On direct elimination of constraints in KKT systems

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Outline of talk

- coupled linear system
  - singular stiffness linear system
  - full rank constraint linear system
- two approaches for solution
  - direct elimination
  - null space projection
- types of constraints and spy plots
  - Dirichlet conditions
  - adaptive conditions
  - rigid body conditions
  - large door model

Outline of talk (continued)

- various topics
  - when not to use direct elimination
  - inertial relief
  - nice basis problem
  - re-use of permutations
  - Lagrange multipliers and residual forces
  - rank-revealing QR factorizations
- summary

Start with a singular linear system

$$K \ u = f \tag{1}$$

- **stiffness matrix** K **is** $n \times n$ **sparse and singular,**
- **displacement vector** u **is** $n \times 1$
  3 translations, 3 rotations
- **force vector** f **is** $n \times 1$
- **solution** u **is not unique.**
- $Ku = f$ **comes from a nonlinear iteration and we expect there to be one equilibrium point**
- **we expect additional information to find a unique solution.**

Add a linear system of constraints

$$C\ u = g \tag{2}$$

- **constraint matrix** C **is** $r \times n$ **sparse,** $r \leq n$
- **displacement vector** u **is** $n \times 1$
  3 translations, 3 rotations
- **right hand size vector** g **is** $r \times 1$
- **equation (2) is satisfied exactly.**
- **impose condition :**
  u **lies in the** $n \times r$ **column space of** C^T
- **now we bifurcate our analysis**
  - **direct elimination**
  - **null space projection**

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Direct elimination (step 1)

- **Form the KKT system**

$$\begin{bmatrix} K_{\mathcal{M},\mathcal{M}} & C^T_{\mathcal{R},\mathcal{M}} \\ C_{\mathcal{R},\mathcal{M}} & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{M}} \\ v_{\mathcal{R}} \end{bmatrix} = \begin{bmatrix} f_{\mathcal{M}} \\ g_{\mathcal{R}} \end{bmatrix} \tag{3}$$

- $K_{\mathcal{M},\mathcal{M}}$ **sparse, semi-positive definite, frequently its rank deficiency is six or less**
- $C_{\mathcal{R},\mathcal{M}}$ **sparse, full rank,** $|\mathcal{R}| \leq |\mathcal{M}|$
- $v_{\mathcal{R}}$, **Lagrange multipliers**
- **indefinite linear** $(n+r) \times (n+r)$ **system**
- **with large rigid bodies, very indefinite,** r **can be much greater than** $(n-r)$

Null space projection (step 1)

- **find** $n \times (n-r)$ **matrix** Z **such that** $C\ Z = 0$

- **<u>For example</u>, full size** LQ **factorization**

$$C = \begin{bmatrix} L & 0 \end{bmatrix} \begin{bmatrix} Q^T \\ Z^T \end{bmatrix} \tag{4}$$

- L **is** $r \times r$, Q **is** $n \times r$, Z **is** $n \times (n-r)$
- $Q^T Q = I$, $Z^T Z = I$, **and** $Q^T Z = 0$
- **write displacements** u **as** $u = Q\ \alpha_{\mathcal{D}} + Z\ \alpha_{\mathcal{I}}$

Null space projection (step 2)

- **constraint equation**

$$\begin{aligned} Cu = g &\Longrightarrow C(Q\ \alpha_{\mathcal{D}} + Z\ \alpha_{\mathcal{I}}) = g \\ &\Longrightarrow CQ\ \alpha_{\mathcal{D}} = g \textbf{ since } CZ = 0 \\ &\Longrightarrow LQ^T Q\ \alpha_{\mathcal{D}} = g \Longrightarrow \alpha_{\mathcal{D}} = L^{-1} g \end{aligned} \tag{5}$$

- **write displacements** u **as** $u = Z\alpha_{\mathcal{I}} + QL^{-1}g$
- **insert into stiffness equation**

$$Ku = K(Z\alpha_{\mathcal{I}} + QL^{-1}g) = f$$

- **modify right hand side**

$$KZ\,\alpha_{\mathcal{I}} = f + \Delta f = f - KQL^{-1}g$$

Null space projection (step 3)

- **impose Galerkin condition**

$$
\begin{aligned}
Z^T K Z \, \alpha_{\mathcal{I}} &= Z^T (f - KQL^{-1} g) \\
&= \left(Z^T f \right) - \left(Z^T K Q \right) \left(L^{-1} g \right) \qquad (6)
\end{aligned}
$$

- $(n-r) \times (n-r)$ **matrix** $Z^T K Z$ **is positive definite**

Direct elimination (step 2)

- **analyze constraint matrix** $C_{\mathcal{R},\mathcal{M}}$

$$C_{\mathcal{R},\mathcal{M}}\, u_{\mathcal{M}} = g_{\mathcal{R}} \tag{7}$$

- **find permutation matrices** $P_{\mathcal{S},\mathcal{R}}$ **and** $P_{\mathcal{M},\mathcal{N}}$

$$\begin{aligned} C_{\mathcal{S},\mathcal{N}}\, u_{\mathcal{N}} &= \left(P_{\mathcal{S},\mathcal{R}} C_{\mathcal{R},\mathcal{M}} P_{\mathcal{M},\mathcal{N}}\right)\left(P^T_{\mathcal{M},\mathcal{N}} u_{\mathcal{M}}\right) \\ &= P_{\mathcal{S},\mathcal{R}}\, g_{\mathcal{R}} = g_{\mathcal{S}} \end{aligned} \tag{8}$$

- **find block structure,** $C_{\mathcal{S},\mathcal{D}}$ **nonsingular** $r \times r$

$$\left[C_{\mathcal{S},\mathcal{I}}\ C_{\mathcal{S},\mathcal{D}}\right] \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = g_{\mathcal{S}} \tag{9}$$

this is the "nice basis problem"

Direct elimination (step 3)

- **compute inverse $C_{\mathcal{D},\mathcal{S}}$, where $C_{\mathcal{D},\mathcal{S}}\ C_{\mathcal{S},\mathcal{D}} = I_{\mathcal{D},\mathcal{D}}$**
- **premultiply with $C_{\mathcal{D},\mathcal{S}}$**

$$C_{\mathcal{D},\mathcal{S}} \begin{bmatrix} C_{\mathcal{S},\mathcal{I}} & C_{\mathcal{S},\mathcal{D}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = C_{\mathcal{D},\mathcal{S}}\, g_{\mathcal{S}}$$

