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MIXED AND MIXED-HYBRID ELEMENTS FOR THE DIFFUSION EQUATION

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ABSTRACT

To solve the diffusion equation, one often uses a Lagrangian finite element method. We want to introduce the mixed elements which allow a simultaneous approximation of the same order for the flux and its gradient. Though the linear systems are not positive definite, it is possible to make them so by eliminating some of the unknowns.

I. INTRODUCTION

Among the classical methods for solving the neutron diffusion equation, the finite element method allows an efficient numerical treatment. Today there is an accumulated experience of many years in the use of Lagrangian finite elements in computer codes : /CRONOS/FINELM.

The aim of this work is to introduce other finite elements ; the approximations obtained for the flux and its gradient by the mixed and mixed - hybrid elements not only are simultaneous but also of the same order. The linear systems are not positive definite but the elimination of some unknowns suppresses this problem. It has been shown that some mixed elements are equivalent to nodal schemes ; that may help to prove the convergence of higher degree nodal methods.

We present the theorical methods and some numerical results obtained with mixed elements.

II. THEORICAL BASIS OF THE MIXED METHOD

A. Variational formulation and approached problem

The mixed-dual variational form of the problem is the following [1,7] :

$$(\mathcal{P})\quad\left|\begin{array}{ll} \text{Find } (\vec{p},u)\in H_{o,\Gamma_1}(\text{div},\Omega)\times L^2(\Omega) \text{ so that :} & \\ \displaystyle\int_\Omega \frac{1}{D}\,\vec{p}\cdot\vec{q} + \text{div}\,\vec{q}\,u = 0 & \forall\vec{q}\in H_{o,\Gamma_1}(\text{div},\Omega) \\ \displaystyle\int_\Omega -\text{div}\,\vec{p}\,v + \Sigma uv = \int_\Omega fv & \forall v\in L^2(\Omega) \end{array}\right.$$

with Ω being a bounded domain of $\mathbb{R}^n (n = 2 \text{ or } 3)$, $\partial\Omega = \Gamma_o \cup \Gamma_1$, meas $(\Omega_o) > 0$ and

$H_{o,\Gamma_1}(\text{div},\Omega) = \{\vec{q}\in H(\text{div},\Omega)/\vec{q}\cdot\vec{n} = 0 \text{ on } \Gamma_1\}$

We have the following result :

If $D,\Sigma\in L^\infty(\Omega)$, $D(x)\geq \nu > 0$ and $\Sigma(x) \geq 0$ a.e. in Ω, $f\in L^2(\Omega)$ then

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problem ($\mathcal{P}$) has a unique solution, which is $(D\vec{\nabla}u, u)$ where u is the solution of the variational problem :

$$(Q)\left|\begin{array}{l}\text{Find } u\in H^1_{o,\Gamma_o}(\Omega) = \{v\in L^2(\Omega)/\ v = 0 \text{ on } \Gamma_o\} \text{ so that :}\\ \int_\Omega D\vec{\nabla}u\cdot\vec{\nabla}v + \Sigma uv = \int_\Omega fv \qquad \forall v\in H^1_{o,\Gamma_o}(\Omega)\end{array}\right.$$

The spaces H_{o,Γ_1} (div, Ω) and $L^2(\Omega)$ are approximated by finite dimensional spaces :

$$Q_h = \{\vec{q}_h\in H_{o,\Gamma_1}(\text{div},\Omega)/\vec{q}_{h/K}\in Q_K \quad \forall\, K\in T_h\}$$

$$V_h = \{v_h\in L^2(\Omega)/v_{h/K}\in P_K \quad \forall\, K\in T_h\}$$

built on a triangulation T_h, P_K and Q_K being polynomial spaces. For the sake of simplicity we shall restrict ourselves to the 2D case. Suppose that Ω is a union of rectangles and $(T_h)_h$ is a regular family of 'triangulations' made of rectangles. Let T_h be one of the triangulations.

For Q_K and P_K, the spaces of Raviart and Thomas[2] are often chosen :

$$Q_K = P_{k+1,k} \times P_{k,k+1} \qquad P_K = P_{k,k}$$

with k being a given integer and $P_{\ell,m} = \{P\in\mathbb{R}[X,Y]/\deg_x P\leq \ell \quad \deg_y P\leq m\}$.

