Solveurs performants pour les fonctionnelles énergétiques

Résumé des travaux de recherche effectués au
Scientific Computing Laboratory, University of Minnesota
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Overview

1. **The constrained optimization problem**
   - Construction of the hybrid model
   - energy-based minimization
2. **Solving the saddle-point linear system**
   - Nullspace projection
   - Iterative methods & block preconditioning
   - Numerical results
3. **Conclusions and perspectives**

1. **The constrained optimization problem**
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Construction of the hybrid model

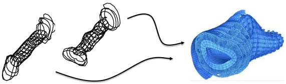
Ingredients

- Hybrid model = numerical model + experimental model
- Finite element numerical model of the structure with the mass matrix $M = M(\theta) \in R^n$ and the stiffness matrix $K = K(\theta) \in R^n$
- Each numerical couple of eigenvalue and eigenvector $(\omega_\theta, \varphi_\theta)$ satisfies :

$$(K(\theta) - \omega_\theta^2 M(\theta))\varphi_\theta = 0, \varphi_\theta \neq 0$$

- Experimental modal basis is available $(\omega_{exp}, \phi_{exp})$

➜ Expansion of the experimental modes on the numerical model in order to compute the response



Constrained optimization problem

- φ is the best estimation of φ_θ, minimizing the distance with the ϕ_{exp} at the pulsation ω_{exp}.
- ψ is an error in stiffness in the model. It satisfies :

$$K(\theta)\psi = (K(\theta) - \omega_{exp}^2 M(\theta))\varphi,$$

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$$C\varphi = 0, \qquad C\psi = 0$$

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- Quadratic problem ➜ Model error + numerical/experimental distance

$$e_\omega(\varphi,\psi,\theta) = \frac{1}{2}\psi^T K(\theta)\psi + \frac{r}{2(1-r)}(\Pi\varphi - \phi_{exp})^T K_r(\Pi\varphi - \phi_{exp})$$

Constrained optimization problem

- Minimizing the cost function :

$$\begin{cases} f_\omega(\varphi,\psi,\lambda,\lambda_1,\lambda_2,\theta) = e_\omega(\varphi,\psi,\theta) + c_\omega(\varphi,\psi,\lambda,\lambda_1,\lambda_2,\theta) \\ c_\omega(\varphi,\psi,\lambda,\lambda_1,\lambda_2,\theta) = \lambda^T((K(\theta)-\omega_{exp}^2 M(\theta))\varphi - K(\theta)\psi) - \lambda_1^T C\psi + \lambda_2^T(C\psi \end{cases}$$

- Stationarity conditions :

$$\begin{cases} \frac{\partial f_\omega}{\partial \varphi} = 0 \iff \frac{r}{1-r}\Pi^T K_r(\Pi\varphi - \phi_{exp}) + (K(\theta)-\omega_{exp}^2 M(\theta))\lambda - C^T\lambda_2 = 0 \\ \frac{\partial f_\omega}{\partial \psi} = 0 \iff K(\theta)\psi - K(\theta)\lambda + C^T\lambda_2 - C^T\lambda_1 = 0 \\ \frac{\partial f_\omega}{\partial \lambda} = 0 \iff -K(\theta)\psi + (K(\theta)-\omega_{exp}^2 M(\theta))\varphi = 0 \\ \frac{\partial f_\omega}{\partial \lambda_1} = 0 \iff C\psi = 0 \\ \frac{\partial f_\omega}{\partial \lambda_2} = 0 \iff C\psi - C\varphi = 0 \end{cases}$$

Searching a solution in the whole space

- Minimizing the cost function yields the following saddle-point linear system :

$$\begin{bmatrix} -K(\theta) & -C^T & K(\theta)-\omega_{exp}^2 M(\theta) & C^T \\ -C & 0 & C & 0 \\ K(\theta)-\omega_{exp}^2 M(\theta) & C^T & \frac{r}{1-r}\Pi^T K_r \Pi & 0 \\ C & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \psi \\ \lambda_1 \\ \varphi \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{r}{1-r}\Pi^T K_r \phi_{exp} \\ 0 \end{bmatrix}$$

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- If we consider the constrained stiffness and mass matrices :