- **simpler constraint system**

$$\begin{bmatrix} C_{\mathcal{D},\mathcal{I}} & I_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = g_{\mathcal{D}} \tag{10}$$

- **simpler KKT system**

$$\begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} & C_{\mathcal{D},\mathcal{I}}^T \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \\ C_{\mathcal{D},\mathcal{I}} & I_{\mathcal{D},\mathcal{D}} & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \\ v_{\mathcal{D}} \end{bmatrix} = \begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \\ g_{\mathcal{D}} \end{bmatrix} \tag{11}$$

Direct elimination (step 4)

- **reduced linear system**

$$\widehat{K}_{\mathcal{I},\mathcal{I}}\, u_{\mathcal{I}} = \widehat{f}_{\mathcal{I}} \tag{12}$$

- **Eliminate trailing block rows and columns**

$$\widehat{K}_{\mathcal{I},\mathcal{I}} = K_{\mathcal{I},\mathcal{I}} - \begin{bmatrix} C^T_{\mathcal{D},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \end{bmatrix} \begin{bmatrix} K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \\ I_{\mathcal{D},\mathcal{D}} & 0 \end{bmatrix}^{-1} \begin{bmatrix} K_{\mathcal{D},\mathcal{I}} \\ C_{\mathcal{D},\mathcal{I}} \end{bmatrix}$$

$$\widehat{f}_{\mathcal{I}} = f_{\mathcal{I}} - \begin{bmatrix} C^T_{\mathcal{D},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \end{bmatrix} \begin{bmatrix} K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \\ I_{\mathcal{D},\mathcal{D}} & 0 \end{bmatrix}^{-1} \begin{bmatrix} f_{\mathcal{D}} \\ g_{\mathcal{D}} \end{bmatrix}$$

- **Block inverse**

$$\begin{bmatrix} K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \\ I_{\mathcal{D},\mathcal{D}} & 0 \end{bmatrix}^{-1} = \begin{bmatrix} 0 & I_{\mathcal{D},\mathcal{D}} \\ I_{\mathcal{D},\mathcal{D}} & (-K_{\mathcal{D},\mathcal{D}}) \end{bmatrix}$$

Direct elimination (step 5)

- **should not be a surprise, since**

$$\begin{bmatrix} I_{\mathcal{D},\mathcal{D}} & K_{\mathcal{D},\mathcal{D}} \\ 0 & I_{\mathcal{D},\mathcal{D}} \end{bmatrix}^{-1} = \begin{bmatrix} I_{\mathcal{D},\mathcal{D}} & -K_{\mathcal{D},\mathcal{D}} \\ 0 & I_{\mathcal{D},\mathcal{D}} \end{bmatrix}$$

and

$$\begin{bmatrix} I_{\mathcal{D},\mathcal{D}} & 0 \\ K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \end{bmatrix}^{-1} = \begin{bmatrix} I_{\mathcal{D},\mathcal{D}} & 0 \\ -K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \end{bmatrix}$$

- **reduced linear system** $\widehat{K}_{\mathcal{I},\mathcal{I}}\, u_{\mathcal{I}} = \widehat{f}_{\mathcal{I}}$

$$\widehat{K}_{\mathcal{I},\mathcal{I}} = K_{\mathcal{I},\mathcal{I}} + \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} & C^T_{\mathcal{D},\mathcal{I}} \end{bmatrix} \begin{bmatrix} 0 & -I_{\mathcal{D},\mathcal{D}} \\ -I_{\mathcal{D},\mathcal{D}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} K_{\mathcal{D},\mathcal{I}} \\ C_{\mathcal{D},\mathcal{I}} \end{bmatrix}$$

$$\widehat{f}_{\mathcal{I}} = f_{\mathcal{I}} + \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} & C^T_{\mathcal{D},\mathcal{I}} \end{bmatrix} \begin{bmatrix} 0 & -I_{\mathcal{D},\mathcal{D}} \\ -I_{\mathcal{D},\mathcal{D}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} f_{\mathcal{D}} \\ g_{\mathcal{D}} \end{bmatrix}$$

Null space projection (step 4)

- **If we start with the simpler constraints**

$$\begin{bmatrix} C_{\mathcal{D},\mathcal{I}} & I_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = g_{\mathcal{D}} \tag{13}$$

and permuted and blocked stiffness equation

$$\begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = \begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \end{bmatrix} \tag{14}$$

- **orthogonal, not orthonormal subspaces**

$$\mathsf{Q}_{\mathcal{N},\mathcal{D}} = \begin{bmatrix} C^T_{\mathcal{D},\mathcal{I}} \\ I_{\mathcal{D},\mathcal{D}} \end{bmatrix}, \mathsf{Z}_{\mathcal{N},\mathcal{I}} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix},$$

$$\mathsf{Q}^T_{\mathcal{N},\mathcal{D}}\mathsf{Z}_{\mathcal{N},\mathcal{I}} = 0, \qquad \mathsf{Q}^T_{\mathcal{N},\mathcal{D}}\mathsf{Q}_{\mathcal{N},\mathcal{D}} \neq I, \qquad \mathsf{Z}^T_{\mathcal{N},\mathcal{I}}\mathsf{Z}_{\mathcal{N},\mathcal{I}} \neq I$$

Null space projection (step 5)

- **split solution**

$$\begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = \mathsf{Z}_{\mathcal{N},\mathcal{I}}\, u_{\mathcal{I}} + \begin{bmatrix} 0_{\mathcal{I}} \\ g_{\mathcal{D}} \end{bmatrix} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix} u_{\mathcal{I}} + \begin{bmatrix} 0_{\mathcal{I}} \\ g_{\mathcal{D}} \end{bmatrix} \tag{15}$$

- **insert into stiffness equation** $Ku = f$

$$\begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \left(\begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix} u_{\mathcal{I}} + \begin{bmatrix} 0_{\mathcal{I}} \\ g_{\mathcal{D}} \end{bmatrix} \right) = \begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \end{bmatrix} \tag{16}$$

$$\begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix} u_{\mathcal{I}} = \begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \end{bmatrix} - \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{D}} \end{bmatrix} g_{\mathcal{D}} \tag{17}$$

Null space projection (step 6)

- **impose Galerkin condition, solve**

$$\widehat{K}_{\mathcal{I},\mathcal{I}}\, u_{\mathcal{I}} = \widehat{f}_{\mathcal{I}} \tag{18}$$

where

$$\widehat{K}_{\mathcal{I},\mathcal{I}} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix}^T \begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix} \tag{19}$$

and

$$\widehat{f}_{\mathcal{I}} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix}^T \left(\begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \end{bmatrix} - \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{D}} \end{bmatrix} g_{\mathcal{D}} \right) \tag{20}$$