Thus, for example, for each rectangle we can take as unknowns : for u_h $(k+1)^2$ inner values, and for $\vec{p}_h$ the value of $\vec{p}_h\cdot\vec{n}$ at $(k+1)$ distinct points on each edge and the moments :

$$\int_K p_{h1}(x,y)x^iy^j \qquad 0\leq i\leq k-1 \qquad 0\leq j\leq k$$
$$\int_K p_{h2}(x,y)x^iy^j \qquad 0\leq i\leq k \qquad 0\leq j\leq k-1$$

With the above specifications the approached problem ($\mathcal{P}_h$) has a unique solution $(\vec{p}_h, u_h)$; and assuming some regularity conditions on D, Σ and f, we have the following theorem of convergence :

$$\|u-u_h\|_{o,\Omega}\leq C\,\|u\|_2\,h \qquad \text{if } k = 0$$
$$\qquad\qquad C\,\|u\|_{k+1}h^{k+1} \qquad \text{if } k\geq 1$$
$$\|p-p_h\|_{o,\Omega}\leq C\,\|u\|_{k+2}h^{k+1}$$
$$\|\text{div}(p-p_h)\|_{o,\Omega}\leq C\,\|u\|_{k+3}\,h^{k+1}$$

with C being a positive constant independant of T_h and u.

second example : modified R.T. method

$$Q_K = P_{\ell+1,o} \times P_{o,\ell+1} \qquad P_K = P_{\ell,o} + P_{o,\ell}$$

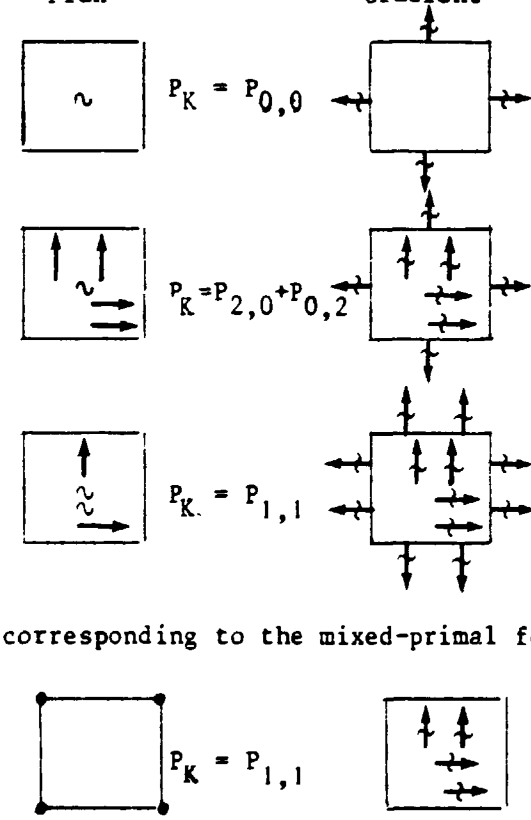
Then the approximations are of order 1.

The mixed elements method provides simultaneously an approximation of u and $\vec{\nabla} u$; this is in distinction to the classical finite elements method in which the approximation of $\vec{\nabla} u$ is given by discretizing the one of u , thus loosing one crder of approximation.

In the mixed methods, the two approximations are of the same order (generally if $P_{\ell,\ell} \subset P_K$, the approximations of u and $\vec{p}$ are of order $\ell + 1$; they may be of order ℓ).

B. Description of some mixed elements

The different finite elements bases can be represented in terms of the unknowns as follow :



	Flux		Gradient	
First order				
MXOL5		$P_K = P_{0,0}$		$Q_K = P_{1,0} \times P_{0,1}$
MXPC13		$P_K = P_{2,0} + P_{0,2}$		$Q_K = P_{3,0} \times P_{0,3}$
Second order				
MXLP16		$P_K = P_{1,1}$		$Q_K = P_{2,1} \times P_{1,2}$

Mixed element corresponding to the mixed-primal formulation :

MDL08		$P_K = P_{1,1}$		$Q_K = P_{0,1} \times P_{1,0}$

We denote by : • a point value
∿ a mean value
→ an x - moment
↑ an y - moment | for the flux approximation.

III. THEORICAL BASIS OF THE MIXED-HYBRID METHOD

The mixed-hybrid method is derived from the mixed method.

