Finite Elements For Engineers

Lecture 3: Solving Linear Algebraic Equations

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System Equations

$$\mathbf{K}_{n\times n}\mathbf{D}_{n\times 1} = \mathbf{F}_{n\times 1}$$

- **K** is symmetric, banded/skyline/sparse, positive definite
- In general, solution time is proportional to n^3
- This step requires the most time as problem size increases (50-95% of the total)
- Memory storage requirement is also very large (16,000 equations full storage = 1.91 GB)

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Notes

- Problem can have multiple RHS vectors
- Truncation and round-off errors are important

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How good is the solution?

$$\mathbf{KD} = \mathbf{F}$$

$$\mathbf{R} = \mathbf{KD} - \mathbf{F} \approx 0$$

Error magnitude is a function of the condition number of **A.**

$$cond(\mathbf{K}) = \frac{\lambda_{\max}}{\lambda_{\min}}$$

Error Measures

$$\varepsilon_{rel} = \frac{\|\mathbf{R}\|}{\|\mathbf{F}\|}$$

$$\varepsilon_{abs} = \|\mathbf{R}\|$$

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Equation Solvers for KD=F

- Direct
  - Gaussian Elimination (any nonsingular **K**)
  - Cholesky Factorization (**K** is symmetric and positive definite)
- Iterative
  - Preconditioned Conjugate Gradient Method

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Imposing Non-Homogenous EBC

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \Rightarrow \begin{aligned} A_{11}x_1 + A_{12}x_2 + A_{13}x_3 &= b_1 \\ A_{21}x_1 + A_{22}x_2 + A_{23}x_3 &= b_2 \\ A_{31}x_1 + A_{32}x_2 + A_{33}x_3 &= b_3 \end{aligned}$$

Modified Form

$x_2 = c$

$$A_{11}x_1 + \qquad A_{13}x_3 = b_1 - A_{12}x_2 = b_1 - A_{12}c$$

$$A_{31}x_1 + \qquad A_{33}x_3 = b_3 - A_{32}x_2 = b_3 - A_{32}c$$

Final Form

$$\begin{bmatrix} A_{11} & 0 & A_{13} \\ 0 & 1 & 0 \\ A_{31} & 0 & A_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 - A_{12}c \\ c \\ b_3 - A_{32}c \end{Bmatrix}$$

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Example

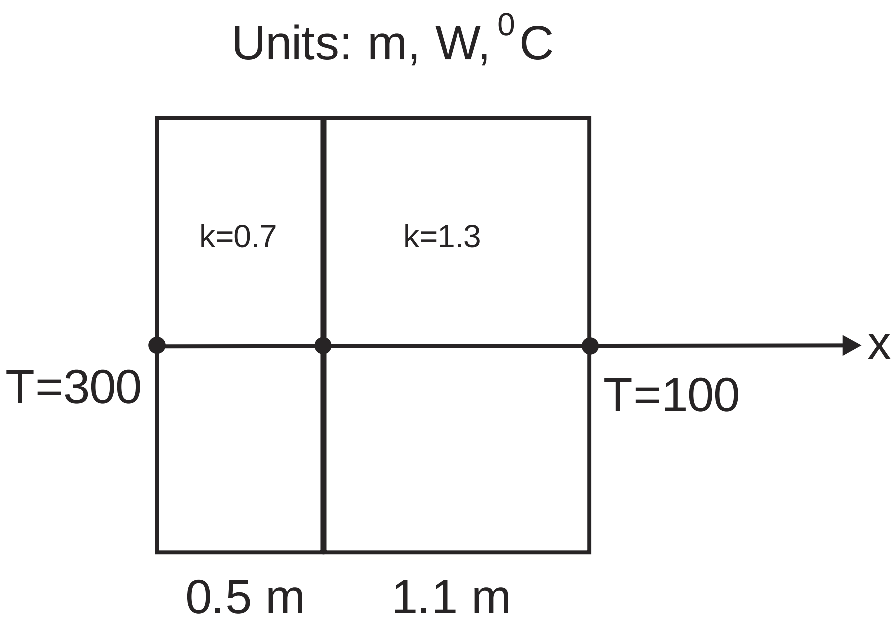

Figure shows a two layer composite wall with thicknesses as 0.5 m and 1.1 m. The outside face is maintained at 300^{0}C and the inside face at 100^{0}C. The thermal conductivities are given as

$$k_1 = 0.7 \frac{W}{m \cdot {}^\circ C}, \quad k_2 = 1.3 \frac{W}{m \cdot {}^\circ C}$$

Compute the temperature distribution in the wall.