Equivalent reduced linear systems

- **from direct elimination**

$$\widehat{K}_{\mathcal{I},\mathcal{I}} = K_{\mathcal{I},\mathcal{I}} + \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} & C_{\mathcal{D},\mathcal{I}}^T \end{bmatrix} \begin{bmatrix} 0 & -I_{\mathcal{D},\mathcal{D}} \\ -I_{\mathcal{D},\mathcal{D}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} K_{\mathcal{D},\mathcal{I}} \\ C_{\mathcal{D},\mathcal{I}} \end{bmatrix}$$

$$\widehat{f}_{\mathcal{I}} = f_{\mathcal{I}} + \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} & C_{\mathcal{D},\mathcal{I}}^T \end{bmatrix} \begin{bmatrix} 0 & -I_{\mathcal{D},\mathcal{D}} \\ -I_{\mathcal{D},\mathcal{D}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} f_{\mathcal{D}} \\ g_{\mathcal{D}} \end{bmatrix}$$

- **from null space projection**

$$\widehat{K}_{\mathcal{I},\mathcal{I}} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix}^T \begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} \end{bmatrix} \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix}$$

$$\widehat{f}_{\mathcal{I}} = \begin{bmatrix} I_{\mathcal{I},\mathcal{I}} \\ -C_{\mathcal{D},\mathcal{I}} \end{bmatrix}^T \left(\begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \end{bmatrix} - \begin{bmatrix} K_{\mathcal{I},\mathcal{D}} \\ K_{\mathcal{D},\mathcal{D}} \end{bmatrix} g_{\mathcal{D}} \right)$$

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- types of constraints and spy plots
  - Dirichlet conditions
  - adaptive conditions
  - rigid body conditions
  - large door model

Dirichlet conditions

- $u_{\mathcal{D}} = u^0_{\mathcal{D}}$, **dependent dof given values**
- **constraint matrix**

$$C_{\mathcal{S},\mathcal{N}} = \left[C_{\mathcal{S},\mathcal{I}} \; C_{\mathcal{S},\mathcal{D}}\right] = \left[0_{\mathcal{S},\mathcal{I}} \; I_{\mathcal{S},\mathcal{D}}\right] \tag{21}$$

$$C_{\mathcal{D},\mathcal{N}} = \left[C_{\mathcal{D},\mathcal{I}} \; I_{\mathcal{D},\mathcal{D}}\right] = \left[0_{\mathcal{D},\mathcal{I}} \; I_{\mathcal{D},\mathcal{D}}\right] \tag{22}$$

- **reduced system**

$$\begin{aligned} \widehat{K}_{\mathcal{I},\mathcal{I}} &= K_{\mathcal{I},\mathcal{I}} \\ \widehat{f}_{\mathcal{I}} &= f_{\mathcal{I}} - K_{\mathcal{I},\mathcal{D}} u^0_{\mathcal{D}} \end{aligned}$$

Adaptive conditions

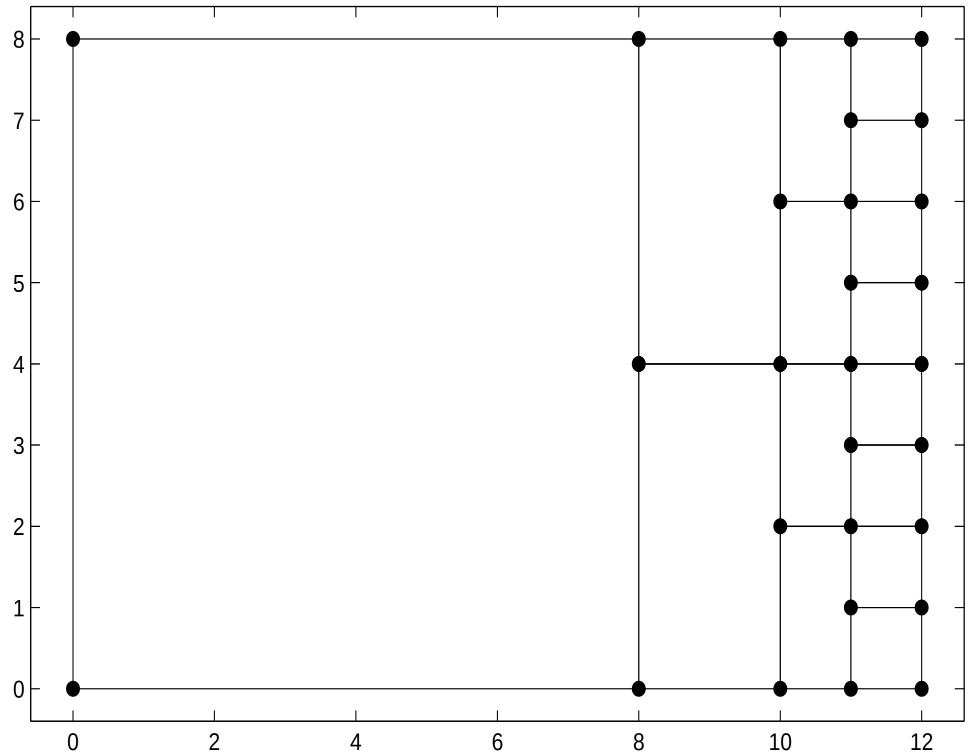
- $u_i = \alpha * u_j + \beta * u_k$
- **linear interpolation between two nodes**
- **constraint matrix**

$$C_{\mathcal{S},\mathcal{N}} = \left[C_{\mathcal{S},\mathcal{I}} \; C_{\mathcal{S},\mathcal{D}}\right] = \left[C_{\mathcal{S},\mathcal{I}} \; I_{\mathcal{S},\mathcal{D}}\right] \quad (23)$$

$$C_{\mathcal{D},\mathcal{N}} = \left[C_{\mathcal{D},\mathcal{I}} \; I_{\mathcal{D},\mathcal{D}}\right] \quad (24)$$

