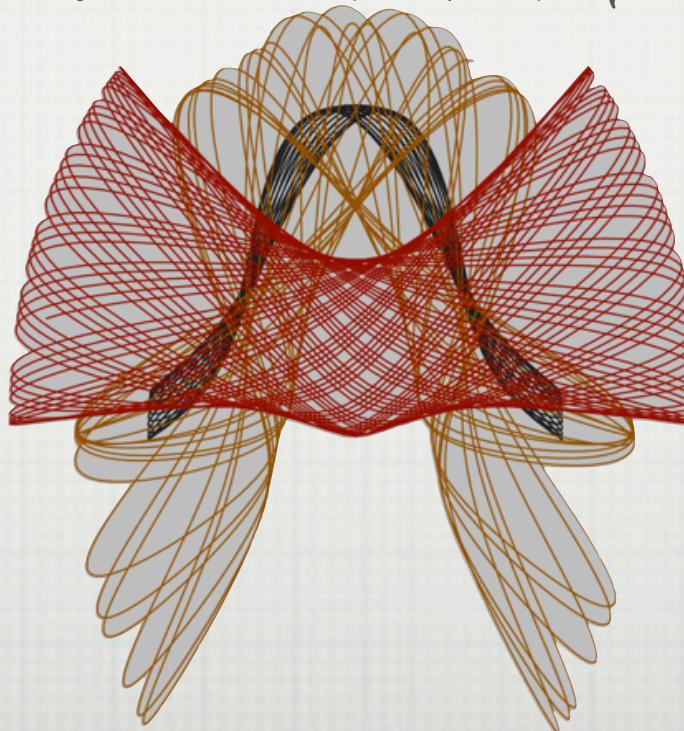


PHY-4810

COMPUTATIONAL PHYSICS

LECTURE 13: MATRIX ALGEBRA



BEFORE WE START...

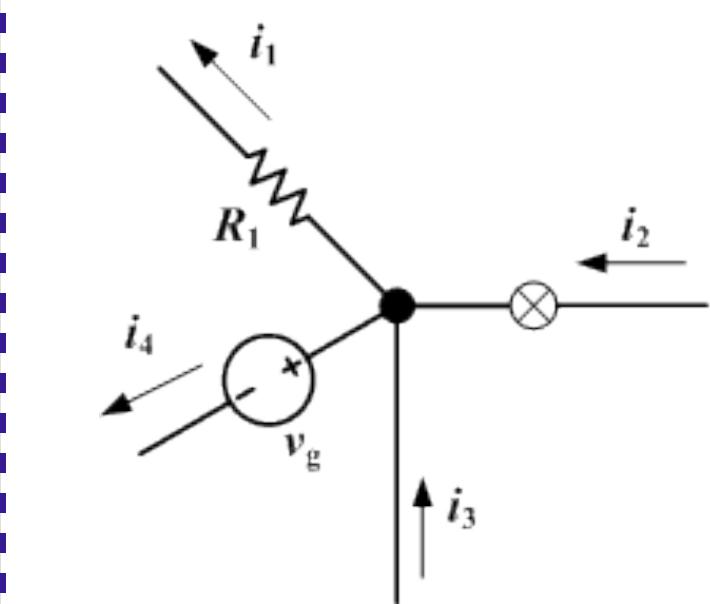
- This is not the easiest material covered so far...
 - I would say it is maybe the hardest...
- Lots of materials...
 - (hopefully) some new...
- Focus on “using” rather than “deriving”...
 - Main ideas behind the derivation will be provided though...
- Bear with me...