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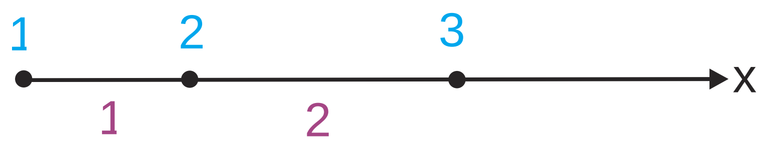
Example

Consistent units (m, W, ^{0}C)



Element Equations

$$\frac{(0.7)(1.0)}{0.5}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} T_1 \\ T_2 \end{Bmatrix} = \begin{Bmatrix} q_1^1 \\ q_2^1 \end{Bmatrix}$$

$$\frac{(1.3)(1.0)}{1.1}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} T_2 \\ T_3 \end{Bmatrix} = \begin{Bmatrix} q_1^2 \\ q_2^2 \end{Bmatrix}$$

System Equations

$$\begin{bmatrix} 1.4 & -1.4 & 0 \\ -1.4 & 1.4+1.18182 & -1.18182 \\ 0 & -1.18182 & 1.18182 \end{bmatrix}\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix} = \begin{Bmatrix} q_1^1 \\ 0 \\ q_2^2 \end{Bmatrix}$$

BCs

$$T_1 = 300$$

$$T_3 = 100$$

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Example

$$\begin{bmatrix} 1.4 & -1.4 & 0 \\ -1.4 & 2.58182 & -1.18182 \\ 0 & -1.18182 & 1.18182 \end{bmatrix} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix} = \begin{Bmatrix} q_1^1 \\ 0 \\ q_2^2 \end{Bmatrix}$$

System Equations after BCs

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2.58182 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix} = \begin{Bmatrix} 300 \\ 0 + 1.4(300) + (1.18182)(100) \\ 100 \end{Bmatrix} = \begin{Bmatrix} 300 \\ 538.182 \\ 100 \end{Bmatrix}$$

Solution

$$\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix} = \begin{Bmatrix} 300 \\ 208.451 \\ 100 \end{Bmatrix} {}^\circ C$$

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Handling Constraints

Solve equations with special conditions

$$\mathbf{KD} = \mathbf{F}$$

with $\quad c_i D_i + c_j D_j = c$

Minimization Problem

$$\Pi(\mathbf{D}) = \frac{1}{2}\mathbf{D}^{\mathbf{T}}\mathbf{KD} - \mathbf{D}^{\mathbf{T}}\mathbf{F}$$

leads to the solution to

$$\frac{\partial \Pi}{\partial \mathbf{D}} = 0 = \mathbf{KD} - \mathbf{F}$$

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Equations with constraints

$$\Pi(\mathbf{D}) = \frac{1}{2}\mathbf{D}^{\mathbf{T}}\mathbf{K}\mathbf{D} - \mathbf{D}^{\mathbf{T}}\mathbf{F} + \frac{1}{2}C\left(c_i D_i + c_j D_j - c\right)^2$$

Large number

Minimum is when $c_i D_i + c_j D_j - c = 0$

$$\frac{\partial \Pi}{\partial \mathbf{D}} = 0$$

$$C = 10^4 \max\left|K_{pq}\right|, 1 \le p, q \le n$$

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Equations with constraints

$$\begin{bmatrix} A_{11} & & A_{1i} & & A_{1j} & A_{1n} \\ & .. & & & & \\ A_{i1} & & A_{ii}+Cc_i^2 & & A_{ij}+Cc_ic_j & A_{in} \\ & & & .. & & \\ A_{j1} & & A_{ji}+Cc_ic_j & & A_{jj}+Cc_j^2 & A_{jn} \\ & & & & .. & \\ A_{n1} & & A_{ni} & & A_{nj} & A_{nn} \end{bmatrix} \begin{Bmatrix} x_1 \\ \\ x_i \\ \\ x_j \\ \\ x_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ .. \\ b_i + Cc_i \\ .. \\ b_j + Cc_j \\ .. \\ b_n \end{Bmatrix}$$

