NUMERICAL CONTINUATION AND BIFURCATION IN THE PRESENCE OF SYMMETRY IN FREEFEM++ *

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Abstract. We draw the attention to a well documented but often ignored strategy to dealing with bifurcation and path continuation analysis in the presence of symmetry. The essence and key steps of this strategy are illustrated with a simple example of Schnakenberg's system of two Reaction Diffusion equations in a two dimensional domain. The powerful FEM machinery in Freefem++ is the ideal platform and a few group theoretic routines easily enable the Symmetry adapted strategy i.e., the optimal way to exploit the symmetry of the problem.

Key words. Symmetry, reaction diffusion, block diagonalization, Freefem++, fractional step, Dihedral Groups

1. Introduction. The simple example chosen for illustration of the ideas in this presentation is the Schnakenberg reaction diffusion equation in two dimensions.

The main focus is,

1. Numerical analysis for determining the steady states with change in bifurcation parameter (λ), i.e path continuation, and detection of bifurcation points along this path.
2. Exploiting the symmetry in the problem for the above numerical analysis.

The first objective is easily achieved with standard procedures (Newton-Raphson method on the standard weak form) and easily implemented in the platform provided by Freefem++.

The second objective has one (obvious and well known) serious issue. The Jacobian is ill conditioned as we approach a bifurcation point. This issue is neatly resolved by exploiting the symmetry in the problem. Essentially, there exists an optimal symmetry adapted basis (which will not coincide with the standard basis chosen by Freefem++) in which the issue of ill conditioning and bifurcation analysis are simultaneously resolved. All of this can be neatly implemented in Freefem++ with ease.

2. The essential ideas of Group Theoretic approach. The details of this short note can be found in [1], [2], [3], [10], [7]. Nonlinear bifurcation analysis involves a numerical continuation solution of the set of nonlinear equations

$$\mathbf{f}(\lambda, \mathbf{u}) = \mathbf{0},$$
$$\mathbf{f} : \mathbb{R} \times V \mapsto V$$

Often times symmetry in the problem would imply that these equations are equivariant under the action of a Group D_n (say eg, a dihedral group),

$$\mathbf{f}(\lambda, R(D_n)\mathbf{u}) = R(D_n)\mathbf{f}(\lambda, \mathbf{u})$$

Differentiating both sides gives us

$$Df(\lambda, R(D_n)\mathbf{u})R(D_n) = R(D_n)Df(\lambda, \mathbf{u}) \quad (2.1)$$

The three things to note now are

*The Finite Element framework of FreeFem++ enables this elegant journey past multiple bifurcation points

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1. *Looking for symmetric solutions (solutions that possess the symmetry of the dihedral group) means $R(D_n)\mathbf{u} = \mathbf{u}$ i.e, the solution is* invariant *to the action of the group. We substitute this into eq(2.1) to note that*

$$Df(\lambda, \mathbf{u})R(D_n) = R(D_n)Df(\lambda, \mathbf{u})$$

2. *Thus, we conclude from the above equation that along the symmetric solutions path, the Jacobian (a linear operator) commutes with the actions of the group.*
3. **The fundamental theorem of Group Theoretic application** *asserts that linear operators which commute with the group can be block diagonalized in a suitable "symmetry adapted basis". This proof is constructive. We can use this to construct the symmetry adapted basis.*

In this symmetry adapted basis, the block diagonal Jacobian and the incremental equations for a Newton-Raphson iteration in the nonlinear FEM analysis takes the form

$$\begin{bmatrix} \mathbf{K}_{\mathbf{V^{(1)}}} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{\mathbf{V^{(2)}}} & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{K}_{\mathbf{V^{(p)}}} \end{bmatrix} \begin{bmatrix} w^{(1)} \\ w^{(2)} \\ \vdots \\ w^{(p)} \end{bmatrix} = \begin{bmatrix} -\mathbf{f}_\lambda \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix}$$

and tracing out the complete symmetric solutions would only require the solutions of the first block, i.e.,

$$\mathbf{K}_{\mathbf{V^{(1)}}}\mathbf{w_1} = -\mathbf{f}_\lambda$$

The other matrices $\mathbf{K}_{\mathbf{V}^{(\mu)}}\,(\mu = \mathbf{2}, \mathbf{3}, \dots, \mathbf{p})$ are only associated with the occurence of a bifurcation point when one of these blocks goes singular. Thus, block diagonalization circumvents the illconditioning encountered near bifurcation solution points. $V^{(\mu)}$ are vector subspaces that are in 1-1 correspondence with the number of irreducible representations of the finite group D_n and $V^{(1)}$ is the subspace corresponding to the one dimensional trivial representation of the group and inherits the complete symmetry of the group. Thus, all the solutions that we seek lie in this vector subspace $V^{(1)}$.