A triangulation T_h is given.

By relaxing the continuity condition on $H_{o,\Gamma_1}(\mathrm{div}, \Omega)$ we obtain the mixed-hybrid variational formulation[6] :

$$
(\mathcal{PH}) \left| \begin{array}{ll}
\text{Find } (\vec{p}, u, \lambda) \in H_{0,\Gamma_1}(\mathrm{div},T) \times L^2(\Omega) \times L^2(\partial T) \text{ so that} & \\
\int_\Omega \frac{1}{D} \vec{p}\cdot\vec{q} + \sum_{K\in T_h} \int_K u \,\mathrm{div}\, \vec{q} - \int_K \lambda \vec{q}\cdot\vec{n} = 0 & \forall \vec{q} \in H(\mathrm{div}, T) \\
\sum_{K\in T_h} \int_K - \mathrm{div}\, \vec{p}\, v + \int_\Omega \Sigma\, u\, v = \int_\Omega f\, v & \forall v \in L^2(\Omega) \\
\sum_{K\in T_h} \int_{\partial K} \mu\, \vec{p}\cdot\vec{n} = 0 & \forall \mu \in L^2_{o,\Gamma_o}(\partial T)
\end{array} \right.
$$

with the following notations : $\Omega = \bigcup_{K\in T_h} K \qquad T = \bigcup_{K\in T_h} \mathring{K} \qquad \partial T = \bigcup_{K\in T_h} \partial K$

$$H(\mathrm{div}, T) = \{\vec{q} \in L^2(\Omega) / \ \forall K \in T_h \quad \vec{q}_{/K} \in H(\mathrm{div},K)\}$$

$$L^2_{0,\Gamma_0}(\partial T) = \{\mu \in L^2(\partial T) / \mu_{/\Gamma_o} = 0\}$$

Problem $(\mathcal{PH})$ has a unique solution : u is the solution of (Q), $\vec{p} = D\vec{\nabla}u$ and $\lambda = u_{/\partial T}$ (($\vec{p}$, u) is the solution of ($\mathcal{P}$))

The spaces H(div, T), $L^2(\Omega)$ and $L^2_{o,\Gamma_o}(\partial T)$ are approximated by finite dimensional subspaces $\overline{Q}_h$, $\overline{V}_h$ and $\overline{L}_h$, the elements of which have polynomial restrictions on each K.

The triangulation of Ω is supposed to be composed of rectangles. The approximation spaces of Raviart and Thomas are the following.

$$\overline{Q}_h = \{\vec{q}_h \in H(\mathrm{div},T) / \forall K \in T_h \quad \vec{q}_{h/K} \in P_{k+1,k} \times P_{k,k+1}\}$$

$$\overline{V}_h = \{v_h \in L^2(\Omega) / \forall K \in T_h \quad v_{h/K} \in P_{k,k}\}$$

$$\overline{L}_h = \{\lambda_h \in L^2_{o,\Gamma_o}(\Omega) / \forall K \in T_h \quad \lambda_{h/\partial K} \in P_k(\partial K)\}$$

The corresponding approached problem $(\mathcal{PH}_h)$ has then a unique solution $(\overline{\vec{p}}_h, \overline{u}_h, \overline{\lambda}_h)$. Moreover we have $\overline{\vec{p}}_h = \vec{p}_h$ and $\overline{u}_h = u_h$, $(\vec{p}_h, u_h)$ being the solution of problem $(\mathcal{P}_h)$ with the choice of the R.T. spaces. The approximation of $\pi_h u$ by $\overline{\lambda}_h$ is of order k + 2 ($\pi_h u$ = orthogonal projection of $u_{/\partial T}$ following the norm : $||\mu||^2 = \int_{\partial T} |\mu|^2$) .

IV. MATRICES - ELIMINATION OF UNKNOWNS

A. Mixed Method

1. We consider $\vec{B}$ a basis of Q_h and B' a basis of V_h. The matrix of the linear system corresponding to $(\mathcal{P}_h)$ relatively to the basis ($\vec{B}$, B') of $Q_h \times V_h$ is of the form:

$$M = \begin{pmatrix} M_1 & M_2 \\ M_2^T & M_3 \end{pmatrix}$$ where M_1 is the matrix of the bilinear form : $(\vec{p}_h, \vec{q}_h) \to \int_\Omega \frac{1}{D} \vec{p}_h \cdot \vec{q}_h$

M_2 is the matrix of : $(\vec{q}_h, u_h) \to \int_\Omega \operatorname{div} \vec{q}_h \, u_h$

M_3 is the matrix of : $(u_h, v_h) \to -\int_\Omega \Sigma u_h \, v_h$

M_1 is symetric positive definite, M_3 is symetric negative.