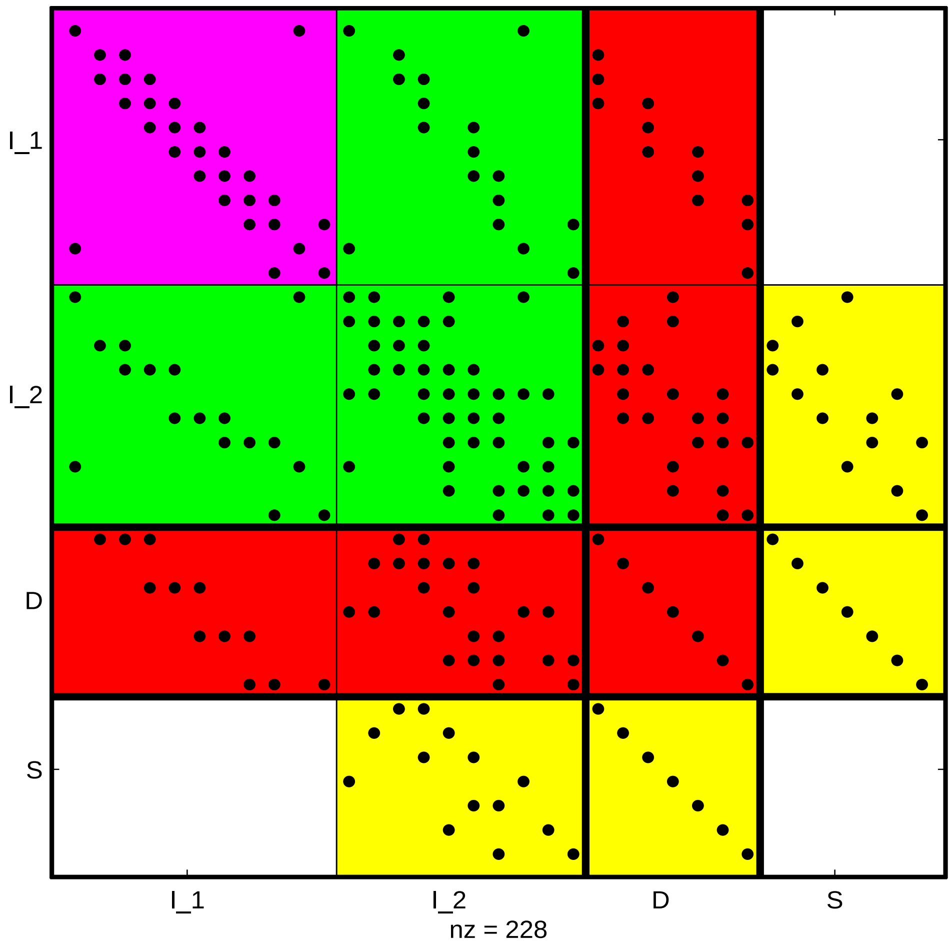
- **idea extends to tied contact,
slave node linear combination of 3-4 nodes**

Adaptive conditions : mesh



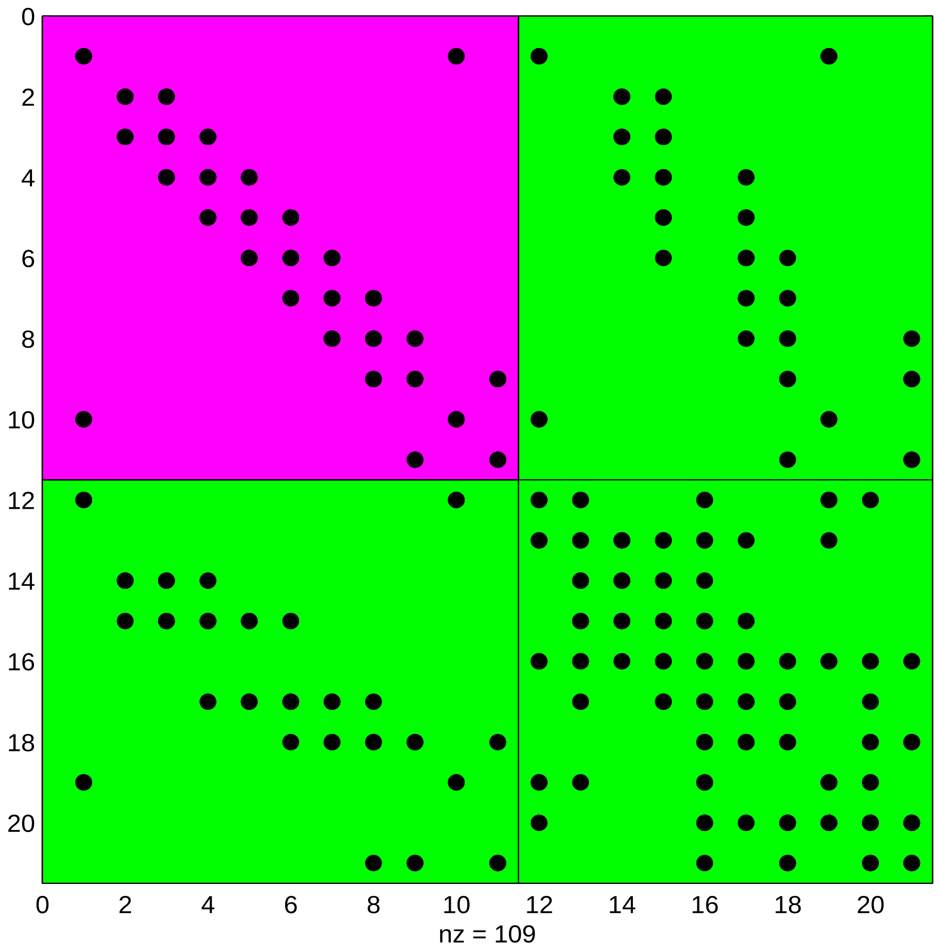
$$\mathbf{u_i} = \frac{1}{2}\left(\mathbf{u_j} + \mathbf{u_k}\right)$$