MOTIVATION: KIRCHHOFF'S LAWS



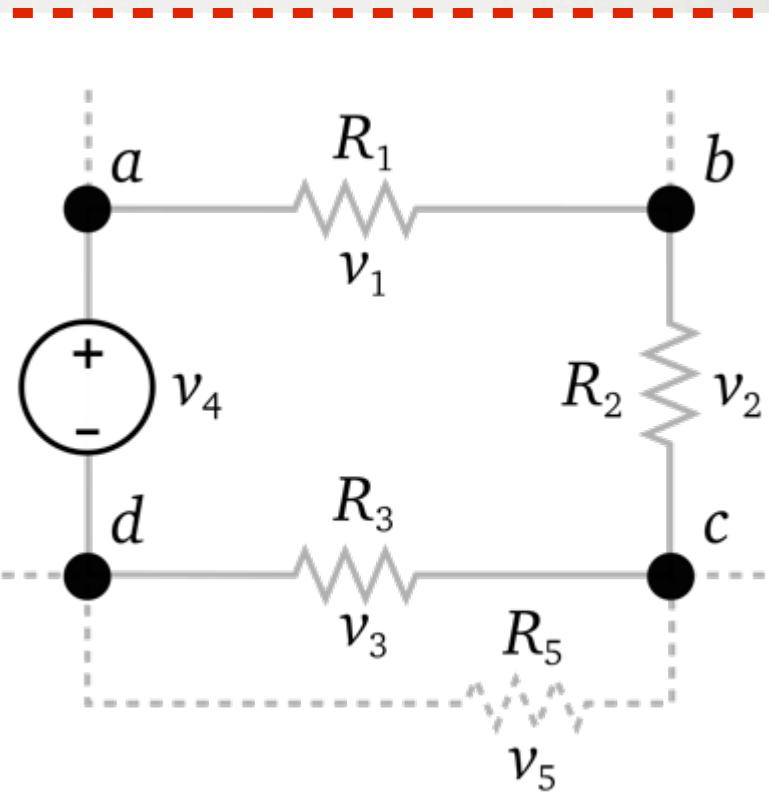
Gustav Robert Kirchhoff

CURRENT LAW



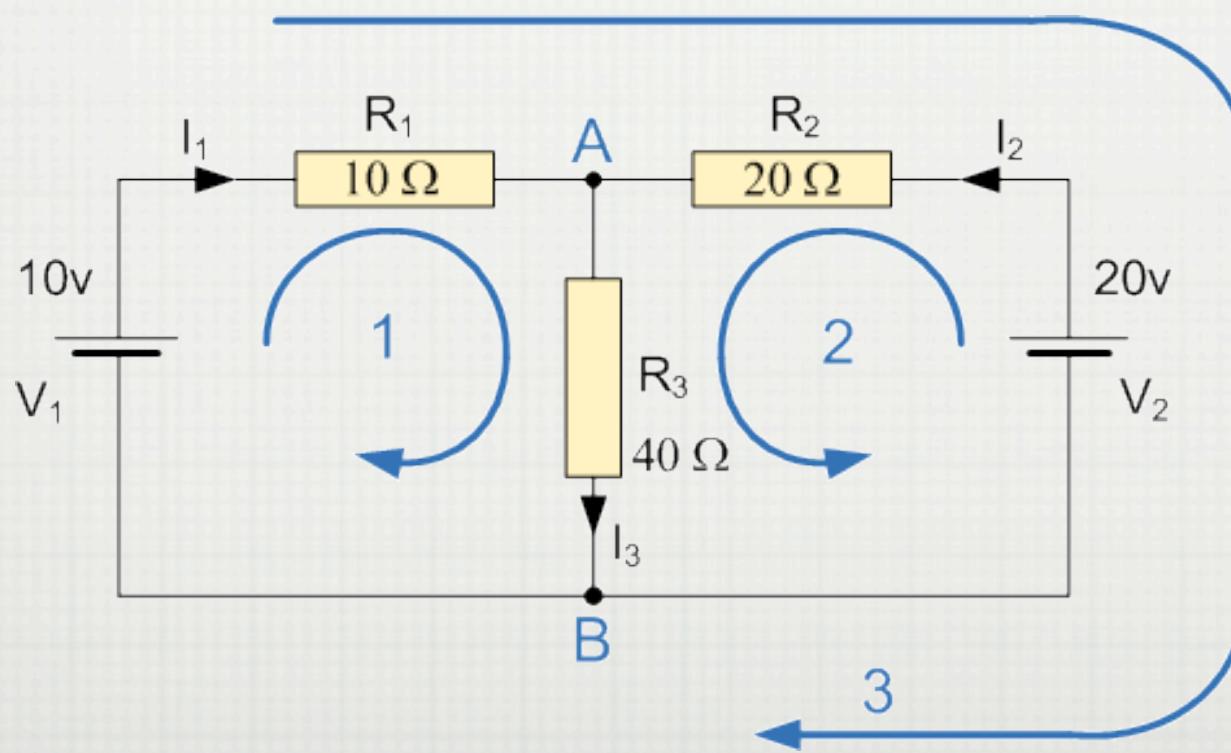
$$\sum_{k=1}^n I_k = 0$$

VOLTAGE LAW

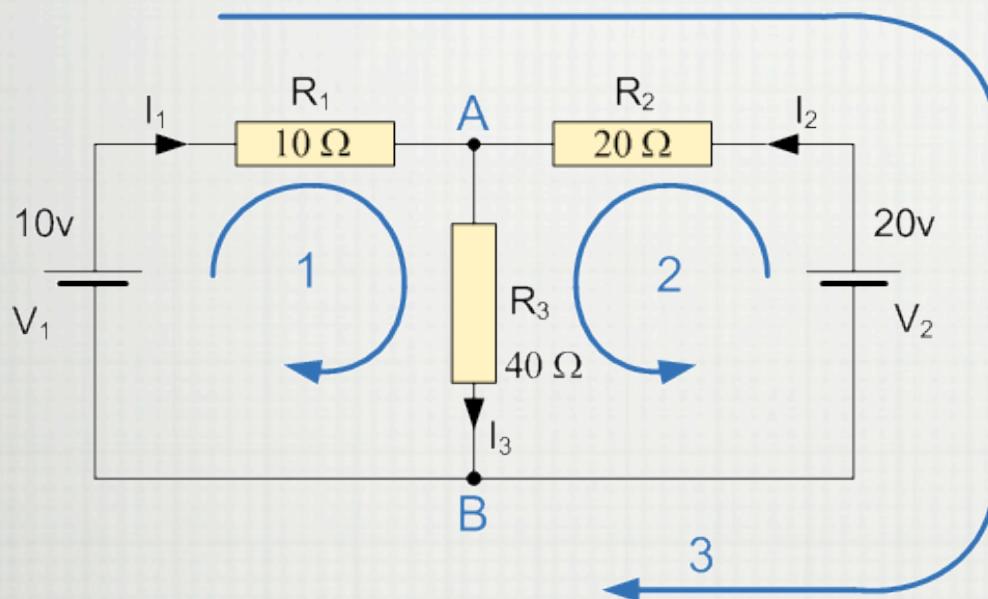


$$\sum_{k=1}^n V_k = 0$$

EXAMPLE



EXPLICITLY



* NODE A

$$I_1 + I_2 = I_3$$

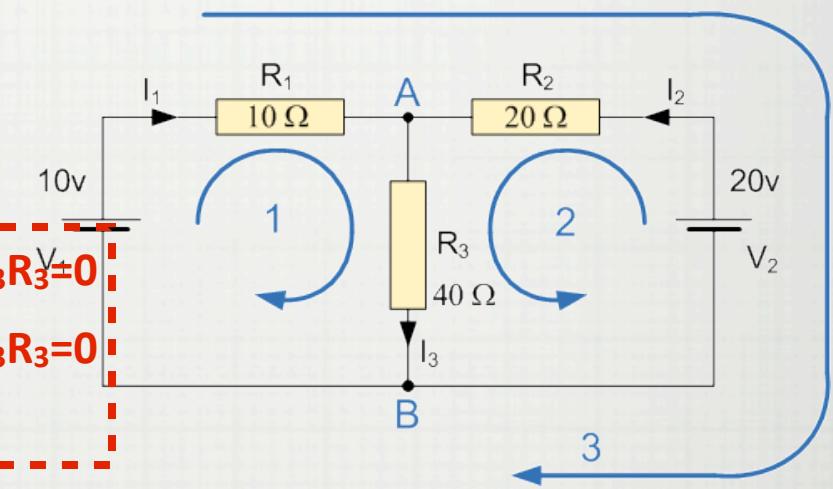
- Loop 1:
 - Drop at the battery: $+V_1$
 - Drop at R_1 : $-I_1 R_1$
 - Drop at R_3 : $-I_3 R_3$
 - $V_1 - I_1 R_1 - I_3 R_3 = 0$

- Loop 2:
 - Drop at the battery: $+V_2$
 - Drop at R_2 : $-I_2 R_2$
 - Drop at R_3 : $-I_3 R_3$
 - $V_2 - I_2 R_2 - I_3 R_3 = 0$

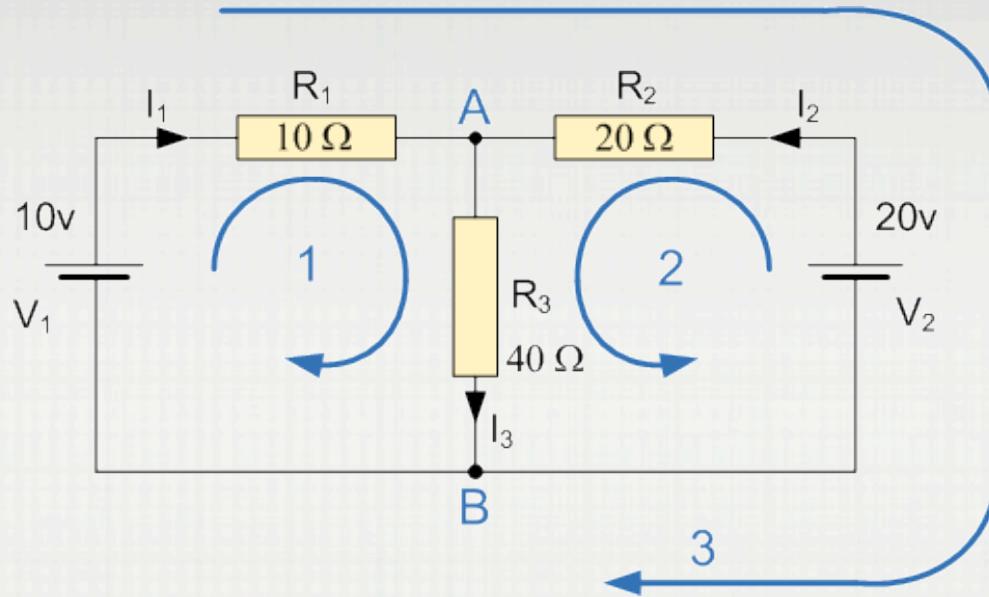
MATRIX FORM

$$\begin{pmatrix} R_1 & 0 & R_3 \\ 0 & R_2 & R_3 \\ 1 & 1 & -1 \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix}$$

• $V_1 - I_1 R_1 - I_3 R_3 = 0$
 • $V_2 - I_2 R_2 - I_3 R_3 = 0$
 • $I_1 + I_2 = I_3$



$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} R_1 & 0 & R_3 \\ 0 & R_2 & R_3 \\ 1 & 1 & -1 \end{pmatrix}^{-1} \begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix}$$

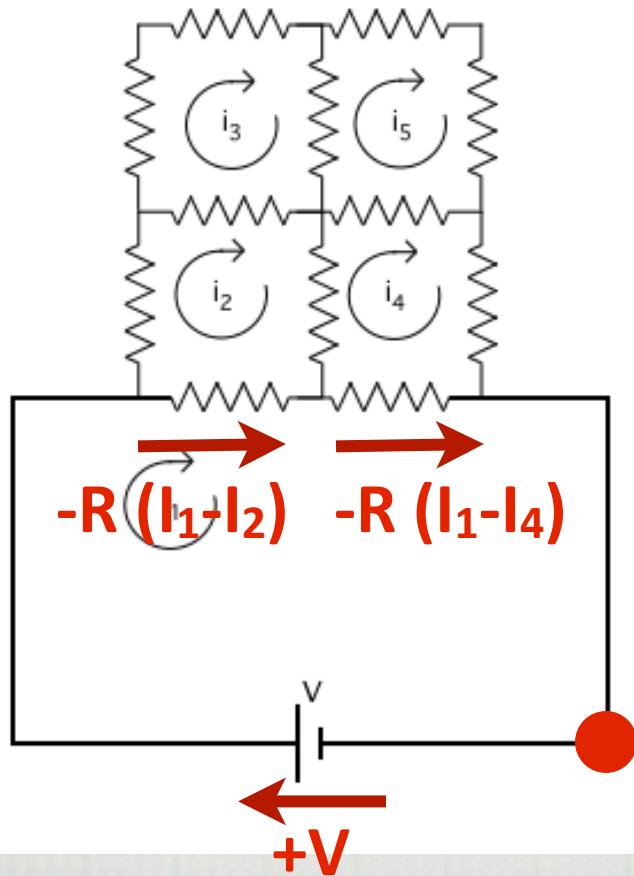


$$\begin{pmatrix} 1 & 0 & 4 \\ 0 & 2 & 4 \\ 1 & 1 & -1 \end{pmatrix}^{-1} = \frac{-1}{14} \begin{pmatrix} -6 & 4 & -8 \\ 4 & -5 & -4 \\ -2 & -1 & -2 \end{pmatrix} \quad \begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$$

SOLUTION:

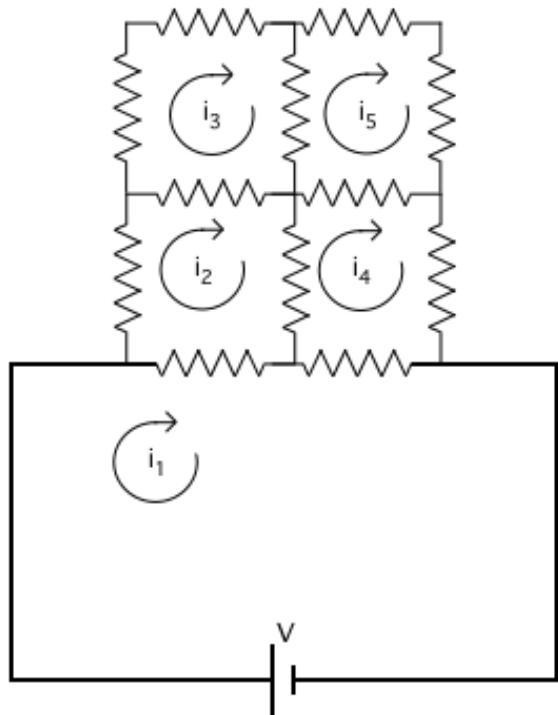
$$\boxed{\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} -1/7 \\ 3/7 \\ 2/7 \end{pmatrix}}$$

MORE COMPLICATED PROBLEMS



- Loop 1: $V - R(i_1 - i_2) - R(i_1 - i_4) = 0$
- Loop 2: $0 = R i_2 + R(i_2 - i_3) + R(i_2 - i_4) + R(i_2 - i_1)$
- Loop 3: $0 = 2 R i_3 + R(i_3 - i_5) + R(i_3 - i_2)$
- Loop 4: $0 = R i_4 + R(i_4 - i_1) + R(i_4 - i_2) + R(i_4 - i_5)$
- Loop 5: $0 = 2 R i_5 + R(i_5 - i_4) + R(i_5 - i_3)$