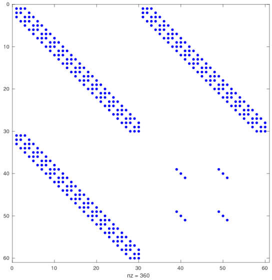
$$\widetilde{K} = \begin{bmatrix} K(\theta) & C^T \\ C & 0 \end{bmatrix}, \quad \widetilde{M} = \begin{bmatrix} M(\theta) & 0 \\ 0 & 0 \end{bmatrix}$$

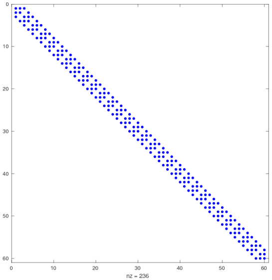
Then :

$$\begin{bmatrix} -\widetilde{K}(\theta) & \widetilde{K}(\theta)-\omega_{exp}^2 \widetilde{M}(\theta) \\ \widetilde{K}(\theta)-\omega_{exp}^2 \widetilde{M}(\theta) & \frac{r}{1-r}\widetilde{\Pi}^T \widetilde{K}_r \widetilde{\Pi} \end{bmatrix} \begin{bmatrix} \widetilde{\psi} \\ \widetilde{\varphi} \end{bmatrix} = \begin{bmatrix} \widetilde{0} \\ \frac{r}{1-r}\widetilde{\Pi}^T \widetilde{K}_r \widetilde{\phi}_{exp} \end{bmatrix}$$

Searching a solution in the whole space

- Nonsingular matrix
- But : Large band, bad fill-in ratio, highly indefinite ...



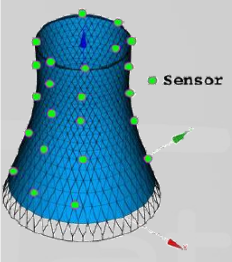


The pattern of the studied saddle point matrix (left) and a finite element matrix in (right)

Searching a solution in the whole space

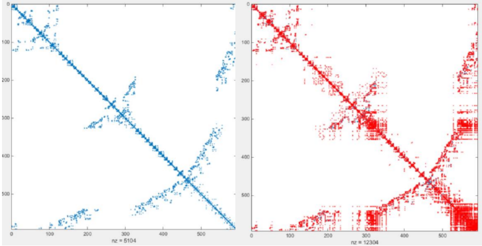
Mechanical solvers

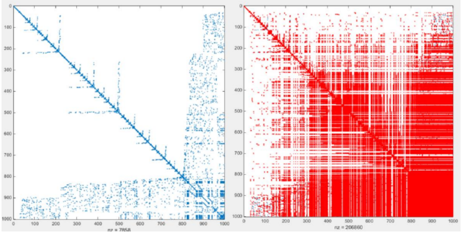
- for an industrial structure model with more than 10^6 dofs and few hundreds of measurement points (i.e. $N \approx 10^6$ and $n \approx 100$), *MD Nastran*® provides a huge computation cost for a single calculation.



Searching a solution in the whole space

Direct mechanical solvers





Searching the solution in the kinematic conditions nullspace

The linear system could be described in equivalent form as follows :

$$\mathcal{A} = \begin{bmatrix} -A & -C^T & B^T & C^T \\ -C & 0 & C & 0 \\ B & C^T & T & 0 \\ C & 0 & 0 & 0 \end{bmatrix} \equiv \left[\begin{array}{cc|cc} -A & B^T & -C^T & C^T \\ B & T & C^T & 0 \\ \hline -C & C & 0 & 0 \\ C & 0 & 0 & 0 \end{array}\right] = \begin{bmatrix} \widetilde{A} & \widetilde{C}^T \\ \widetilde{C} & 0 \end{bmatrix}$$

where $A = K(\theta) \in \mathbb{R}^{n\times n}$, $B = K(\theta) - \omega_{exp}^2 M(\theta) \in \mathbb{R}^{n\times n}$ and $T = \frac{r}{1-r}\Pi^T K_r \Pi$.