Adaptive conditions : KKT system



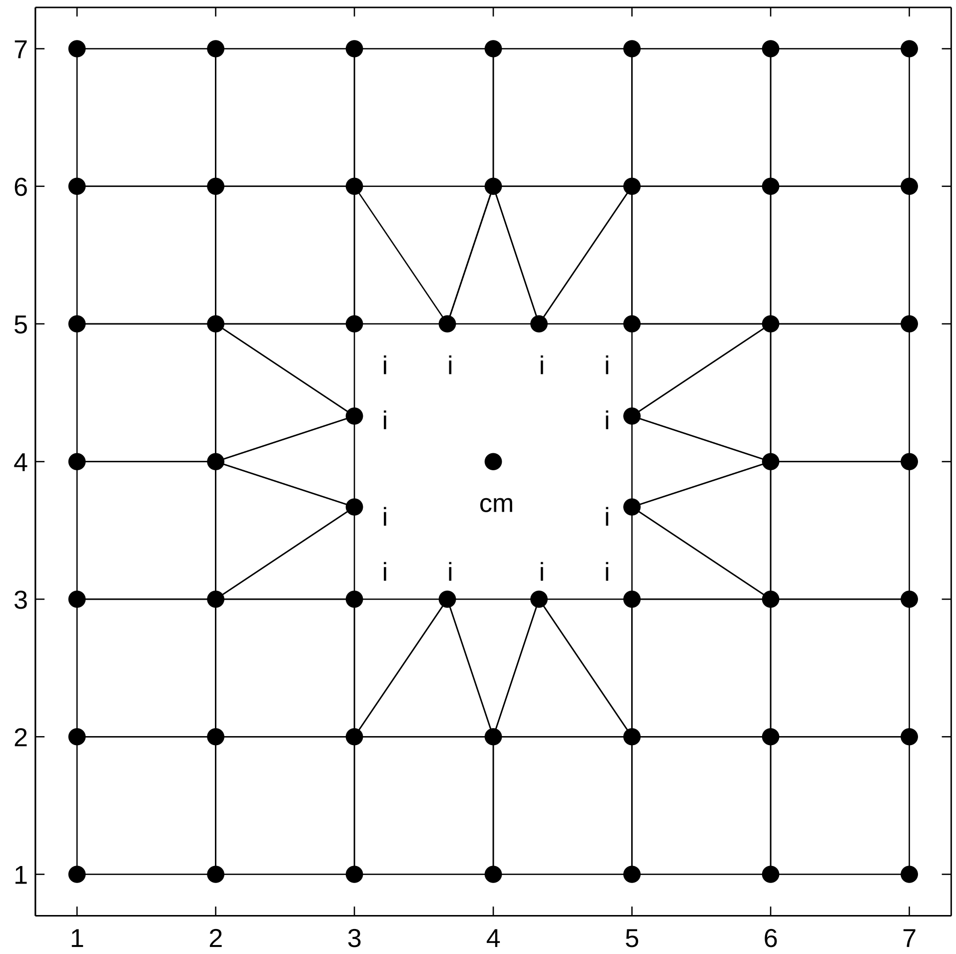
- **magenta – stiffness matrix not modified**
- **green – stiffness matrix modified**
- **red – stiffness matrix not modified**
- **yellow – constraint matrix**

Adaptive conditions : Reduced system



- **magenta – stiffness matrix not modified**
- **green – stiffness matrix modified**

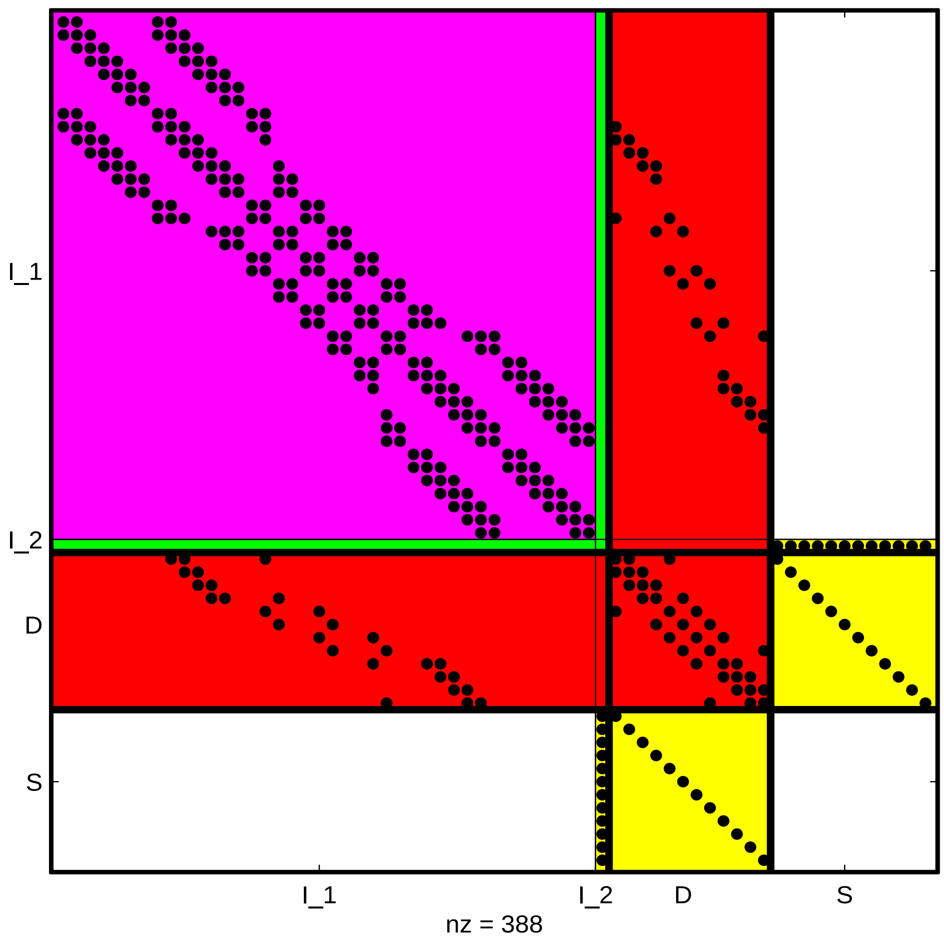
Rigid body conditions : mesh



$$\mathbf{u_i} = T_{\mathbf{i,cm}} \mathbf{u_{cm}}$$

$$T_{\mathbf{i,cm}} = \begin{bmatrix} 1 & 0 & 0 & 0 & * & * \\ 0 & 1 & 0 & * & 0 & * \\ 0 & 0 & 1 & * & * & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Rigid body conditions : KKT system