- Loop 1: $V = 2i_1 - i_2 - i_4$
- Loop 2: $0 = -i_1 + 4i_2 - i_3 - i_4$
- Loop 3: $0 = 4i_3 - i_5 - i_2$
- Loop 4: $0 = 4i_4 - i_1 - i_2 - i_5$
- Loop 5: $0 = 4i_5 - i_4 - i_3$



CURRENTS=

$$i_1 = 1.6$$

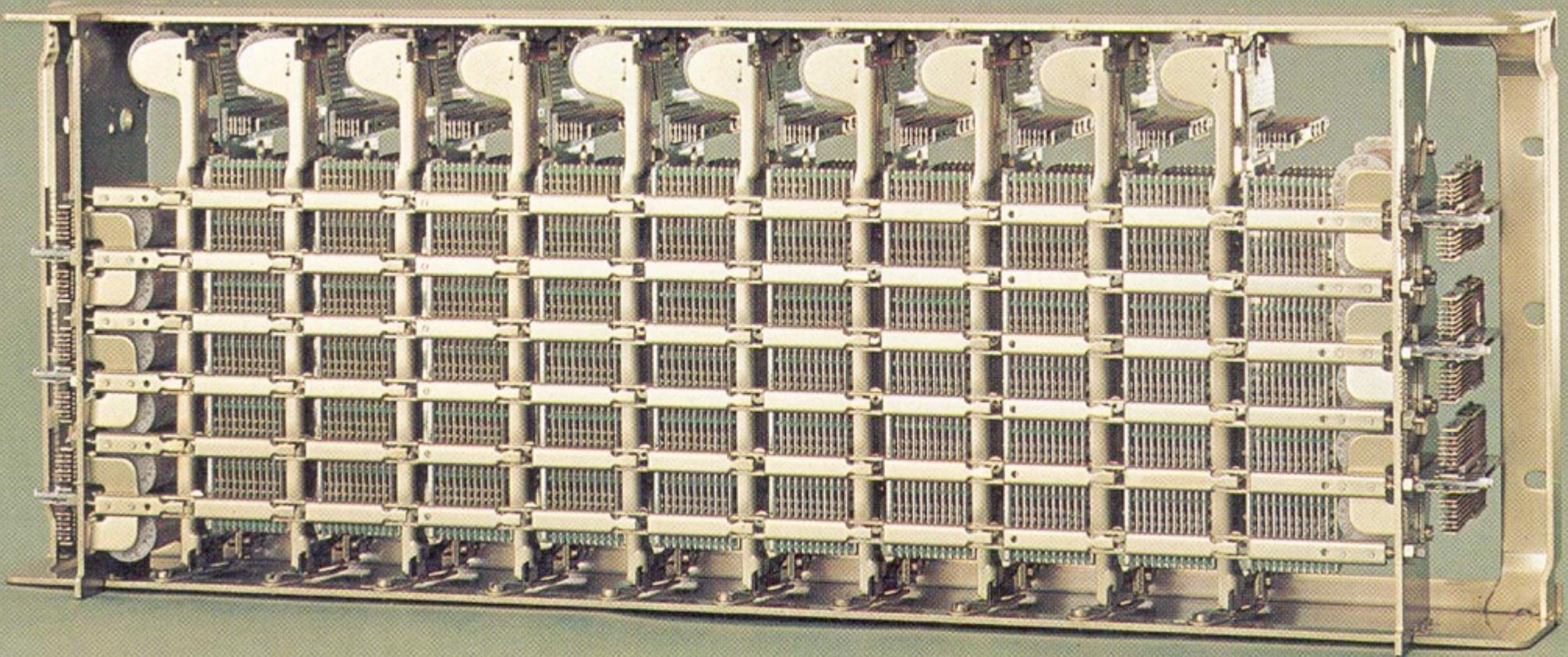
$$i_2 = 0.6$$

$$i_3 = 0.2$$

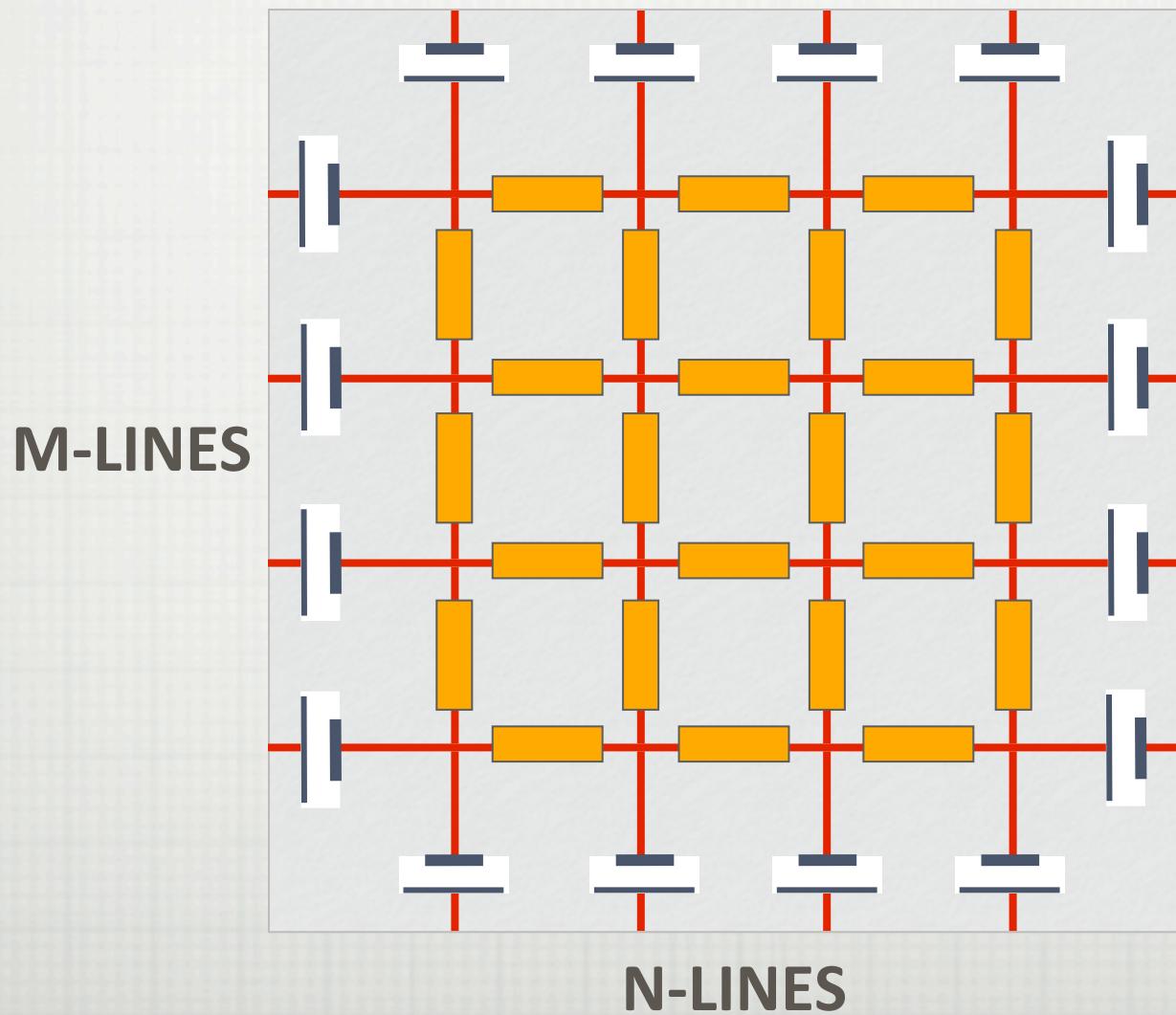
$$i_4 = 0.6$$

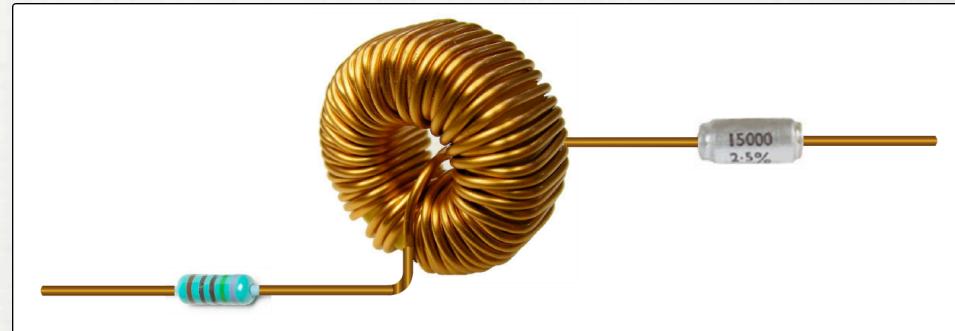
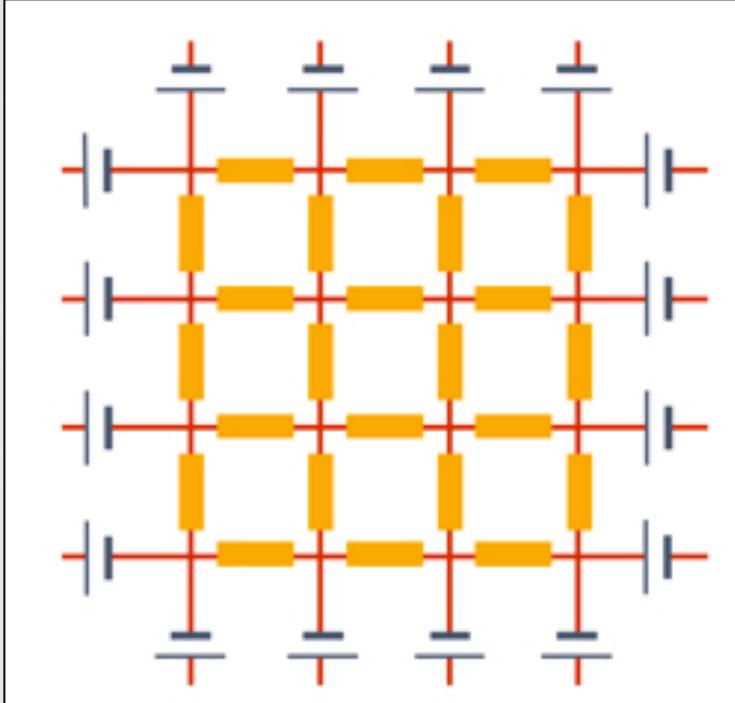
$$i_5 = 0.2$$