3. The algorithm. A simplified version of the numerical algorithm is as follows,

A new solution $[u_{k+1}, \lambda_{k+1}]$ is sought.

1. Define an initial guess for $[u_{k+1}, \lambda_{k+1}]$.
2. Compute the Jacobian and residue $\mathbf{f}$ with respect to the standard coordinate system in Freefem++.
3. Solve the linear equations restricted to the subspace $V^{(1)}$.

$$\underbrace{\mathbf{Q}_1^T\mathbf{K}\mathbf{Q}_1}_{\mathbf{K_{V^{(1)}}}}\underbrace{\mathbf{Q}_1^T w}_{w^{(1)}} = \underbrace{\mathbf{Q}_1^T\mathbf{f}}_{\mathbf{f}^{(1)}} \Rightarrow \mathbf{K}_{V^{(1)}}w^{(1)} = \mathbf{f}^{(1)}$$

   by computing $\mathbf{K}_{\mathbf{V^{(1)}}}, \mathbf{f^{(1)}}$ with the orthogonal transformation to the symmetry basis $\mathbf{Q}_1$. Thus, $\mathbf{u}_{k+1}^{(1)} = \mathbf{Q}_1^T\mathbf{u}_{k+1}$
4. Using the Newton Raphson method by transforming between the standard computational basis (that Freefem++) uses and the symmetry basis via the orthogonal symmetry transformation $\mathbf{Q_1}$.

5. **Bifurcation analysis**: The other orthogonal Jacobian blocks are evaluated at the converged solution point to check for occurence of a bifurcation (the necessary condition of the *Implicit function theorem*.
6. *Visualization of results* We transform back to standard computational basis via $\mathbf{u}_{k+1} = \mathbf{Q}_1 \mathbf{u}_{k+1}^{(1)}$.

4. Some results. We briefly discuss some simple numerical results obtained from the implementatios in Freefem++ that convey the essence of this paper. The system of equations is as the Schnakenberg system of reaction diffusion on a rectangular domain,

$$\begin{aligned}\frac{\partial u_1}{\partial t} &= -\triangle u_1 + u_1 - u_1^2 u_2 \\ \frac{\partial u_2}{\partial t} &= -d\triangle u_2 - \lambda + u_1^2 u_2\end{aligned}$$

4.1. The Symmetric Mesh and the Symmetry Transformation matrix. A simple symmetric mesh is shown in fig(1).

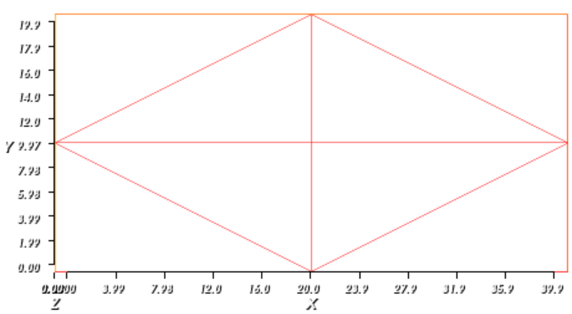

FIG. 1. *The simplest Symmetric mesh with D_2 Symmetry (Freefem++)*

The degrees of freedom with Neumann boundary conditions are 18 and this leads to a Jacobian of 18×18. The similarity transformation matrix $\mathbf{Q}$ contructed from the *fundamental theorem of Group Theoretic applications* [7], is as follows. This theorem has been used to derive the detailed formulae for symmetric matrices in [1] and [2], eg, the actual similarity transformation for this simple mesh is an 18×18 matrix that is printed verbatim in the appendix.

4.2. The Jacobian (along the solution path) in standard computational basis and Symmetry adapted basis. We show here the structure of the Jacobian along the homogenous solution ($u_1 = \lambda, u_2 = \frac{1}{\lambda}$). This homogenous solution definitely has the full symmetry of the domain (in this case the symmetry of a rectangle (D_2)) The structure of the Jacobian in the standard computational basis and in the symmetry adapted basis is shown in fig(2) and fig(3) respectively.