If moreover we put together the nodes corresponding to the x - axis component of $\vec{p}_h$ on one side, the ones corresponding to the y - axis component of $\vec{p}_h$ on the other side, M_1 is block-diagonal :

$$M_1 = \begin{pmatrix} A & 0 \\ 0 & A' \end{pmatrix}$$

The matrix A is itself block-diagonal if the nodes are numbered element by element and this line by line of rectangl[illegible] of T_h, the blocks of A corresponding to the lines of rectangles. The same is true for A'.

Contrary to the classical finite elements method, the matrix is not positive definite. So for solving the system, one cannot use the usual iterative methods (block Jacobi, block S.O.R....) without taking precautions. Then we think of trying to eliminate some of the unknowns in order to obtain a positive definite system.

2. Elimination of the flux

We have to solve a linear system $M\vec{X} = \vec{W}$ (S) with

$M = \begin{pmatrix} M_1 & M_2 \\ M_2^T & M_3 \end{pmatrix}$ M_1 being symetric positivie definite and M_3 symetric negative.

We'll note $\vec{X} = \binom{X}{Y}$, X corresponds to $\vec{p}_h$ and Y to u_h .

We note $\vec{W} = \binom{U}{V}$ and notice that $U = 0$.

Assume that M_3 is invertible and consequently negative definite (that is the cas if for example there exists a constant $\Sigma_o > 0$ so that $\Sigma(x) \geq 0$ a.e. in Ω) ; that is not necessarily realized in practice.

$\vec{X} = \binom{X}{Y}$ is the solution of (S) $\Leftrightarrow \begin{cases} Y = M_3^{-1} (V - M_2^T X) \\ (M_1 - M_2 M_3^{-1} M_2^T)X = - M_2 M_3^{-1} V \end{cases}$

M_3^{-1} is symetric negative definite because such is M_3 , therefore

$M_2 M_3^{-1} M_2^T$ is symetric negative ; moreover M_1 is symetric positive definite so $M_1 - M_2 M_3^{-1} M_2^T$ is symetric positive definite.

3. Elimination of the gradient

$\vec{X} = \binom{X}{Y}$ is the solution of (S) $\Leftrightarrow \begin{cases} X = - M_1^{-1} M_2 Y \\ (- M_3 + M_2^T M_1^{-1} M_2) Y = V \end{cases}$

We note $\bar{\mathcal{R}} = M_2^T M_1^{-1} M_2 - M_3$

As M_1^{-1} is symetric positive definite, $M_2^T M_1^{-1} M_2$ is symetric positive ; M_3 is symetric negative then is symetric positive.

We'll assume that, for example, for each K of the triangulation we have $\Sigma/_K = 0$ or $\Sigma/_K \geq \nu_K > 0$ (ν_K being a constant depending on K). It necessary by changing the order of the basis functions so that to number at first the ones corresponding to rectangles K in which $\Sigma(X) \geq \nu_K > 0$, we can write :

$$- M_3 = \begin{pmatrix} \mathcal{M}_1 & 0 \\ 0 & 0 \end{pmatrix}$$

with $\mathcal{M}_1$ being symetric positive definite, and possibly $M_3 = 0$.

We note by passing that the writing of $- M_3$ in the form $\begin{pmatrix} \mathcal{M}_1 & 0 \\ 0 & 0 \end{pmatrix}$ is valid as soon as for each K the bilinear form :

$(u_K, v_K) \in L^2(K)^2 \to \int_K u_K v_K$ is either null or positive definite.

We'll now show that $\bar{\mathcal{R}}$ is positive define.

We note $Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$.