The fundamental nullspace basis of $\widetilde{C}$, is described using :

- $\widetilde{Z} \in \mathbb{R}^{2n\times 2(n-m)}$ such that $range(\widetilde{Z}) = Ker(\widetilde{C})$
- $\widetilde{Y} \in \mathbb{R}^{2n\times 2m}$ such that $Im(\widetilde{Y}) = Im(\widetilde{C}^T)$. We can take $\widetilde{Y} = \widetilde{C}^T$ which is the description of $Im(\widetilde{C}^T)$ in canonical basis.

$$NB = \begin{bmatrix} \widetilde{C}^T & \widetilde{Z} & 0 \\ 0 & 0 & \mathbb{I}_{2m} \end{bmatrix}$$

Searching the solution in the kinematic conditions nullspace

- The equivalent linear system is as follows :

$$\mathcal{A} \equiv \begin{bmatrix} \widetilde{C} & 0 \\ \widetilde{Z}^T & 0 \\ 0 & \mathbb{I}_{2m} \end{bmatrix} \begin{bmatrix} \widetilde{A} & \widetilde{C}^T \\ \widetilde{C} & 0 \end{bmatrix} \begin{bmatrix} \widetilde{C}^T & \widetilde{Z} & 0 \\ 0 & 0 & \mathbb{I}_{2m} \end{bmatrix} = \begin{bmatrix} \widetilde{C}\widetilde{A}\widetilde{C}^T & \widetilde{C}\widetilde{A}\widetilde{Z} & \widetilde{C}\widetilde{C}^T \\ \widetilde{Z}^T\widetilde{A}\widetilde{C}^T & \widetilde{Z}^T\widetilde{A}\widetilde{Z} & 0 \\ \widetilde{C}\widetilde{C}^T & 0 & 0 \end{bmatrix}$$

Searching the solution in the kinematic conditions nullspace

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$$\mathcal{A} \equiv \begin{bmatrix} \widetilde{C} & 0 \\ \widetilde{Z}^T & 0 \\ 0 & \mathbb{I}_{2m} \end{bmatrix} \begin{bmatrix} \widetilde{A} & \widetilde{C}^T \\ \widetilde{C} & 0 \end{bmatrix} \begin{bmatrix} \widetilde{C}^T & \widetilde{Z} & 0 \\ 0 & 0 & \mathbb{I}_{2m} \end{bmatrix} = \begin{bmatrix} \widetilde{C}\widetilde{A}\widetilde{C}^T & \widetilde{C}\widetilde{A}\widetilde{Z} & \widetilde{C}\widetilde{C}^T \\ \widetilde{Z}^T\widetilde{A}\widetilde{C}^T & \widetilde{Z}^T\widetilde{A}\widetilde{Z} & 0 \\ \widetilde{C}\widetilde{C}^T & 0 & 0 \end{bmatrix}$$

- Let $Z \in R^{n\times(n-m)}$ be a matrix such that $range(Z) = Ker(C)$. It is trivial to see that $\widetilde{Z} = \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix}$ where $Im(Z) = Ker(C)$. We obtain that :

$$\widetilde{Z}^T\widetilde{A}\widetilde{Z} = \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix}^T \begin{bmatrix} -A & B \\ B & T \end{bmatrix} \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix} = \begin{bmatrix} -Z^TAZ & Z^TBZ \\ Z^TBZ & Z^TTZ \end{bmatrix}$$

Searching the solution in the kinematic conditions nullspace

Computing a sparse nullspace basis of C

- Using skinny LU technique : Perform LU on the "skinny" matrix C^T

$$PC^TQ = \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} U_1$$

where P and Q are permutations, and define the nulspace to be :

$$Z = P^T \begin{bmatrix} -L_1^{-T} L_2^T \\ \mathbb{I} \end{bmatrix}$$

- Implementation of a fast sparse nullspace basis generation algorithm on SuperLU

Searching the solution in the kinematic conditions nullspace

- The reduced linear system to solve is :

$$\begin{bmatrix} -Z^T AZ & Z^T BZ \\ Z^T BZ & Z^T TZ \end{bmatrix} \begin{bmatrix} x_{Z1} \\ x_{Z2} \end{bmatrix} = \begin{bmatrix} -A_Z & B_Z \\ B_Z & T_Z \end{bmatrix} \begin{bmatrix} x_{Z1} \\ x_{Z2} \end{bmatrix} = \begin{bmatrix} 0 \\ f_Z \end{bmatrix}$$

- The coefficient matrix is also a saddle point one, where $\mathbb{A}_{\mathbb{Z}}$ is SPD, $\mathbb{B}_{\mathbb{Z}}$ is a symmetric indefinite matrix that shares the same pattern as $\mathbb{A}_{\mathbb{Z}}$, and $\mathbb{T}_{\mathbb{Z}}$ is symmetric positive semidefinite, composed of a dense $c \times c$ sub-block scattered into a $n \times n$ matrix, where $c << n$ is the number of sensors.