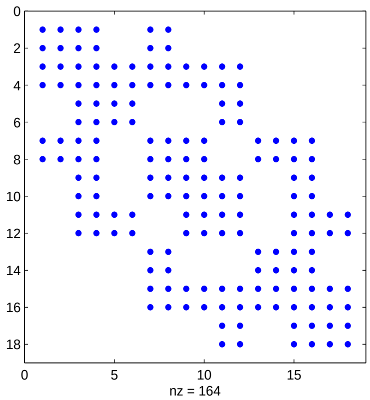

FIG. 2. *Structure of the Jacobian in Standard Computational basis for the simplest mesh.*

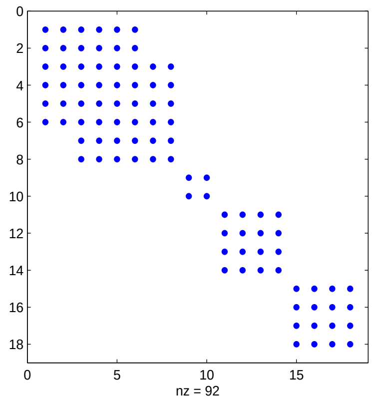

FIG. 3. *Structure of the Jacobian in the Symmetry adapted basis for the simplest mesh*

Thus, the original Jacobian is of size 18×18 and the block diagonal matrix consists of four blocks corresponding to the four irreducible representation of the dihedral group D_2.

The same is repeated for a practical mesh shown in fig(7). The degrees of freedom are now 3362×3362 and once again we have 4 blocks. The first block that is associated with the full symmetry (happens to be the block associated with the trivial 1-dimensional representation) is of size 882×882

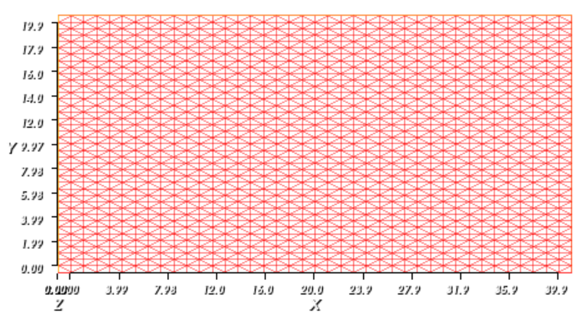

FIG. 4. *The Symmetric mesh with D_2 Symmetry for a practical mesh (Freefem++)*

4.3. Continuation along the path of complete symmetry. As discussed in the paper, the numerical continuation along the full symmetry path will only require computations involving the first block in the block diagonalization. In our practical example, this will be a

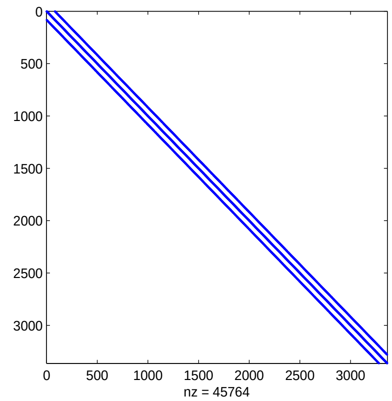

FIG. 5. *Structure of the Jacobian in Standard Computational basis along the homogenous solution path*

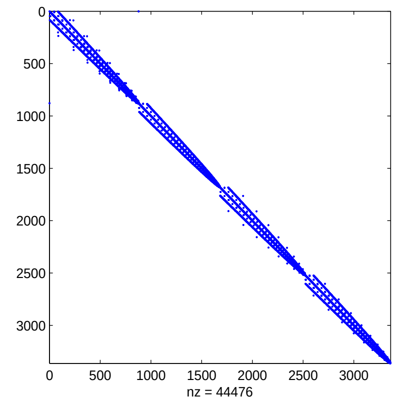

FIG. 6. *Structure of the Jacobian in the Symmetry adapted basis along the homogenous solution path*

882×882 matrix. We show here a non-homogenous steady state solution (this solution with spots retained the original D_2 symmetry of the domain), and the corresponding Jacobian in standard computational and in symmetry coordinates. Thus, using the path following algorithm along this path of solutions will require the solution of a smaller problem restricted to the subspace associated with the first block. This first block structure is shown in the figure (9). This is of size 882×882

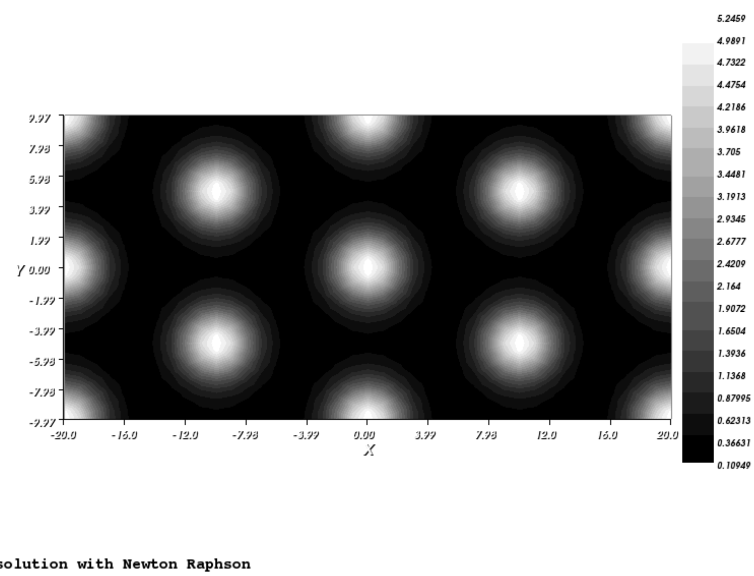

FIG. 7. *The steady non-homogenous solution (spotted patterns) obtained by Newton Raphson (in Freefem++) convergence aided by an initial guess via a long time transient analysis with the fractional step method in Freefem++.*