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Example

$$\begin{bmatrix} 10 & -5 & 2 \\ -5 & 20 & 5 \\ 2 & 5 & 15 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 58 \\ 57 \end{Bmatrix} \text{ with } 2x_1 + x_3 = 3$$

Modified Equations

$$\begin{bmatrix} 10+20\left(10^4\right)2^2 & -5 & 2+20\left(10^4\right)(2)(1) \\ -5 & 20 & 5 \\ 2+20\left(10^4\right)(2)(1) & 5 & 15+20\left(10^4\right)1^2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6+20\left(10^4\right)(3)(2) \\ 58 \\ 57+20\left(10^4\right)(3)(1) \end{Bmatrix}$$

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Gaussian Elimination

Original Equations

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} & K_{1i} & K_{1n} \\ K_{21} & K_{22} & K_{23} & K_{2i} & K_{2n} \\ K_{31} & K_{32} & K_{33} & K_{3i} & K_{3n} \\ \\ K_{i1} & K_{i2} & K_{i3} & K_{ii} & K_{in} \\ \\ K_{n1} & K_{n2} & K_{n3} & K_{ni} & K_{nn} \end{bmatrix} \begin{Bmatrix} D_1 \\ D_2 \\ D_3 \\ \\ D_i \\ \\ D_n \end{Bmatrix} = \begin{Bmatrix} F_1 \\ F_2 \\ F_3 \\ \\ F_i \\ \\ F_n \end{Bmatrix}$$

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Direct Solvers

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Gaussian Elimination

- To obtain another equivalent **Ax=b**
  - **We can interchange two rows.**
  - **Multiply both sides by a constant.**
  - **Multiply one equation by a constant and add it to another equation.**

$$\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \times \\ \times \\ \times \end{Bmatrix} \Rightarrow \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} \times \\ \times \\ \times \end{Bmatrix}$$

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Gaussian Elimination

Forward Elimination

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} & & K_{1i} & & K_{1n} \\ 0 & K_{22}^{(1)} & K_{23}^{(1)} & & K_{2i}^{(1)} & & K_{2n}^{(1)} \\ 0 & 0 & K_{33}^{(2)} & & K_{3i}^{(2)} & & K_{3n}^{(2)} \\ & & & & & & \\ 0 & 0 & 0 & & K_{ii}^{(i-1)} & & K_{in}^{(i-1)} \\ & & & & & & \\ 0 & 0 & 0 & & 0 & & K_{nn}^{(n-1)} \end{bmatrix} \begin{Bmatrix} D_1 \\ D_2 \\ D_3 \\ \\ D_i \\ \\ D_n \end{Bmatrix} = \begin{Bmatrix} F_1 \\ F_2^{(1)} \\ F_3^{(2)} \\ \\ F_i^{(i-1)} \\ \\ F_n^{(n)} \end{Bmatrix}$$

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Gaussian Elimination

Backward Substitution

$$D_n = \frac{F_n}{K_{nn}}$$

$$D_i = \frac{F_i - \sum_{j=i+1}^{n} K_{ij} D_j}{K_{ii}} \qquad i = n-1, n-2, \ldots, 1$$

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```
// ===========================================================================
// ===========================================================================
// ============================ GAUSS ELIMINATION ============================
// ===========================================================================
// ===========================================================================
template <class T>
int GaussElimination (CMatrix<T>& A, CMatrix<T>& x,
                      const CMatrix<T>& b, T TOL)
// --------------------------------------------------------------------------
// Function: Solves A x = b
// Input:    A, x, and b
// Output:   A and x are modified. return value is zero if a solution exists
//           Otherwise the eqn. number is returned.
// --------------------------------------------------------------------------
{
    // solves A x = b
    int i, j, k, ii;
    double c;

    // number of equations to solve
    int n = A.GetRows();
    if (n != A.GetColumns() || n != x.GetRows() || n != b.GetRows() ||
        x.GetColumns() != b.GetColumns())
        return 1;