Iterative solution of the reduced system

The constraint preconditioner

- We use the following decomposition of the constraint preconditioner :

$$P = \begin{bmatrix} -G_Z & B_Z \\ B_Z & T_Z \end{bmatrix} = \begin{bmatrix} \mathbb{I}_{n-m} & 0 \\ -B_Z G_Z^{-1} & S_Z \end{bmatrix} \begin{bmatrix} -G_Z & B_Z \\ 0 & \mathbb{I}_{n-m} \end{bmatrix}$$

$$P^{-1} = \begin{bmatrix} -G_Z^{-1} & G_Z^{-1} B_Z \\ 0 & \mathbb{I}_{n-m} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{n-m} & 0 \\ S_Z^{-1} B_Z G_Z^{-1} & S_Z^{-1} \end{bmatrix}$$

where $S_Z = T_Z + B_Z G_Z^{-1} B_Z$ is the shur complement of $-G_Z$.

Iterative solution of the reduced system

The constraint preconditioner P_1

- A_Z is positive definite, we take $G_Z = L_A L_A^T$ a Cholesky decomposition as an approximation. We use $D = Diag(A_Z)$ instead of G_Z in the shur complement which admits a Cholesky factorisation $\widetilde{S}_Z = L_S L_S^T$.
- Applying these approximations, we get the preconditioner P_1 :

$$P_1^{-1} \equiv \begin{bmatrix} -L_A^{-T} L_A^{-1} & L_A^{-T} L_A^{-1} B_Z \\ 0 & \mathbb{I}_{n-m} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{n-m} & 0 \\ L_S^{-T} L_S^{-1} B_Z D^{-1} & L_S^{-T} L_S^{-1} \end{bmatrix}$$

Iterative solution of the reduced system

The constraint preconditioner P_2

- An other way to approximate the Shur complement in our case, is to observe that :

$$S_Z = T_Z + B_Z A_Z^{-1} B_Z = \underbrace{T_Z + K_Z}_{\substack{\text{Approx.} \\ \widetilde{S_Z}}} - 2\omega_{exp}^2 M_Z + \omega_{exp}^4 M_Z K_Z^{-1} M_Z$$

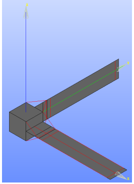
- Applying these approximations, we get the preconditioner P_2 :

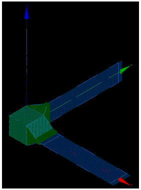
$$P_2^{-1} \equiv \begin{bmatrix} -L_A^{-T} L_A^{-1} & L_A^{-T} L_A^{-1} B_Z \\ 0 & \mathbb{I}_{n-m} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{n-m} & 0 \\ L_S^{-T} L_S^{-1} B_Z D^{-1} & L_S^{-T} L_S^{-1} \end{bmatrix}$$

Iterative solution of the reduced system

Numerical results

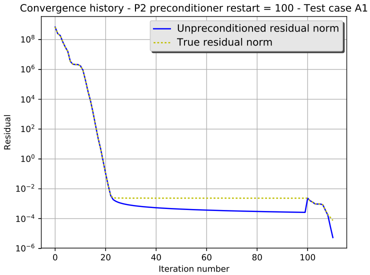
- We use Petsc (block user implementation) to solve the above linear system. We apply Flexible GMRES method with this setting : restart = depends on each preconditioner, maximum iterations = 10.000, seeked precision = 1e-05.
- Academic application : A three-beam structure.