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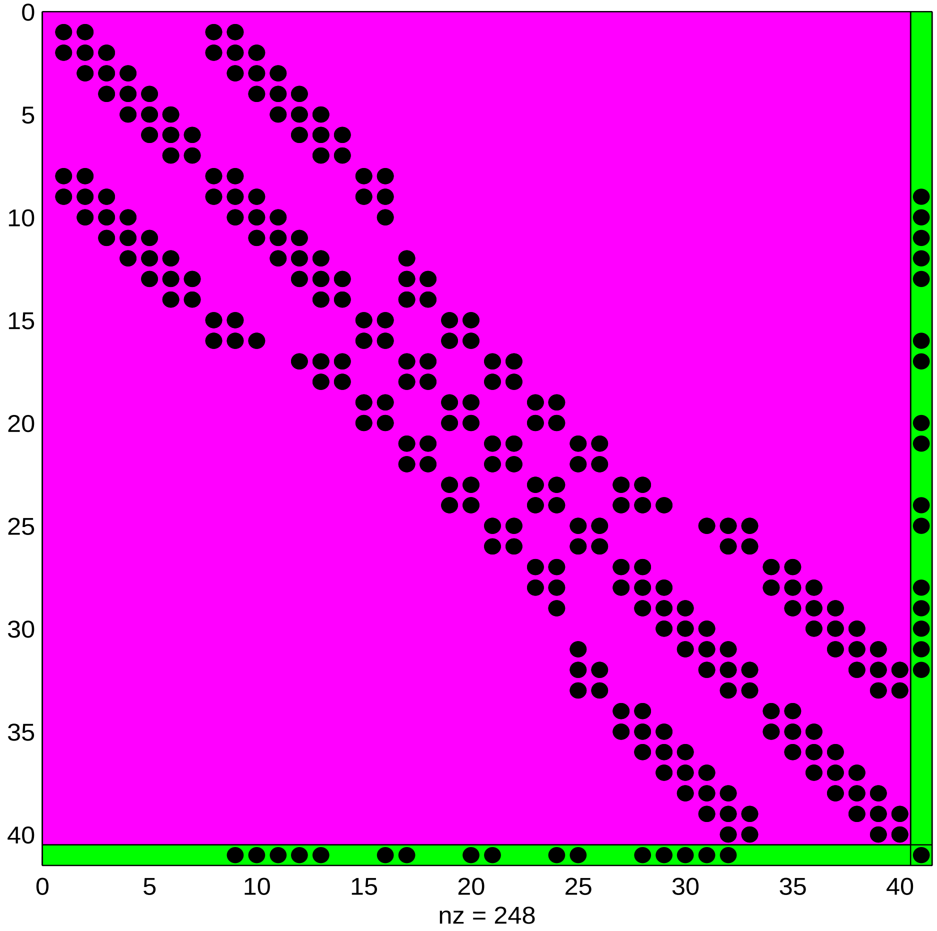
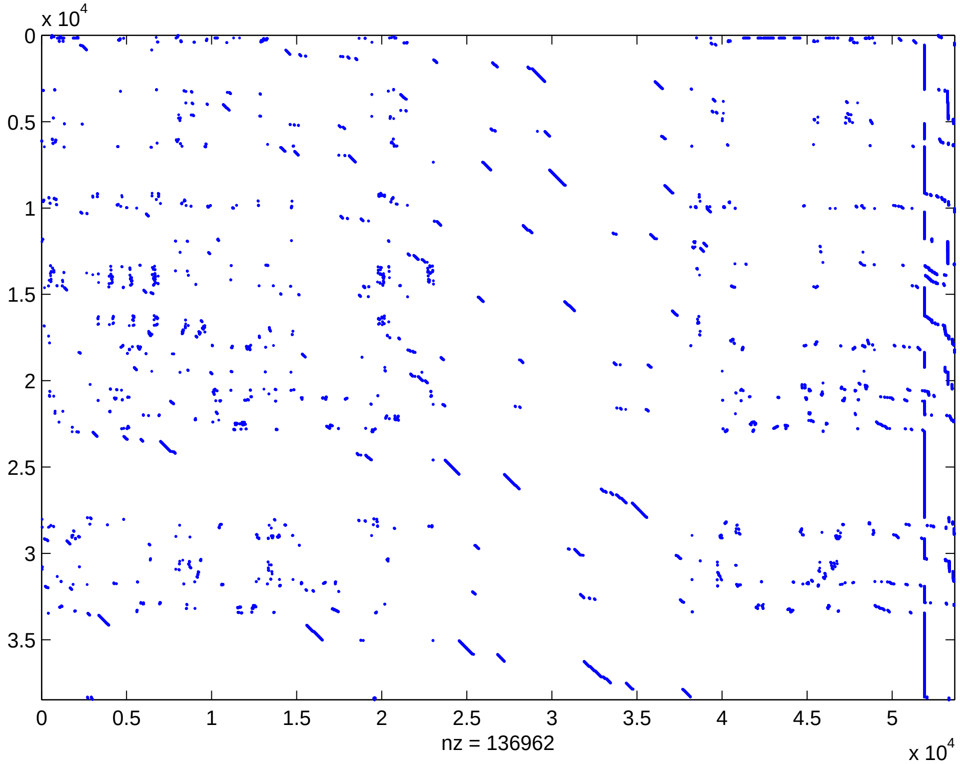
Rigid body conditions : Reduced system



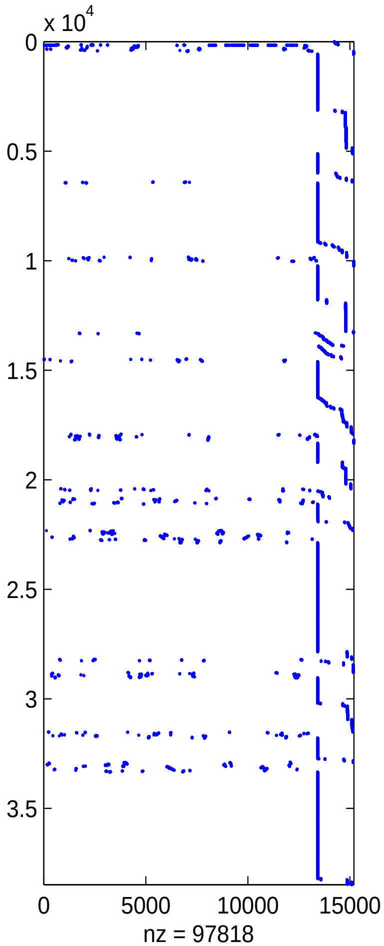
- **magenta – stiffness matrix not modified**
- **green – stiffness matrix modified**