    // x initially contains b
    x = b;

    // forward elimination
    for (k=1; k <= n-1; k++)
    {
        for (i=k+1; i <= n; i++)
        {
            // singular matrix?
            if (fabs(A(k,k)) <= TOL)
            {
                return k;
            }
            c = A(i,k)/A(k,k);
            for (j=k+1; j <= n; j++)
            {
                A(i,j) -= c * A(k,j);
            }
            x(i,1) -= c * x(k,1);
        }
    }

    // back substitution
    x(n,1) /= A(n,n);

    for (ii=1; ii <= n-1; ii++)
    {
        i = n - ii;
        double sum = 0.0;
        for (j=i+1; j <= n; j++)
        {
            sum += A(i,j) * x(j,1);
        }
        x(i,1) = (x(i,1) - sum)/A(i,i);
    }

    return 0;
}
```


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Example

$$\begin{bmatrix} 8 & -1 \\ 4 & 7 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 18 \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \end{Bmatrix}$$

Multiply first equation by (-4/8) and add to second

$$\begin{bmatrix} 8 & -1 \\ 0 & 7.5 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 6 \\ 15 \end{Bmatrix} \Rightarrow \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \end{Bmatrix}$$

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Cholesky Factorization

Factorize K $\mathbf{K} = \mathbf{L}\hat{\mathbf{D}}\mathbf{L}^{T} \Rightarrow \mathbf{L}\hat{\mathbf{D}}\mathbf{L}^{T}\mathbf{D} = \mathbf{F}$

Solution Steps

Form $\mathbf{L}$ and $\hat{\mathbf{D}}$

Solve $\mathbf{LQ} = \mathbf{F}$ for $\mathbf{Q}$

Solve $\hat{\mathbf{D}}\mathbf{L}^{T}\mathbf{D} = \mathbf{Q}$ for $\mathbf{D}$

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Cholesky Factorization

$$\begin{bmatrix} K_{11} & K_{12} & . & K_{1n} \\ K_{12} & K_{22} & . & K_{2n} \\ . & . & . & . \\ K_{1n} & K_{2n} & . & K_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & . & 0 \\ L_{21} & 1 & . & 0 \\ . & . & . & . \\ L_{n1} & L_{n2} & . & 1 \end{bmatrix} \begin{bmatrix} \hat{D}_1 & 0 & . & 0 \\ 0 & \hat{D}_2 & . & 0 \\ . & . & . & . \\ 0 & 0 & . & \hat{D}_n \end{bmatrix} \begin{bmatrix} 1 & L_{21} & . & L_{n1} \\ 0 & 1 & . & L_{n2} \\ . & . & . & . \\ 0 & 0 & . & 1 \end{bmatrix}$$

$$= \left[\begin{array}{c|c|c|c|c} \hat{D}_1 & \hat{D}_1 L_{21} & \hat{D}_1 L_{31} & . & \hat{D}_1 L_{n1} \\ \hline & \hat{D}_2 L_{21}^2 & \hat{D}_1 L_{21} L_{31} + \hat{D}_2 L_{32} & . & \hat{D}_1 L_{21} L_{n1} + \hat{D}_2 L_{n2} \\ \hline & & \hat{D}_1 L_{31}^2 + \hat{D}_2 L_{32}^2 + \hat{D}_3 & . & \hat{D}_1 L_{31} L_{n1} + \hat{D}_2 L_{32} L_{n2} + \hat{D}_3 L_{n3} \\ \hline & & & . & . \\ \hline sym & & & & \hat{D}_1 L_{n1}^2 + \hat{D}_2 L_{n2}^2 + \ldots + \hat{D}_n \end{array}\right]$$

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Cholesky Factorization

$$\hat{\mathbf{D}}\mathbf{L}^{\mathbf{T}} = \begin{bmatrix} \hat{D}_1 & \hat{D}_1 L_{12} & . & \hat{D}_1 L_{1n} \\ & \hat{D}_2 & . & \hat{D}_2 L_{2n} \\ & & . & . \\ \mathbf{0} & & & \hat{D}_n \end{bmatrix}$$