Then :

$$Y^T \bar{\mathcal{R}} Y = 0 \Leftrightarrow \begin{cases} (M_2 Y)^T M_1^{-1} (M_2 Y) = 0 \\ - Y^T M_3 Y = 0 \end{cases} \Leftrightarrow \begin{cases} M_2 Y = 0 \\ Y_1^T \bar{\mathcal{R}} Y_1 = 0 \end{cases} \Leftrightarrow \begin{cases} M_2 Y = 0 \\ Y_1 = 0 \end{cases}$$

$$Y^T \bar{\mathcal{R}} Y = 0 \quad \begin{cases} M_2 Y = 0 \\ {}_1 Y_1 = 0 \end{cases} \Leftrightarrow \begin{cases} M_2 Y = 0 \\ M_3 Y = 0 \end{cases} \Leftrightarrow M\binom{0}{Y} = \binom{0}{0} \Leftrightarrow Y = 0.$$

So, particularly, if $\forall K \in T_h$ $\Sigma/_K$ is constant then the system obtained after elimination of the gradient is positive definite.

B. Mixed-hybrid method

A basis of $\bar{Q}_h \times \bar{V}_h \times \bar{L}_h$ is chosen in a natural way from bases of $\bar{Q}_h$, $\bar{V}_h$ and $\bar{L}_h$. The matrix of the corresponding system obtained from problem $(\mathcal{PH}_h)$ has the following form :

$$M = \begin{pmatrix} A & B & C \\ B^T & E & 0 \\ C^T & 0 & 0 \end{pmatrix}$$ with A being symetric positive definite
E being symetric negative.

Matrix A is invertible, so it is possible to eliminate the gradient. The matrix obtained after this elimination is the symetric matrix :

$$M_G = \begin{pmatrix} B^T A^{-1} B - E & B^T A^{-1} C \\ C^T A^{-1} B & C^T A^{-1} \end{pmatrix}$$

We are going to show that M_G is symetric positive definite.

For a given $\binom{Y}{Z}$, we note that $Y' = BY$ and $Z' = CZ$,

Then :

$$\binom{Y}{Z}^T M_G \binom{Y}{Z} = Y'^T A^{-1} Y' - Y^T EY + Y'^T A^{-1} Z' + Z'^T A^{-1} Y' + Z'^T A^{-1} Z'$$

$$\binom{Y}{Z}^T M_G \binom{Y}{Z} = (Y' + Z')^T A^{-1} (Y' + Z') - Y^T EY \geq 0$$

and :

$$\binom{Y}{Z}^T M \binom{Y}{Z} = 0 \Leftrightarrow \begin{cases} Y' + Z' = 0 \\ Y = 0 \end{cases} \Leftrightarrow \begin{cases} Y = 0 \\ CZ = 0 \end{cases} \Leftrightarrow Y = 0 \text{ and } M \begin{pmatrix} 0 \\ 0 \\ Z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\binom{Y}{Z}^T M \binom{Y}{Z} = 0 \Leftrightarrow Y = 0 \text{ and } Z = 0$$

So M_G is symetric positive definite.

M_G being symetric positive it is possible to eliminate either the flux or the Lagrange multipliers and the system obtained after such an elimination is still positive definite.

V. EQUIVALENCES

One can think of comparing the mixed method with other numerical methods for solving the diffusion equation, especially with the nodal methods.

If the coefficients D and Σ are constant on each node of the triangulation, then at the first order the mixed-hybrid method with Lobatto numerical integration is equivalent to the block-centered finite differences method.

The modified R.T. method with post-processing has been shown to be equivalent to the classical non conforming finite element method with transverse integration,[5] which is itself equivalent to the physical nodal method[3,4]. If for the physical nodal method we choose as unknown on the interfaces the current and not the flux, we obtain exactly the mixed method, with u_h locally in $P_{\ell,0} + P_{0,\ell}$ and $\vec{p}_h$ $P_{\ell+1,0} \times P_{0,\ell+1}$.

VI. NUMERICAL TEST

A. Description of some finite elements

Lagrangian elements :

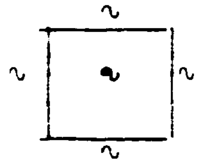
CL16# and CL16R are the cubic Lagrangian elements, the first with Gauss integration, the second with quasi-diagonalization of the mass-matrix.

PL9# and PL9R are the parabolic Lagrangian elements, the first with Gauss integration the second with quasi-diagonalization of the mass matrix.

LL4 is the linear Lagrangian element.

