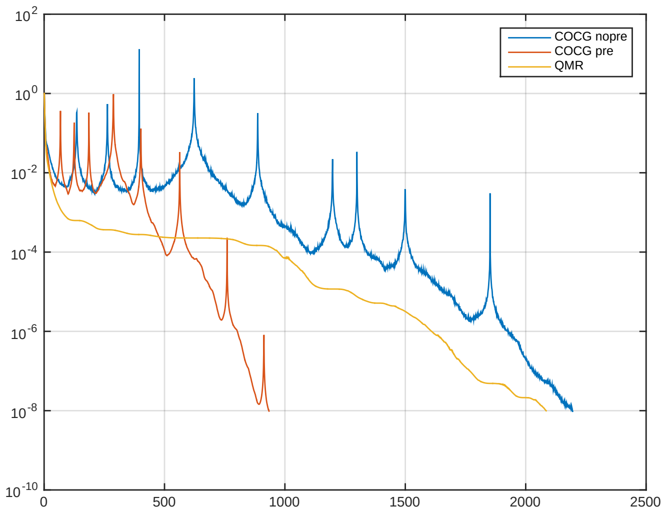


Fig. 6. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem with only PEC and PMC boundary conditions, 181k elements.

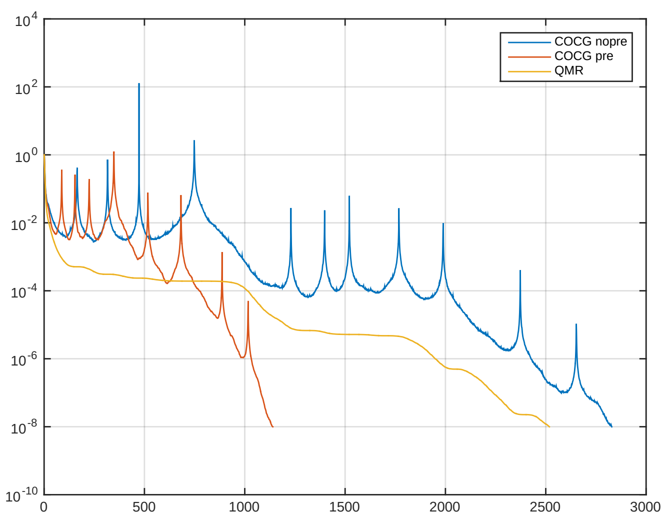


Fig. 7. Convergence of unpreconditioned COCG, preconditioned COCG, unpreconditioned QMR on the problem with only PEC and PMC boundary conditions, 300k elements.

### D. Computational requirements

On the 181k element mesh, solving (3) with a direct solver required about 2.9 GB of RAM, while solving (7) with iterative solvers required slightly less than 1 GB of RAM. On the mesh with 300k elements, 5.6 GB and 1.9 GB were required respectively. Memory savings increase with increasing system sizes. On (3) it was impossible to reach convergence with iterative solvers, while in (7) convergence can be reached in few hundreds iterations. The presented technique allows for huge memory savings and problems with millions of unknowns become solvable on a common laptop computer.

## V. Conclusions

It is well known that simulating wave propagation in the frequency domain is a challenging problem, because of the properties of the matrices that arise from the discretization.

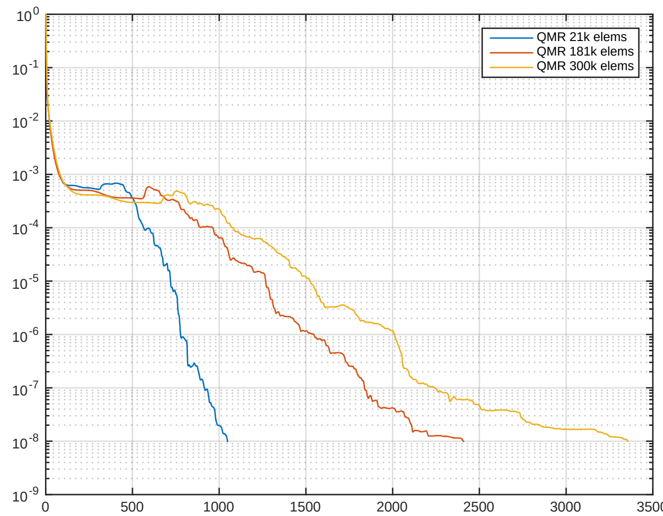


Fig. 8. Convergence of QMR on problem with impedance boundary conditions. Convergence rate for all the mesh sizes are shown in same graph.

In this work we studied the use of regularization techniques to obtain linear systems treatable by iterative solvers. We observed that in absence of impedance boundary conditions, introducing the regularization is very effective and allows to solve huge problems on modest machines. Introducing regularization in presence of impedance conditions, however, appears to be a far more delicate subject. The technique we proposed seems to be quite effective, but it is not optimal since it requires an user-specified parameter.

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