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Example

$$\begin{bmatrix} 3.5120 & 0.7679 & 0 & 0 & 0 \\ 0.7679 & 3.1520 & 0 & -2 & 0 \\ 0 & 0 & 3.5120 & -0.7679 & 0.7679 \\ 0 & -2 & -0.7679 & 3.1520 & -1.1520 \\ 0 & 0 & 0.7679 & -1.1520 & 3.1520 \end{bmatrix} \begin{Bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ 0 \end{Bmatrix}$$

Solution: Factorization

1st Col

$$\hat{D}_1 = K_{11} = 3.5120$$

$$L_{21} = \frac{K_{21}}{\hat{D}_1} = \frac{0.7679}{3.5120} = 0.21865$$

$$L_{31} = L_{41} = L_{51} = 0$$

2nd Col

$$\hat{D}_2 = K_{22} - L_{21}^2 \hat{D}_1 = 2.9841$$

$$L_{32} = \frac{K_{32} - L_{31}\hat{D}_1 L_{21}}{\hat{D}_2} = 0$$

$$L_{42} = \frac{K_{42} - L_{41}\hat{D}_1 L_{21}}{\hat{D}_2} = -0.670219$$

$$L_{52} = 0$$

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Example

Forward Substitution: LQ=F

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.21865 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -0.670219 & -0.21865 & 1 & 0 \\ 0 & 0 & 0.21865 & -0.598724 & 1 \end{bmatrix} \begin{Bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ 0 \end{Bmatrix}$$

Solution

$$\mathbf{Q} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ -0.023949 \end{Bmatrix}$$

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Example

Backward Substitution: $\left(\hat{\mathbf{D}}\mathbf{L}^{\mathbf{T}}\mathbf{D} = \mathbf{Q}\right)$

$$\begin{bmatrix} 3.5120 & 0.21865 & 0 & 0 & 0 \\ 0 & 2.9841 & 0 & -0.670219 & 0 \\ 0 & 0 & 3.5120 & -0.21865 & 0.21865 \\ 0 & 0 & 0 & 1.64366 & -0.598724 \\ 0 & 0 & 0 & 0 & 2.3949 \end{bmatrix} \begin{Bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ -0.04 \\ -0.023949 \end{Bmatrix}$$

Solution

$$\begin{Bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{Bmatrix} = \begin{Bmatrix} 0.00444367 \\ -0.0203232 \\ -0.00444367 \\ -0.0303232 \\ -0.01 \end{Bmatrix}$$

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Algorithm

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Step 1: Cholesky Factorization. Loop through rows, $i = 1, \ldots, n$.

Step 2: Set $\hat{D}_i = K_{ii} - \sum_{j=1}^{i-1} L_{ij}^2 \hat{D}_j$. If $\hat{D}_i < \varepsilon$, stop. The matrix is not positive definite.

Step 3: For $j = i+1, \ldots, n$, set $L_{ji} = \dfrac{K_{ji} - \sum_{k=1}^{i-1} L_{jk} \hat{D}_k L_{ik}}{\hat{D}_i}$.

Step 4: End loop i. This ends the factorization phase.

Step 5: Forward Substitution. Set $Q_1 = F_1$.

Step 6: For $i = 2, \ldots, n$, set $Q_i = F_i - \sum_{j=1}^{i-1} L_{ij} Q_j$. This ends the Forward Substitution phase.

Step 7: Backward Substitution. Set $D_n = \dfrac{Q_n}{\hat{D}_n}$.

Step 8: For $i = n-1, \ldots, 1$, set $D_i = \dfrac{Q_i}{\hat{D}_i} - \sum_{j=i+1}^{n} L_{ij} D_j$. This ends the Backward Substitution phase.

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Storage Schemes for **K**

- Full matrix
- Banded matrix