$$\begin{pmatrix} 2 & -1 & 0 & -1 & 0 \\ -1 & 4 & -1 & -1 & 0 \\ 0 & -1 & 4 & 0 & -1 \\ -1 & -1 & 0 & 4 & -1 \\ 0 & 0 & -1 & -1 & 4 \end{pmatrix} \begin{pmatrix} i_1 \\ i_2 \\ i_3 \\ i_4 \\ i_5 \end{pmatrix} = \begin{pmatrix} V \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$



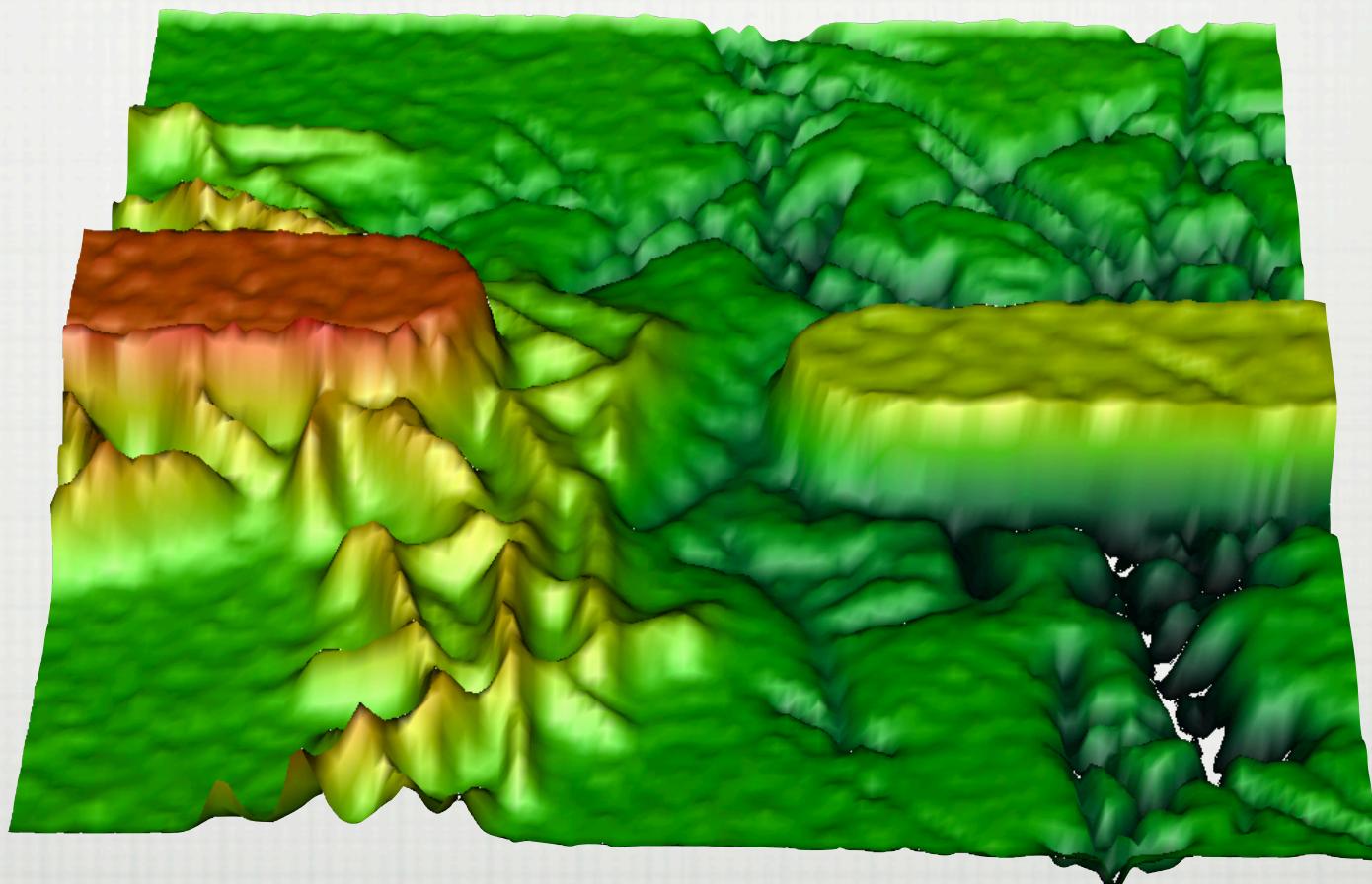
OUR OBJECTIVE





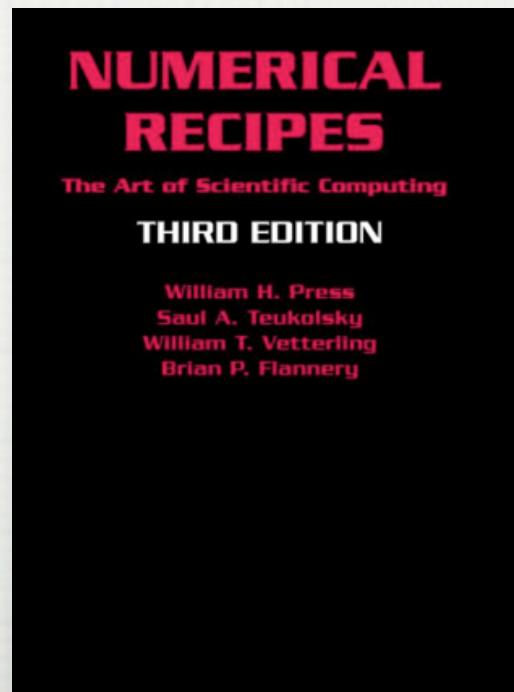
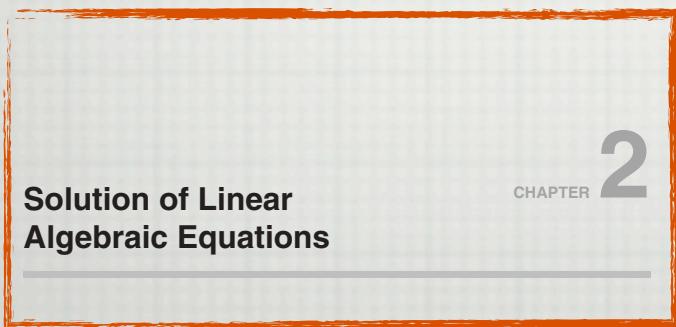
- ➡ can be any type of “impedance”, z
 - ➡ (explicitly dependent on V)
 - ➡ (capacitive)
 - ➡ (inductive)
 - ➡ (resistive)
 - ➡ ...
- ➡ number of resistors in excess of thousands!

EQUIVALENT CIRCUIT MODEL



MAIN REFERENCE FOR THIS LECTURE

- Numerical Recipes (chapter 2 is loaded on LMS)
- Chapter 2; Libraries used: gaussj; cholesky, LU, sparse (on LMS)



Course Content

- Landau/Paez/Bordeianu
Copy of textbook used in class. No distribution allowed!!!
- Subroutines Discussed in class
- Latex quick help
This includes a sample homework file
- Files for C++ refresher
- Numerical Recipes for HW5
- Slides 2013
- Calendar

$$Ax = b$$

$$x = A^{-1} b$$

TYPICAL FORM OF A SYSTEM OF LINEAR EQUATIONS

$$a_{00}x_0 + a_{01}x_1 + a_{02}x_2 + \cdots + a_{0,N-1}x_{N-1} = b_0$$

$$a_{10}x_0 + a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,N-1}x_{N-1} = b_1$$

$$a_{20}x_0 + a_{21}x_1 + a_{22}x_2 + \cdots + a_{2,N-1}x_{N-1} = b_2$$

...

...

$$a_{M-1,0}x_0 + a_{M-1,1}x_1 + \cdots + a_{M-1,N-1}x_{N-1} = b_{M-1}$$

MATRIX NOTATION

$$\boxed{\mathbf{A} = \begin{bmatrix} a_{00} & a_{01} & \dots & a_{0,N-1} \\ a_{10} & a_{11} & \dots & a_{1,N-1} \\ \dots & & & \\ a_{M-1,0} & a_{M-1,1} & \dots & a_{M-1,N-1} \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_0 \\ b_1 \\ \dots \\ b_{M-1} \end{bmatrix}}$$

$$\boxed{\mathbf{A} \cdot \mathbf{x} = \mathbf{b}}$$

SINGULAR VERSUS NON-SINGULAR

- **Singular system: (determinant=0)**
 - “Row degeneracy” (i.e. one row is a linear combination of other rows)
 - equivalent to an “Under-determined system”
- Numerically:
 - Rows could be degenerate within roundoff-error!
 - Accumulated roundoff errors during solution yield singular system, especially if N is large
- Algorithms seek to
 - Avoid accumulating round-off errors
 - Accelerate calculations by taking advantage of form of matrix
 - Accelerate calculations by taking advantage of theorems of linear algebra
- Good news: it is easy to check solution!