Door model, 1,288,044 dof, 38,478 constraints

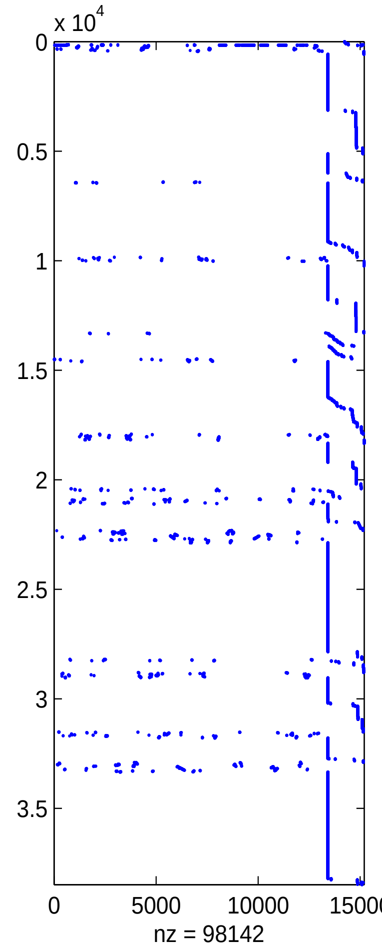


- constraints distributed across 16 processors
- C has 38,478 rows and 53,673 nonzero columns
- 2,916 tied contact
- 5 interpolation constraints
- 297 rigid bodies, 35,532 rows

Door model, 1,288,044 dof, 38,478 constraints



- $|C_{\mathcal{S},\mathcal{D}}| = 39144$, **almost diagonal**
- $|C_{\mathcal{D},\mathcal{S}}| = 39144$, **no-fill inverse**
- $|C_{\mathcal{S},\mathcal{I}}| = 97818$, **(on left)**
- $|C_{\mathcal{D},\mathcal{I}}| = 98142$, **(on right)**



Outline of talk

- **various topics**
  - **when not to use direct elimination**
  - **inertial relief**
  - **nice basis problem**
  - **re-use of permutations**
  - **Lagrange multipliers and residual forces**
  - **rank-revealing QR factorizations**

When is direct elimination a bad idea?

- **When $C_{\mathcal{D},\mathcal{I}}$ is dense, or has one or more dense rows, then $\widehat{K}_{\mathcal{I},\mathcal{I}}$ is dense**
- **Expand $C_{\mathcal{D},\mathcal{I}} = C_{\mathcal{D},\mathcal{S}}\ C_{\mathcal{S},\mathcal{I}}$**
  - **we want $C_{\mathcal{D},\mathcal{S}}$ to be sparse**
  - **only possible when $C_{\mathcal{S},\mathcal{D}}$ has many components, i.e., diagonal or block diagonal**
  - **$C_{\mathcal{D},\mathcal{S}}$ has a good block triangular form with small diagonal blocks**
  - **also want $C_{\mathcal{S},\mathcal{I}}$ to be sparse**
- **Interesting ordering problem, much different from ordering stiffness matrix K**

Example : Inertial relief, $C_{\mathcal{E},\mathcal{I}}$ and $C_{\mathcal{E},\mathcal{D}}$ dense

- **rows and columns : eliminate $\mathcal{D}$, keep $\mathcal{E}$**

$$\begin{bmatrix} K_{\mathcal{I},\mathcal{I}} & K_{\mathcal{I},\mathcal{D}} & C^T_{\mathcal{D},\mathcal{I}} & C^T_{\mathcal{E},\mathcal{I}} \\ K_{\mathcal{D},\mathcal{I}} & K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} & C^T_{\mathcal{E},\mathcal{D}} \\ C_{\mathcal{D},\mathcal{I}} & I_{\mathcal{D},\mathcal{D}} & 0 & 0 \\ C_{\mathcal{E},\mathcal{I}} & C_{\mathcal{E},\mathcal{D}} & 0 & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \\ v_{\mathcal{D}} \\ v_{\mathcal{E}} \end{bmatrix} = \begin{bmatrix} f_{\mathcal{I}} \\ f_{\mathcal{D}} \\ g_{\mathcal{D}} \\ g_{\mathcal{E}} \end{bmatrix} \tag{25}$$

- **reduce to then solve for $u_{\mathcal{I}}$ and $v_{\mathcal{E}}$.**

$$\begin{bmatrix} \widehat{K}_{\mathcal{I},\mathcal{I}} & \widehat{C}^T_{\mathcal{E},\mathcal{I}} \\ \widehat{C}_{\mathcal{E},\mathcal{I}} & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ v_{\mathcal{E}} \end{bmatrix} = \begin{bmatrix} \widehat{f}_{\mathcal{I}} \\ \widehat{g}_{\mathcal{E}} \end{bmatrix} \tag{26}$$

- **recover $u_{\mathcal{D}}$ and $v_{\mathcal{D}}$**

$$\begin{bmatrix} K_{\mathcal{D},\mathcal{D}} & I_{\mathcal{D},\mathcal{D}} \\ I_{\mathcal{D},\mathcal{D}} & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{D}} \\ v_{\mathcal{D}} \end{bmatrix} = \begin{bmatrix} f_{\mathcal{D}} \\ g_{\mathcal{D}} \end{bmatrix} - \begin{bmatrix} K_{\mathcal{D},\mathcal{I}} & C^T_{\mathcal{E},\mathcal{D}} \\ C_{\mathcal{D},\mathcal{I}} & 0 \end{bmatrix} \begin{bmatrix} u_{\mathcal{I}} \\ v_{\mathcal{E}} \end{bmatrix} \tag{27}$$

Nice basis problem $C_{\mathcal{R},\mathcal{M}} u_{\mathcal{M}} = g_{\mathcal{R}}$

- **Given** $r \times n$ **matrix** $C_{R,M}$ **find**
  - **permutations** $P_{\mathcal{S},\mathcal{R}}$ **and** $P_{\mathcal{N},\mathcal{M}}$

$$\left(P_{\mathcal{S},\mathcal{R}} C_{\mathcal{R},\mathcal{M}} P^T_{\mathcal{N},\mathcal{M}}\right)\left(P_{\mathcal{N},\mathcal{M}} u_{\mathcal{M}}\right) = \left(P_{\mathcal{S},\mathcal{R}} g_{\mathcal{R}}\right) \quad (28)$$

$$C_{\mathcal{S},\mathcal{N}}\ u_{\mathcal{N}} = g_{\mathcal{S}} \quad (29)$$

  - **find independent** $\mathcal{I}$ **and dependent** $\mathcal{D}$ **dof**

$$\left[C_{\mathcal{S},\mathcal{I}}\ C_{\mathcal{S},\mathcal{D}}\right] \begin{bmatrix} u_{\mathcal{I}} \\ u_{\mathcal{D}} \end{bmatrix} = g_{\mathcal{S}} \quad (30)$$

    with $C_{\mathcal{S},\mathcal{D}}$ **square, nonsingular**
  - **inverse** $C_{\mathcal{D},\mathcal{S}} = C^{-1}_{\mathcal{S},\mathcal{D}}$ **is sparse, well conditioned**