Nodal element :

NDP5R



Gauss-Radan integration of order 4
$P_K = P_{2,0} + P_{0,2}$

The element NDP5R is equivalent to the mixed-element MXOL5.

B. A numerical test has been carried out on 2D IAEA Benchmark.

The reference calculation is based on the element CL16# with a 2 x 2 mesh, the eigenvalue being : 1,033937.

A second test has been carried out on a reactor with plutonium recycling. The reference calculation is based on the element CL16R with a 4 x 4 mesh, the eigenvalue being 0,978110.

The results are respectively put in table I and table II. In these tables the fith and sixth columns give the maximum and the mean square errors in the power assembly.

TABLE I

Finite Element	Mesh	Eignvalue	Error on the eigenvalue (p.c.m.)	ΔP_{max} (%)	$\overline{P}_i$ (%)	Computing time on CRAY - XMP (s)	Memory place (words)
CL16#	2x2	1,033937				4,27	304 532
PL9#	1x1	1,034121	17,78	3,72	1,78	0,59	21 497
	2x2	1,033955	1,71	2,93	1,40	1,68	97 925
PL9R	1x1	1,035105	112,98	14,52	8,61	0,58	21 497
	2x2	1,034037	9,66	5,00	2,62	1,68	97 925
NDP5R	1x1	1,033297	61,87	13,32	7,96	0,39	9 196
	2x2	1,033367	55,12	10,07	5,61	0,88	39 802
MXOL5	1x1	1,033190	72,29	13,59	8,08	0,43	9 407
	2x2	1,033331	58,58	10,14	5,69	0,94	40 629
MXPL13	1x1	1,034135	19,12	2,65	1,02	1,61	45 755
	2x2	1,033995	5,56	2,26	1,01	3,54	190 353
MXLP16	1x1	1,033228	68,62	8,78	4,58	1,48	66 709
	2x2	1,033779	15,28	1,21	0,56	4,33	303 909
MDL08	1x1	1,036719	269,06	71,17	29,98	0,54	20 238
	2x2	1,033600	32,62	3,19	1,51	1,65	84 604

TABLE II

Finite Element	Mesh	Eigenvalue	Error on the eigenvalue (p.c.m.)	ΔP_{max} (%)	$\overline{P}_i$ (%)	Computing time on CRAY - XMP (s)	Memory place (words)
CL16R	4x4	0,978110				33,73	1 371 225
PL9#	1x1	0,976311	183,89	5,61	2,85	0,89	20 870
	2x2	0,977819	29,75	1,19	0,50	2,93	123 310
LL4	1x1	0,989605	807,21	49,71	18,66	0,44	5 223
	2x2	0,980254	219,22	16,67	5,96	0,86	17 693
MX L5	1x1	0,979360	127,76	25,45	11,65	0,69	9 490
	2x2	0,977266	86,34	12,33	4,35	1,65	37 679
MXPC13	1x1	0,978448	34,55	6,93	3,01	2,53	73 001
	2x2	0,978129	1,91	2,49	0,29	8,69	454 518
MXLP16	1x1	0,976775	136,52	7,91	2,90	2,55	101 833
	2x2	0,977416	70,93	2,69	1,21	11,35	646 475
MDL08	1x1	0,982301	428,46	25,95	11,07	0,95	19 759
	2x2	0,970368	178,13	5,29	2,85	3,46	153 132

The best mixed element seems to be MXPC13 ; though of lower order it gives as good results as MXLP16 and takes less memory place and less time.

VII. CONCLUSION

The mixed elements method gives approximations of the flux and its gradient simultaneously ; moreover these approximations are of the same order. The matrices of the linear systems are not positive definite which leads to difficulties in the numerical solution ; but by eliminating some of the unknowns, it is possible to obtain positive definite systems.

The convergence of physical nodal methods of order 1 have been shown by the equivalence with finite elements methods. Maybe from mixed methods we can find equivalent physical nodal methods of order higher than 1 and so prove the convergence of the latter.

We hope to achieve fast results by preconditioning a mixed element method by a block-centered finite difference scheme.

The mixed method, with an appropriate enumeration of the nodes, of the dissection type, gives well uncoupled equations that may be solved by an iterative method (Block Jacobi, Block Gauss-Seidel...) ; the convergence is fast in cases of symetry. This property of uncoupling should be appropriate for use on parallel computers.

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