SIZE ROUTINELY SOLVABLE

- Dense matrices: a few thousands
- Sparse matrices: a few millions
- Sometime much care has to be taken,
especially for close-to singular problems
(i.e. singular value decomposition)

MAIN ISSUES, IN A NUTSHELL

- Accuracy
- Speed
- Memory Requirement

BY-PRODUCTS OF SOLVING $Ax=B$

- Matrix inverse**
- Determinant**
- Underdetermined systems (fewer equations than unknowns)**
 - > singular value decomposition
- Overdetermined systems (more equations than unknowns)**
 - > linear least-square problem

THERE ARE MANY TOPICS OUT THERE...

- But we can't investigate them all in one lecture**
- My goal is to convince you that depending on the problem you need to carefully choose your linear solver.**
- A clever choice can yield ORDERS of magnitude in improvements (accuracy, time, or most importantly memory consumption)**

EXAMPLE OF SOFTWARE: LAPACK

		SINGLE PRECISION		DOUBLE PRECISION	
TYPE	DESCRIPTION	REAL	COMPLEX	REAL	COMPLEX
General	Solves a general system of linear equations $AX=B$.	SGESV	CGESV	DGESV	ZGESV
	Solves a general system of linear equations $AX=B$ with iterative refinement.	-	-	DSGESV	ZCGESV
	Computes an LU factorization of a general matrix, using partial pivoting with row interchanges.	SGETRF	CGETRF	DGETRF	ZGETRF
	Computes the inverse of a general matrix, using the LU factorization.	SGETRI	CGETRI	DGETRI	ZGETRI
	Solves a general system of linear equations $AX=B$, $A^T X=B$, or $A^H X=B$, using the LU factorization.	SGETRS	CGETRS	DGETRS	ZGETRS
Positive Definite	Solves a symmetric positive definite system of linear equations $AX=B$.	SPOSV	CPOSV	DPOSV	ZPOSV
	Computes the Cholesky factorization of a symmetric positive definite matrix.	SPOTRF	CPOTRF	DPOTRF	ZPOTRF
	Solves a symmetric positive definite system of linear equations $AX=B$, using the Cholesky factorization.	SPOTRS	CPOTRS	DPOTRS	ZPOTRS
Triangular	Solves a triangular system of linear equations $AX=B$, $A^T X=B$, or $A^H X=B$.	STRTRS	CTRTRS	DTRTRS	ZTRTRS
	Computes the inverse of a triangular matrix.	STRTRI	CTRTRI	DTRTRI	ZTRTRI
General Banded	Computes an LU factorization of a real m-by-n band matrix A using partial pivoting with row interchanges.	SGBTRF	CGBTRF	DGBTRF	ZGBTRF
Positive Definite Banded	Computes the Cholesky factorization of a real symmetric positive definite band matrix A.	SPBTRF	CPBTRF	DPBTRF	ZPBTRF

LAPACK: SVD

		SINGLE PRECISION		DOUBLE PRECISION	
TYPE	DESCRIPTION	REAL	COMPLEX	REAL	COMPLEX
General	Computes the singular value decomposition (SVD) of a general rectangular matrix.	SGESVD	CGESVD	DGESVD	ZGESVD
	Reduces a general rectangular matrix to real bidiagonal form by an orthogonal transformation.	SGEBRD	CGEBRD	DGEBRD	ZGEBRD
	Generates the orthogonal transformation matrices from a reduction to bidiagonal form.	SORGBR	CUNGBR	DORGBR	ZORGBR
Bidiagonal	Computes the singular value decomposition (SVD) of a real bidiagonal matrix, using the bidiagonal QR algorithm.	SBDSQR	CBDSQR	DBDSQR	ZBDSQR

SURVEY OF NUMERICAL TECHNIQUES

- Gauss-Jordan Elimination**
- LU decomposition**
- Tridiagonal and band-diagonal systems**
- Iterative Improvement of a solution to linear equations**
- Singular Value Decomposition**
- Sparse Linear Systems**
- Cholesky Decomposition**
- QR Decomposition**

SURVEY OF NUMERICAL TECHNIQUES

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- Singular Value Decomposition**
- Sparse Linear Systems**
- Cholesky Decomposition**
- QR Decomposition**

GAUSS-JORDAN ELIMINATION

- Use same technique as the one you see when you calculate A^{-1} manually
- Up to 3-5 times slower than “more clever” methods (unless you need A^{-1} explicitly)
- Solid method
- Uses pivoting
 - idea #1 : changing row order of A (and corresponding b) does not change the problem
 - idea #2: replacing a row of A by a combination of other row and itself (and corresponding b) does not change the problem
 - idea #3: changing two columns of A (and corresponding order of x) does not change the problem
- see gaussj.h for C++ implementation from Numerical Recipes

PIVOTING

- No pivoting: only operation 2 is used**
- Pivoting means we change order of rows and columns**
- In fact no pivoting means ... roundoff errors will yield unstable algorithm**
- Note that you can have partial and full pivoting**

GJ: REFERENCE CARD (gausj.h)

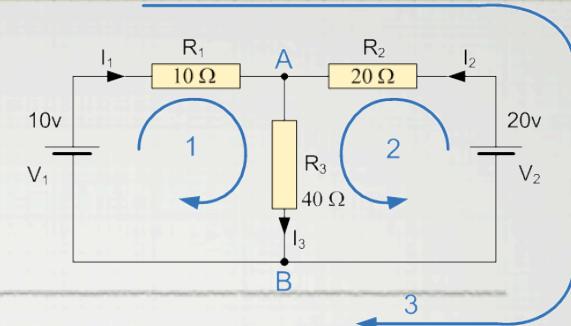
```
void gaussj(MatDoub_IO &a, MatDoub_IO &b)
```

Linear equation solution by Gauss-Jordan elimination, equation (2.1.1) above. The input matrix is $a[0..n-1][0..n-1]$. $b[0..n-1][0..m-1]$ is input containing the m right-hand side vectors. On output, a is replaced by its matrix inverse, and b is replaced by the corresponding set of solution vectors.

Usage:

- MatDoub_IO A(10,10);**
- MatDoub_IO b(10,1);**
- gaussj(a,b);**
- solution is now in b, A^{-1} is in A**

EXAMPLE



```
#include <iostream>
#include <fstream>
#include <cmath>
#include "nr3.h"
#include "gaussj.h"
using namespace std;
int main() {
    int size=3;
    MatDoub_I0 A(size,size);
    MatDoub_I0 b(size,1);

    //Define LHS
    //first row
    A[0][0]=1;
    A[0][1]=0;
    A[0][2]=4;

    //second row
    A[1][0]=0;
    A[1][1]=2;
    A[1][2]=4;

    //third row
    A[2][0]=1;
    A[2][1]=1;
    A[2][2]=-1;

    //Define RHS
    b[0][0]=1;
    b[1][0]=2;
    b[2][0]=0;

    //perform Gauss-Jordan
    gaussj(A,b);

    cout << "Solution is: \n";
    for (int i=0;i<3;i++){
        cout << i << ":" << b[i][0] << endl;
    }
    cout<<"Finished"<<endl;
}
```

$$\begin{pmatrix} 1 & 0 & 4 \\ 0 & 2 & 4 \\ 1 & 1 & -1 \end{pmatrix}^{-1} = \frac{-1}{14} \begin{pmatrix} -6 & 4 & -8 \\ 4 & -5 & -4 \\ -2 & -1 & -2 \end{pmatrix}$$

bash-3.2\$./a.out

Solution is:

0: -0.142857

1: 0.428571

2: 0.285714

Finished

$$\begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$$

$$\boxed{\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix}} = \boxed{\begin{pmatrix} -1/7 \\ 3/7 \\ 2/7 \end{pmatrix}}$$

LU DECOMPOSITION

- We try to decompose A as :

$$\boxed{L \cdot U = A}$$

- With:

$$\begin{bmatrix} \alpha_{00} & 0 & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & \alpha_{33} \end{bmatrix} \cdot \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

ADVANTAGE OF LU DECOMPOSITION?

$$\mathbf{A} \cdot \mathbf{x} = (\mathbf{L} \cdot \mathbf{U}) \cdot \mathbf{x} = \mathbf{L} \cdot (\mathbf{U} \cdot \mathbf{x}) = \mathbf{b}$$

We have now two problems to solve:

1. finding \mathbf{y} such that:

$$\mathbf{L} \cdot \mathbf{y} = \mathbf{b} \quad \text{Simple Forward substitution!}$$

2. finding \mathbf{x} such that:

$$\mathbf{U} \cdot \mathbf{x} = \mathbf{y} \quad \text{Simple Backward substitution!}$$

LU: WHAT'S THE ADVANTAGE?