Nice basis problem $C_{\mathcal{R},\mathcal{M}} u_{\mathcal{M}} = g_{\mathcal{R}}$

- **purely structural based permutations have created singular $C_{\mathcal{S},\mathcal{D}}$ matrices.**
- **use structural and numeric phases to compute the permutations**

$$P_{\mathcal{S},\mathcal{R}} = \begin{bmatrix} I_{\mathcal{S}_1,\mathcal{R}_1} & \\ & P_{\mathcal{S}_2,\mathcal{R}_2} \end{bmatrix} \begin{bmatrix} P_{\mathcal{S}_1,\mathcal{R}_1} & \\ & I_{\mathcal{S}_2,\mathcal{R}_2} \end{bmatrix} \tag{31}$$

$$P_{\mathcal{N},\mathcal{M}} = \begin{bmatrix} I_{\mathcal{N}_1,\mathcal{M}_1} & \\ & P_{\mathcal{N}_2,\mathcal{M}_2} \end{bmatrix} \begin{bmatrix} P_{\mathcal{N}_1,\mathcal{M}_1} & \\ & I_{\mathcal{N}_2,\mathcal{M}_2} \end{bmatrix} \tag{32}$$

  no MPP implementation (not needed yet)
- **structural phase needs a tolerance to bound** $\max |C_{\mathcal{D},\mathcal{S}}|$

Re-using the permutations

- **The operation**

$$\textbf{minimize } \|f - Ku\|_2 \textbf{ subject to } Cu = g$$

  is done inside a nonlinear iteration
- **we can reuse the permutations for several steps**
- **monitor** $\max |C_{\mathcal{D},\mathcal{S}}| / \max |C_{\mathcal{S},\mathcal{D}}|$
- **monitor** $\max |C_{\mathcal{D},\mathcal{I}}| / \max |C_{\mathcal{S},\mathcal{I}}|$
- **as the constraint matrix** C **becomes stale,** $C_{\mathcal{D},\mathcal{S}}$ **and** $C_{\mathcal{D},\mathcal{I}}$ **can become ill-conditioned since the ordering may not be suited for the entries**

Lagrange multipliers

More than just a mathematical construct.

- **residual forces :** $r = f - Ku = C^T v$
- **Lagrange multipliers are residual forces at dependent dof**

$$v_{\mathcal{D}} = r_{\mathcal{D}} = f_{\mathcal{D}} - K_{\mathcal{D},\mathcal{N}} u_{\mathcal{N}} \tag{33}$$

- **residual forces at** $\mathcal{N}$ **:**

$$r_{\mathcal{N}} = C^T_{\mathcal{D},\mathcal{N}} v_{\mathcal{D}} = \begin{bmatrix} C^T_{\mathcal{D},\mathcal{I}} \\ I_{\mathcal{D},\mathcal{I}} \end{bmatrix} v_{\mathcal{D}} = \begin{bmatrix} C^T_{\mathcal{D},\mathcal{I}} v_{\mathcal{D}} \\ v_{\mathcal{D}} \end{bmatrix} \tag{34}$$

- **residual forces at original ordering** $\mathcal{M}$ **:**

$$r_{\mathcal{M}} = P_{\mathcal{M},\mathcal{N}}\, r_{\mathcal{N}} = P_{\mathcal{M},\mathcal{N}}\, C^T_{\mathcal{D},\mathcal{N}}\, v_{\mathcal{D}} \tag{35}$$

Relaxation of full rank constraints

- **full rank property** $\Longrightarrow C_{\mathcal{S},\mathcal{D}}$ **is nonsingular**
- **rank-revealing** QR **factorization of** $C_{\mathcal{R},\mathcal{M}}$

$$C_{\mathcal{R},\mathcal{M}} P_{\mathcal{M},\mathcal{N}} = Q_{\mathcal{R},\mathcal{K}} R_{\mathcal{K},\mathcal{N}} = Q_{\mathcal{R},\mathcal{K}} \begin{bmatrix} R_{\mathcal{K},\mathcal{D}} & R_{\mathcal{I},\mathcal{N}} \end{bmatrix}$$

where $|K| = |D| \leq |R|$

$$\begin{aligned} C_{\mathcal{R},\mathcal{M}} u_{\mathcal{M}} &= g_{\mathcal{R}} \\ \left(C_{\mathcal{R},\mathcal{M}} P_{\mathcal{M},\mathcal{N}}\right)\left(P_{\mathcal{N},\mathcal{M}} u_{\mathcal{M}}\right) &= g_{\mathcal{R}} \\ Q_{\mathcal{R},\mathcal{K}} \begin{bmatrix} R_{\mathcal{K},\mathcal{D}} & R_{\mathcal{K},\mathcal{I}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{D}} \\ u_{\mathcal{I}} \end{bmatrix} &= g_{\mathcal{R}} \\ \begin{bmatrix} R_{\mathcal{K},\mathcal{D}} & R_{\mathcal{K},\mathcal{I}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{D}} \\ u_{\mathcal{I}} \end{bmatrix} &= g_{\mathcal{K}} = Q_{\mathcal{R},\mathcal{K}} g_{\mathcal{R}} \\ \begin{bmatrix} I_{\mathcal{D},\mathcal{D}} & R_{\mathcal{D},\mathcal{I}} \end{bmatrix} \begin{bmatrix} u_{\mathcal{D}} \\ u_{\mathcal{I}} \end{bmatrix} &= g_{\mathcal{D}} = R_{\mathcal{D},\mathcal{K}} g_{\mathcal{K}} \end{aligned}$$

Why $RRQR$ on constraint matrix C?

- **Full rank $\Longrightarrow$ no replicated constraint rows across processors**
- **Useful feature, return information to user on over-constrained system**
  - **presently return information about dof**
  - **$RRQR$ can return information about constraint rows**
- **New feature for engineer — weighted constraint rows**

Summary

- Basic idea : use constraints to reduce system size, often indefinite matrix $\longrightarrow$ definite matrix
- Two approaches are equivalent
  - direct elimination
  - null space projection
- Nice basis problem
  - structural methods inadequate by themselves
  - numeric methods necessary for a robust solution
  - MPP implementation interesting research topic