The non-homogenous solution was obtained with a standard fractional step time stepping scheme (transient analysis carried out for long times to obtain a steady state) in FreeFem++ and the expressions for the Jacobian along the solution paths were also obtained via suitable FreeFem++ implementations. As the solutions on this non homogenous path retains the D_2 symmetry, we again get four blocks as before.

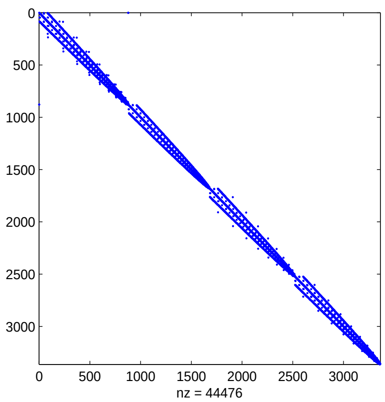

FIG. 8. *Structure of the Jacobian in Symmetry adapted basis for the non-homogenous (spotted) steady state solution*

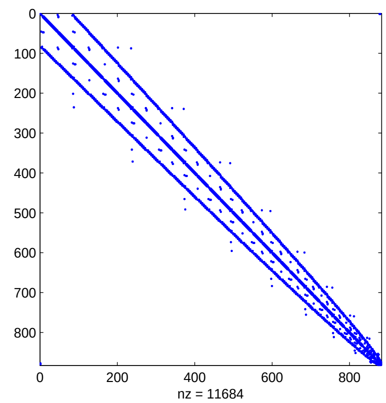

FIG. 9. *Structure of the first block in the block diagonalized Jacobian in the Symmetry adapted basis for the non-homogenous (spotted) steady state solution*

5. Future Objectives and ambitions. Our main objectives and ambition is to design and implement routines that will enable a class of symmetric problems to be analyzed by the symmetry adapted basis algorithms, in particular a well conditioned path following and symmetry bifurcation analysis. We hope this will be a useful *Open Source Tool* for researchers. The plan is build this on the powerful Freefem++ platform.

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Appendix

The similarity transformation matrix Q for the elementary mesh is printed below. We can obtain similar matrices for all D_n symmetric meshes by using the formulae in [1] and [2].

Q=

Columns 1 through 12

0	0	0	0	0	0	0.5000	0	0.5000
0	0	0	0	0	0	0	0.5000	0
0	0	0.7071	0	0	0	0	0	0
0	0	0	0.7071	0	0	0	0	0
0	0	0	0	0	0	0.5000	0	-0.5000
0	0	0	0	0	0	0	0.5000	0
0	0	0	0	0.7071	0	0	0	0
0	0	0	0	0	0.7071	0	0	0
1.0000	0	0	0	0	0	0	0	0
0	1.0000	0	0	0	0	0	0	0
0	0	0	0	0.7071	0	0	0	0
0	0	0	0	0	0.7071	0	0	0
0	0	0	0	0	0	0.5000	0	-0.5000
0	0	0	0	0	0	0	0.5000	0
0	0	0.7071	0	0	0	0	0	0
0	0	0	0.7071	0	0	0	0	0
0	0	0	0	0	0	0.5000	0	0.5000
0	0	0	0	0	0	0	0.5000	0

Columns 13 through 18

```
   -0.5000         0         0         0   -0.5000         0
         0   -0.5000         0         0         0   -0.5000
         0         0   -0.7071         0         0         0
         0         0         0   -0.7071         0         0
    0.5000         0         0         0   -0.5000         0
         0    0.5000         0         0         0   -0.5000
         0         0         0         0         0         0
         0         0         0         0         0         0
         0         0         0         0         0         0
         0         0         0         0         0         0
         0         0         0         0         0         0
         0         0         0         0         0         0
   -0.5000         0         0         0    0.5000         0
         0   -0.5000         0         0         0    0.5000
         0         0    0.7071         0         0         0
         0         0         0    0.7071         0         0
    0.5000         0         0         0    0.5000         0
         0    0.5000         0         0         0    0.5000
```