- We end up with two trivial problems!
- (1) y can be found by forward substitution

$$y_0 = \frac{b_0}{\alpha_{00}}$$

$$y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j \right] \quad i = 1, 2, \dots, N-1$$

- (2) x can be found by backward substitution

$$x_{N-1} = \frac{y_{N-1}}{\beta_{N-1,N-1}}$$

$$x_i = \frac{1}{\beta_{ii}} \left[y_i - \sum_{j=i+1}^{N-1} \beta_{ij} x_j \right] \quad i = N-2, N-3, \dots, 0$$

LU DECOMPOSITION

$$i < j : \quad \alpha_{i0}\beta_{0j} + \alpha_{i1}\beta_{1j} + \cdots + \alpha_{ii}\beta_{ij} = a_{ij}$$

$$i = j : \quad \alpha_{i0}\beta_{0j} + \alpha_{i1}\beta_{1j} + \cdots + \alpha_{ii}\beta_{jj} = a_{ij}$$

$$i > j : \quad \alpha_{i0}\beta_{0j} + \alpha_{i1}\beta_{1j} + \cdots + \alpha_{ij}\beta_{jj} = a_{ij}$$

- Set $\alpha_{ii} = 1, i = 0, \dots, N - 1$ (equation 2.3.11).
- For each $j = 0, 1, 2, \dots, N - 1$ do these two procedures: First, for $i = 0, 1, \dots, j$, use (2.3.8), (2.3.9), and (2.3.11) to solve for β_{ij} , namely

$$\beta_{ij} = a_{ij} - \sum_{k=0}^{i-1} \alpha_{ik}\beta_{kj} \quad (2.3.12)$$

(When $i = 0$ in 2.3.12 the summation term is taken to mean zero.) Second, for $i = j + 1, j + 2, \dots, N - 1$ use (2.3.10) to solve for α_{ij} , namely

$$\alpha_{ij} = \frac{1}{\beta_{jj}} \left(a_{ij} - \sum_{k=0}^{j-1} \alpha_{ik}\beta_{kj} \right) \quad (2.3.13)$$

Be sure to do both procedures before going on to the next j .

**Crout's algorithm.....
beyond the scope of this course**

LU: REFERENCE CARD (LUDCMP.H)

```
struct LUDcmp
Object for solving linear equations  $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$  using LU decomposition, and related functions.
{
    Int n;
    MatDoub lu;
    VecInt indx;
    Doub d;
    LUDcmp(MatDoub_I &a);
    void solve(VecDoub_I &b, VecDoub_O &x);
    void solve(MatDoub_I &b, MatDoub_O &x);
    void inverse(MatDoub_O &ainv);
    Doub det();
    void mprove(VecDoub_I &b, VecDoub_IO &x);
    MatDoub_I &aref;
};
```

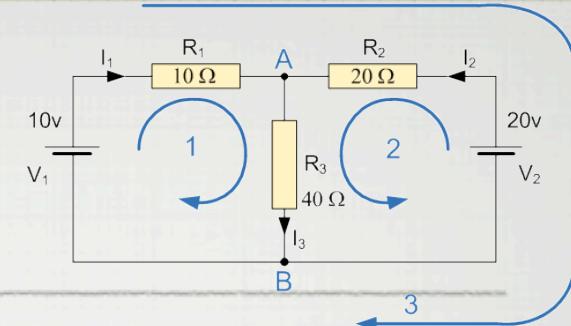
Stores the decomposition.
Stores the permutation.
Used by `det`.
Constructor. Argument is the matrix \mathbf{A} .
Solve for a single right-hand side.
Solve for multiple right-hand sides.
Calculate matrix inverse \mathbf{A}^{-1} .
Return determinant of \mathbf{A} .
Discussed in §2.5.
Used only by `mprove`.

LU: IN PRACTICE

```
const Int n = ...  
MatDoub a(n,n);  
VecDoub b(n),x(n);  
...  
LUDcmp alu(a);  
alu.solve(b,x);
```

- can also compute inverse, and determinant
- if $GJ \sim N^3$; $LU \sim N^3/3$

EXAMPLE



```
#include <iostream>
#include <fstream>
#include <cmath>
#include "nr3.h"
#include "ludcmp.h"

using namespace std;

int main() {
    int size=3;

    MatDoub_IO A(size,size);
    VecDoub b(size), x(size);
    //Define LHS
    //first row
    A[0][0]=1;
    A[0][1]=0;
    A[0][2]=4;

    //second row
    A[1][0]=0;
    A[1][1]=2;
    A[1][2]=4;

    //third row
    A[2][0]=1;
    A[2][1]=1;
    A[2][2]=-1;

    //Define RHS
    b[0]=1;
    b[1]=2;
    b[2]=0;

    //perform LU Decomposition
    LUdcmp alu(A);

    //solve problem
    alu.solve(b,x);

    cout << "LU Solution is: \n";
    for (int i=0;i<3;i++){
        cout << i << ":" << x[i] << endl;
    }
    cout<<"Finished"<<endl;
    return 0;
}
```

$$\begin{pmatrix} 1 & 0 & 4 \\ 0 & 2 & 4 \\ 1 & 1 & -1 \end{pmatrix}^{-1} = \frac{-1}{14} \begin{pmatrix} -6 & 4 & -8 \\ 4 & -5 & -4 \\ -2 & -1 & -2 \end{pmatrix}$$

bash-3.2\$./a.out

LU Solution is:

0: -0.142857

1: 0.428571

2: 0.285714

Finished

$$\begin{pmatrix} V_1 \\ V_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$$

$$\boxed{\begin{pmatrix} I_1 \\ I_2 \\ I_3 \end{pmatrix}} = \boxed{\begin{pmatrix} -1/7 \\ 3/7 \\ 2/7 \end{pmatrix}}$$

CHOLESKY DECOMPOSITION

- If a square matrix A happens to be symmetric and positive-definite, then it has a special, more efficient, triangular decomposition.
- Instead of seeking arbitrary lower and upper triangular factors L and U , Cholesky de- composition constructs a lower triangular matrix L whose transpose L^T can itself serve as the upper triangular part. In other words we have

$$L \cdot L^T = A$$

- This factorization is sometimes referred to as “taking the square root” of the matrix A , though, because of the transpose, it is not literally that. The components of L^T are of course related to those of L by

$$L_{ij}^T = L_{ji}$$

- ❖ SPEEDUP: A FACTOR OF 2 COMPARED TO LU DECOMPOSITION

$$L_{ii} = \left(a_{ii} - \sum_{k=0}^{i-1} L_{ik}^2 \right)^{1/2}$$

$$L_{ji} = \frac{1}{L_{ii}} \left(a_{ij} - \sum_{k=0}^{i-1} L_{ik} L_{jk} \right) \quad j = i + 1, i + 2, \dots, N - 1$$

REFERENCE CARD: CHOLESKY.H

```
struct Cholesky{
```

Object for Cholesky decomposition of a matrix \mathbf{A} , and related functions.

```
Int n;
```

```
MatDoub el;
```

Stores the decomposition.

```
Cholesky(MatDoub_I &a) : n(a.nrows()), el(a) {
```

Constructor. Given a positive-definite symmetric matrix $a[0..n-1][0..n-1]$, construct and store its Cholesky decomposition, $\mathbf{A} = \mathbf{L} \cdot \mathbf{L}^T$.

Example:

```
#include "cholesky.h";

MatDoub lap(4,4); //declaration
VECDOUNB B[4], X[4];

Cholesky Laplace (lap); //class constructor with lap
Laplace.solve(b,x); //compute inverse
```

TRIDIAGONAL AND BAND DIAGONAL

$$\begin{bmatrix} b_0 & c_0 & 0 & \cdots \\ a_1 & b_1 & c_1 & \cdots \\ & \cdots & & \\ \cdots & a_{N-2} & b_{N-2} & c_{N-2} \\ \cdots & 0 & a_{N-1} & b_{N-1} \end{bmatrix} \cdot \begin{bmatrix} u_0 \\ u_1 \\ \cdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} r_0 \\ r_1 \\ \cdots \\ r_{N-2} \\ r_{N-1} \end{bmatrix}$$

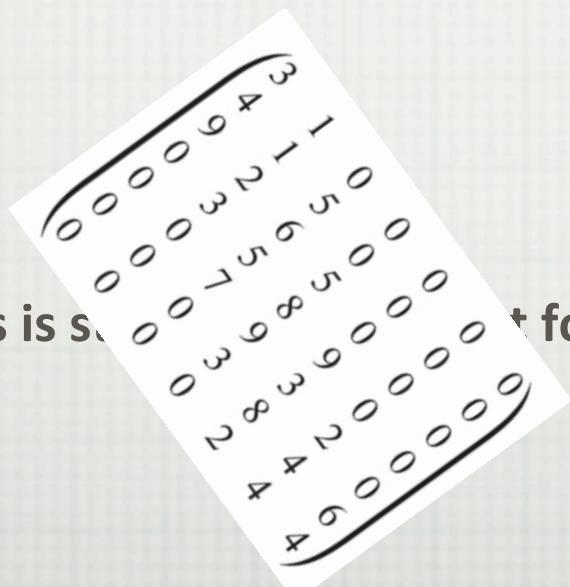
- only store vectors a, b, c, r!

```
void tridag(VecDoub_I &a, VecDoub_I &b, VecDoub_I &c, VecDoub_I &r, VecDoub_O &u)
Solves for a vector u[0..n-1] the tridiagonal linear set given by equation (2.4.1). a[0..n-1],
b[0..n-1], c[0..n-1], and r[0..n-1] are input vectors and are not modified.
```

BAND-DIAGONAL

$$\begin{pmatrix} 3 & 1 & 0 & 0 & 0 & 0 & 0 \\ 4 & 1 & 5 & 0 & 0 & 0 & 0 \\ 9 & 2 & 6 & 5 & 0 & 0 & 0 \\ 0 & 3 & 5 & 8 & 9 & 0 & 0 \\ 0 & 0 & 7 & 9 & 3 & 2 & 0 \\ 0 & 0 & 0 & 3 & 8 & 4 & 6 \\ 0 & 0 & 0 & 0 & 2 & 4 & 4 \end{pmatrix}$$