- Skyline storage (requires additional vector)
- Sparse storage (requires additional vectors)

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Example

Upper triangular, banded matrix

Banded storage

$$\begin{bmatrix} K_{11} & & K_{13} & & \\ & K_{22} & K_{23} & & \\ & & K_{33} & K_{34} & K_{35} \\ & & & K_{44} & \\ Sym & & & & K_{55} \end{bmatrix} \Rightarrow \begin{bmatrix} K_{11} & 0 & K_{13} \\ K_{22} & K_{23} & 0 \\ K_{33} & K_{34} & K_{35} \\ K_{44} & 0 & 0 \\ K_{55} & 0 & 0 \end{bmatrix}$$

HBW=3

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Skyline Storage

$$\begin{bmatrix} K_{11} & & K_{13} & & \\ & K_{22} & K_{23} & & \\ & & K_{33} & K_{34} & K_{35} \\ & & & K_{44} & 0 \\ Sym & & & & K_{55} \end{bmatrix} \Rightarrow \left\{K_{11}, K_{22}, K_{33}, K_{23}, K_{13}, K_{44}, K_{34}, K_{55}, 0, K_{35}\right\}$$

$$\mathbf{D}_{loc} = \left\{1, 2, 3, 6, 8, 11\right\}$$

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Sparse Storage

Compressed Row Format

$$\begin{bmatrix} K_{11} & & K_{13} & & \\ & K_{22} & K_{23} & & \\ & & K_{33} & K_{34} & K_{35} \\ & & & K_{44} & \\ Sym & & & & K_{55} \end{bmatrix}$$

$$\mathbf{K}_{9\times1}^{sparse} = \left\{K_{11}, K_{13}, K_{22}, K_{23}, K_{33}, K_{34}, K_{35}, K_{44}, K_{55}\right\}$$

$$\mathbf{C}_{9\times1}^{sparse} = \{1,3,2,3,3,4,5,4,5\}$$

$$\mathbf{R}_{6\times1}^{sparse} = \{1,3,5,8,9,10\}$$

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Storage Scheme Comparison

Scheme	Integer Locations	Double Precision Locations
Full	0	25
Banded	0	15
Skyline	6	10
Sparse	9+6=15	9

The effects are even more dramatic when the problem size grows larger.

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Summary

- The most expensive (CPU time wise) step is the solution of the system equations. To obtain accurate solutions, double precision arithmetic is necessary.
- This is also the step that consumes the most (memory) resources. However, there are solutions available if one is willing to invest the time and effort.

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Summary

- Direct and iterative solvers have their strengths and weaknesses.
- Advancements in computer hardware and software makes it possible to develop and maintain powerful FE programs.
- It is necessary to understand these issues to be able to use commercial programs wisely.

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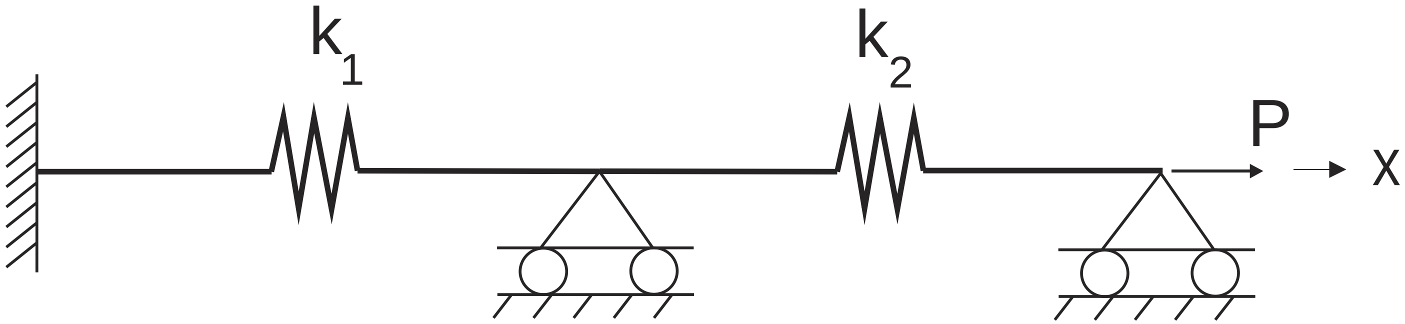
In-Class Exercise



Solve the system equations symbolically.

Case	k_1	k_2	P	Comments
1	10^6	1	1000	Use 4 significant digits
2	(1/6) 10^6	(1/6)	1000	Try single & double precision
3	1	10^6	1000	Try single & double precision

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Further Reading

- Search the web with the following keywords
  - Direct in-core and out-of-core solvers
  - Iterative solvers
  - Sparse and parallel equation solvers

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