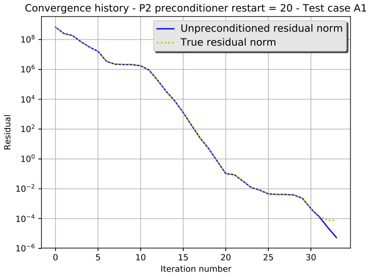




Iterative solution of the reduced system

- **FGMRES parameters : restart parameter**





Iterative solution of the reduced system

- **Benchmark of direct Cholesky preconditioner**

Matrix A_Z	Cholesky direct solve using different packages and ordering methods								
Size = 9,201		PCSetUP				PCApply	KSPSolve		
Nnz = 602,603	Ordering	MatGetOrdering	MatCholFctrSym	MatCholFctrNum	Total	PCApply	PCSetUP + PCApply	Fill-in	Fill Ratio
PETSc	None	0.00	49.01	27.70	76.70	0.03	76.73	16,980,101	28.17
	ND	0.00	1.00	0.48	1.49	0.00	1.49	1,943,372	3.22
	1WD	0.00	7.04	3.25	10.31	0.01	10.32	5,646,066	9.36
	RCM	0.00	5.42	3.20	8.63	0.01	8.64	5,718,474	9.48
	QMD	0.06	1.01	0.45	1.53	0.00	1.54	1,951,034	3.23
	AMD	0.00	0.91	0.42	1.34	0.00	1.35	1,856,094	3.08
MUMPS	AMD	0.00	0.06	0.34	0.41	0.00	0.42	1,920,557	3.18
	AMF	0.00	0.09	0.56	0.65	0.01	0.66	2,215,053	3.67
	METIS	0.00	0.14	0.40	0.55	0.01	0.56	1,871,817	3.10
	PORD	0.00	0.14	0.47	0.61	0.01	0.62	1,944,021	3.22
	QAMD	0.00	0.09	0.51	0.60	0.01	0.61	2,040,667	3.38
	SCOTCH	0.00	0.20	0.41	0.61	0.01	0.62	1,918,287	3.18

Iterative solution of the reduced system

• Nullspace projection test

Matrix A	Physical dofs (n)	Lagrange dofs (m)	System size	System nnz	The constraint matrix C	The nullspace basis Z	CPU Time (sec)	Reduced system size	Reduced system nnz
	Test cases & their nullspace projection								
A_1	10,074	873	21,894	1,798,539	$873 \times 10{,}074$ $nnz = 3{,}387$	$10{,}074 \times 9{,}201$ $nnz = 12{,}890$	1.3e-2	18,402	1,943,373
A_2	13,497	1,089	29,172	2,503,134	$1{,}089 \times 13{,}497$ $nnz = 4{,}146$	$13{,}497 \times 12{,}408$ $nnz = 16{,}977$	2.9e-2	24,816	2,751,990
A_3	1,593	22,791	48,768	4,490,766	$22{,}791 \times 22{,}791$ $nnz = 6{,}062$	$1{,}593 \times 21{,}198$ $nnz = 27{,}847$	6.4e-2	42,396	5,071,433
A_4	64,506	3,273	135,558	13,778,775	$64{,}506 \times 3{,}273$ $nnz = 12{,}555$	$64{,}506 \times 61233$ $nnz = 74{,}794$	18.8e-2	122,466	16,358,756

Iterative solution of the reduced system

- **Parallel test for P_2**

Test case	A_4	Functions & CPU time (sec)						Statistics		
		PCSetUP	PCApply							
The preconditioner			KSPSolve_Low	KSPSolve_0	KSPSolve_Shur	Total	CPU Time (sec)	Iterations	Flops	True residual
P_2	Time (sec)	311.48	255.19	23.25	89.47	368.40				
1 proc	percent (%)	84	69	6	24	99	3.716e+02	37	4.490e+09	9.536e-05
	Count	3	37	37	37	37				
P_2	Time (sec)	41.04	40.65	10.36	13.47	64.79				
4 procs	percent (%)	61	60	15	20	96	6.733e+01	52	2.772e+09	9.531e-05
	Count	3	52	52	52	52				

Conclusions and perspectives

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- The energy-based expansion method generates a nested saddle point system
- Implementation of the nullspace projection + solution method using SuperLU and Petsc on a standalone code in C.
- Significant results using constraint preconditioners on the projected system

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Some perspectives

- Application to industrial structures
- Need to interface different implementations to be used within the mechanical code CodeAster ®