This is sometimes called band form



$$\begin{pmatrix} x & x & 3 & 1 \\ x & 4 & 1 & 5 \\ 9 & 2 & 6 & 5 \\ 3 & 5 & 8 & 9 \\ 7 & 9 & 3 & 2 \\ 3 & 8 & 4 & 6 \\ 2 & 4 & 4 & x \end{pmatrix}$$

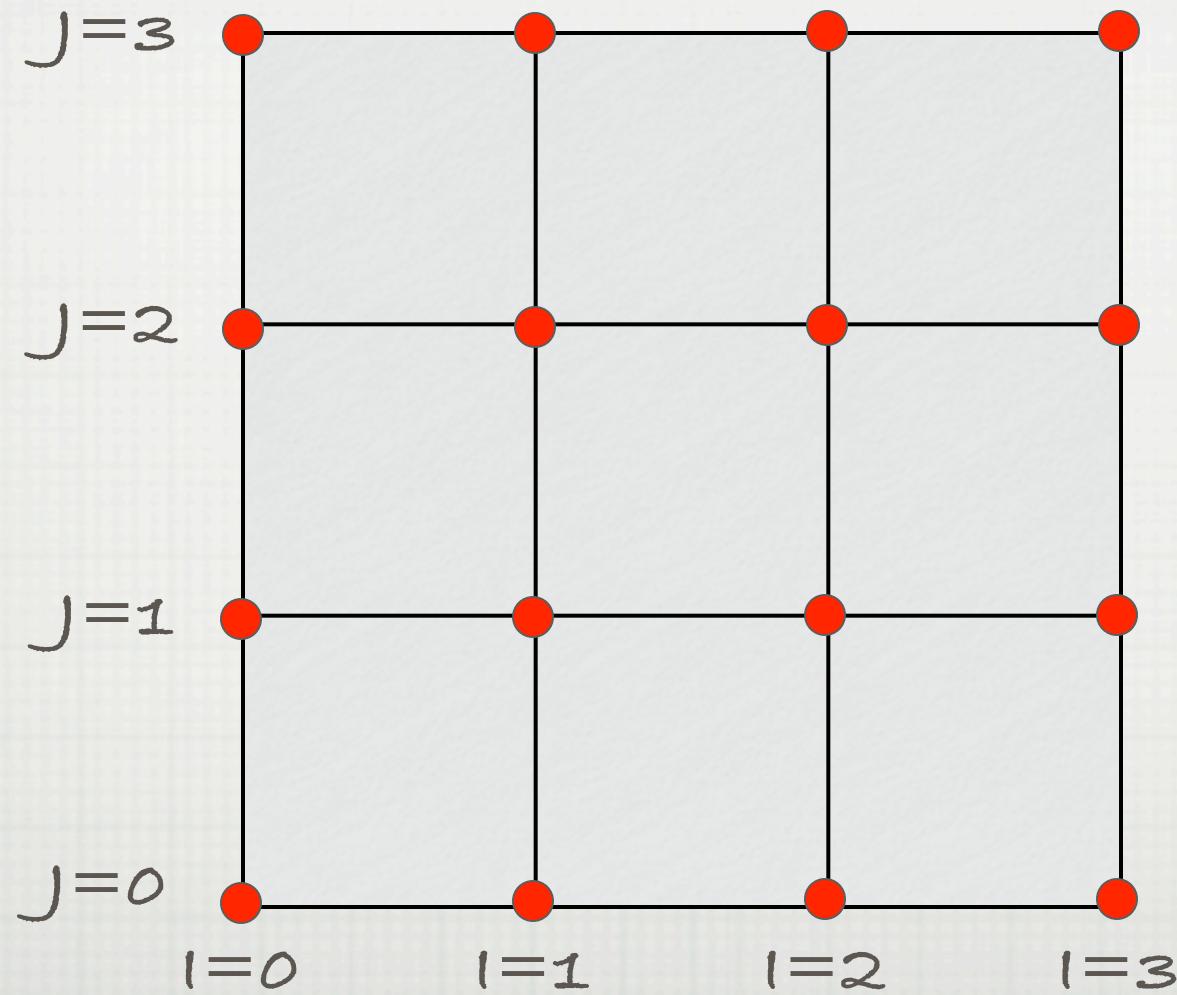
EXPLICIT EXAMPLE: BACK TO LAPLACE

LAPLACE REVISITED (LECTURE 10)

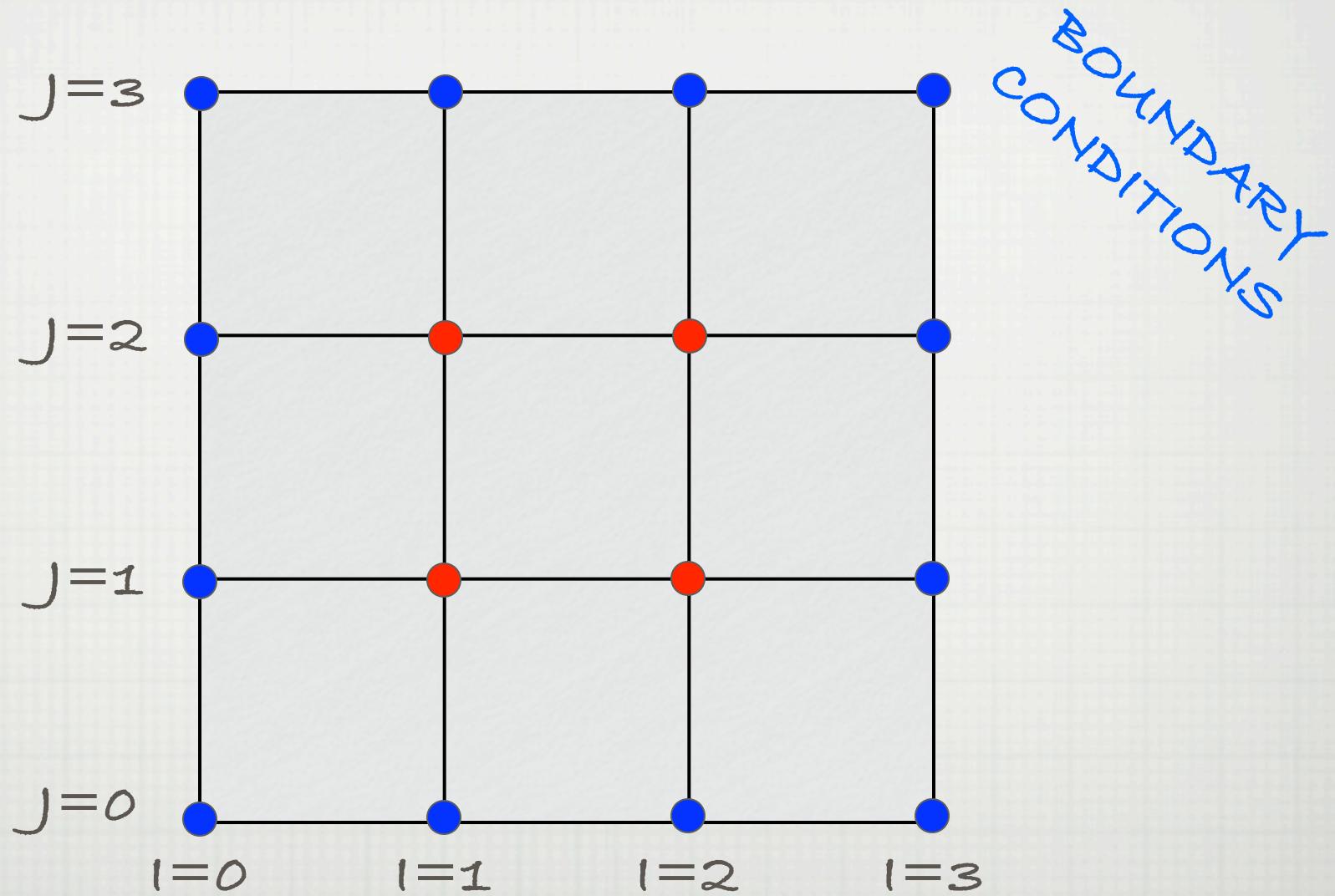
$$\frac{\partial^2 U(x, y)}{\partial x^2} + \frac{\partial^2 U(x, y)}{\partial y^2} = \begin{cases} 0 & \text{Laplace's equation} \\ -4\pi\rho(\mathbf{x}) & \text{Poisson's equation} \end{cases}$$

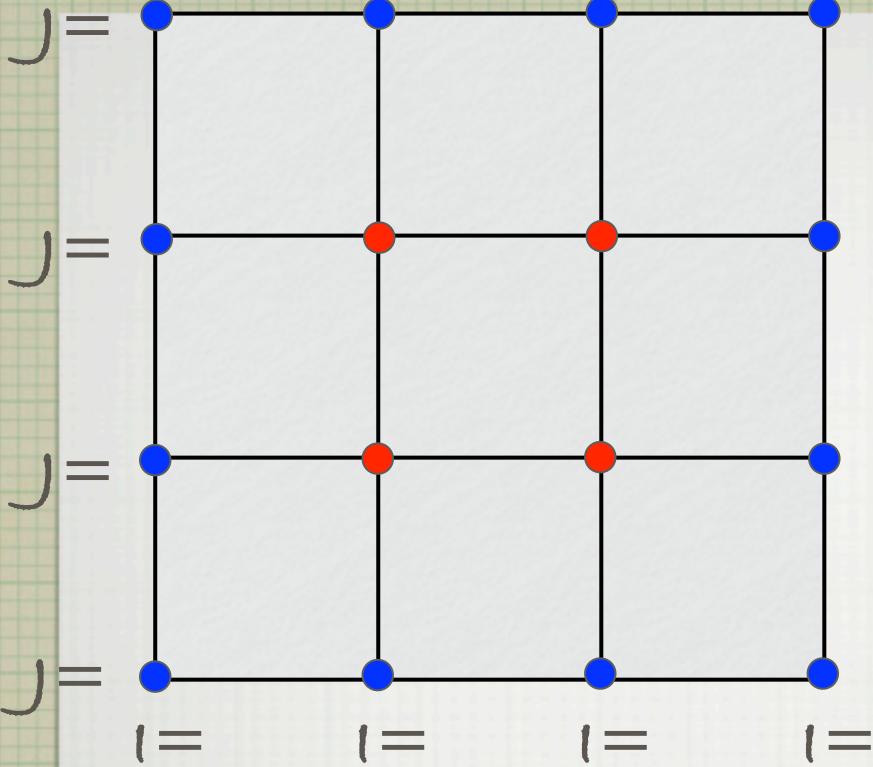
$$U_{i,j} = \frac{1}{4} [U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}] + \pi\rho(i\Delta, j\Delta)\Delta^2$$

$$U_{i,j} = \frac{1}{4} [U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}] + \pi\rho(i\Delta, j\Delta)\Delta^2$$



$$U_{i,j} = \frac{1}{4} [U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}] + \pi\rho(i\Delta, j\Delta)\Delta^2$$





$$U_{i,j} = \frac{1}{4} [U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}]$$

$$\begin{aligned}
 U_{11} &= 1/4(U_{10} + U_{12} + U_{01} + U_{21}) \\
 U_{21} &= 1/4(U_{20} + U_{22} + U_{31} + U_{11}) \\
 U_{12} &= 1/4(U_{11} + U_{13} + U_{02} + U_{22}) \\
 U_{22} &= 1/4(U_{21} + U_{23} + U_{12} + U_{32})
 \end{aligned}$$

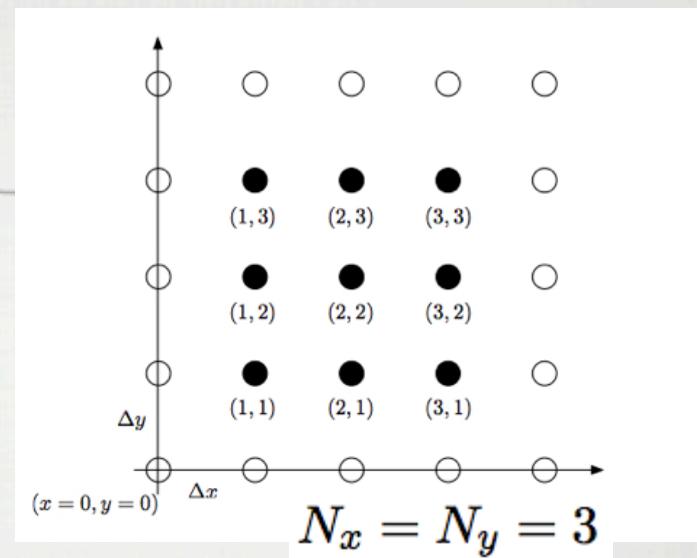
$$\begin{aligned}
U_{11} &= \frac{1}{4}(U_{10} + U_{12} + U_{01} + U_{21}) & 4U_{11} - U_{12} - U_{21} &= U_{10} + U_{01} \\
U_{21} &= \frac{1}{4}(U_{20} + U_{22} + U_{31} + U_{11}) & -U_{11} + 4U_{21} - U_{22} &= U_{20} + U_{31} \\
U_{12} &= \frac{1}{4}(U_{11} + U_{13} + U_{02} + U_{22}) & -U_{11} + 4U_{12} - U_{22} &= U_{13} + U_{02} \\
U_{22} &= \frac{1}{4}(U_{21} + U_{23} + U_{12} + U_{32}) & -U_{12} + 4U_{22} - U_{21} &= U_{23} + U_{32}
\end{aligned}$$

$$\begin{pmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{pmatrix} \begin{pmatrix} U_{11} \\ U_{21} \\ U_{12} \\ U_{22} \end{pmatrix} = \begin{pmatrix} U_{10} + U_{01} \\ U_{20} + U_{31} \\ U_{13} + U_{02} \\ U_{23} + U_{32} \end{pmatrix}$$

$$\begin{pmatrix} U_{11} \\ U_{21} \\ U_{12} \\ U_{22} \end{pmatrix} = \begin{pmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{pmatrix}^{-1} \begin{pmatrix} U_{10} + U_{01} \\ U_{20} + U_{31} \\ U_{13} + U_{02} \\ U_{23} + U_{32} \end{pmatrix}$$

$$\begin{pmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{pmatrix}^{-1} = \begin{pmatrix} 0.292 & 0.0833 & 0.0833 & 0.0417 \\ 0.0833 & 0.292 & 0.0417 & 0.0833 \\ 0.0833 & 0.0417 & 0.292 & 0.0833 \\ 0.0417 & 0.0833 & 0.0833 & 0.292 \end{pmatrix}$$

ONE WAY TO BUILD THE MATRIX



$$\partial^2 x \equiv \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 0 \end{pmatrix}$$

$$\partial^2 y \equiv \begin{pmatrix} -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 \end{pmatrix}$$

$$\frac{\partial^2 f(x_n, y_m)}{\partial x^2} \sim \frac{f(x_n - \Delta x, y_m) - 2 f(x_n, y_m) + f(x_n + \Delta x, y_m)}{\Delta x^2}$$

PUTTING IT ALL TOGETHER (LHS)

$$\nabla^2 \equiv \begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{pmatrix}$$

$$\nabla^2 \equiv \begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{pmatrix}$$

$$\begin{matrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{matrix}$$

$n_y \times (n_x \times n_x)$ blocks along the diagonal

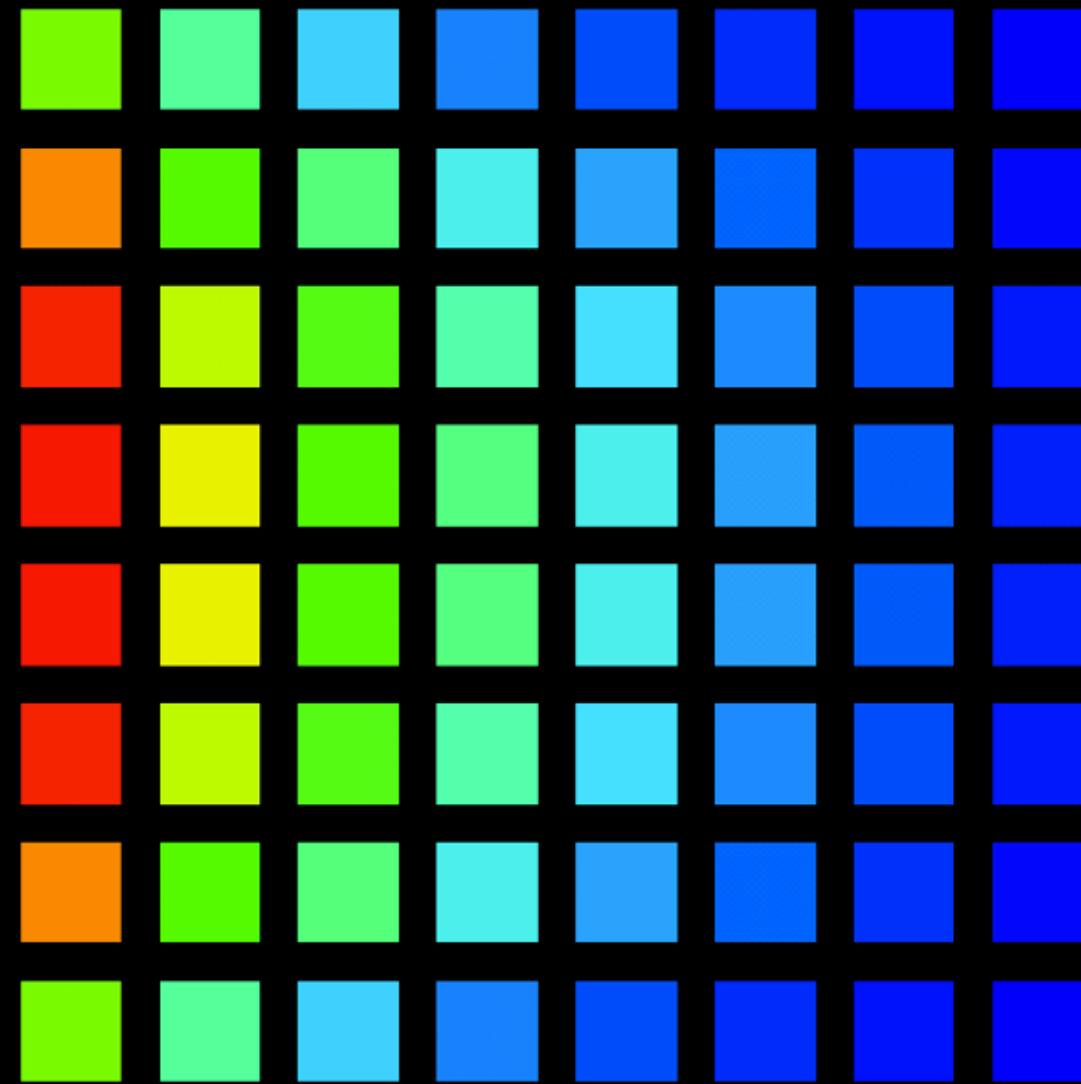
blocks are connected by a diagonal of “1”

5X5 => 25X25

How previous page was written

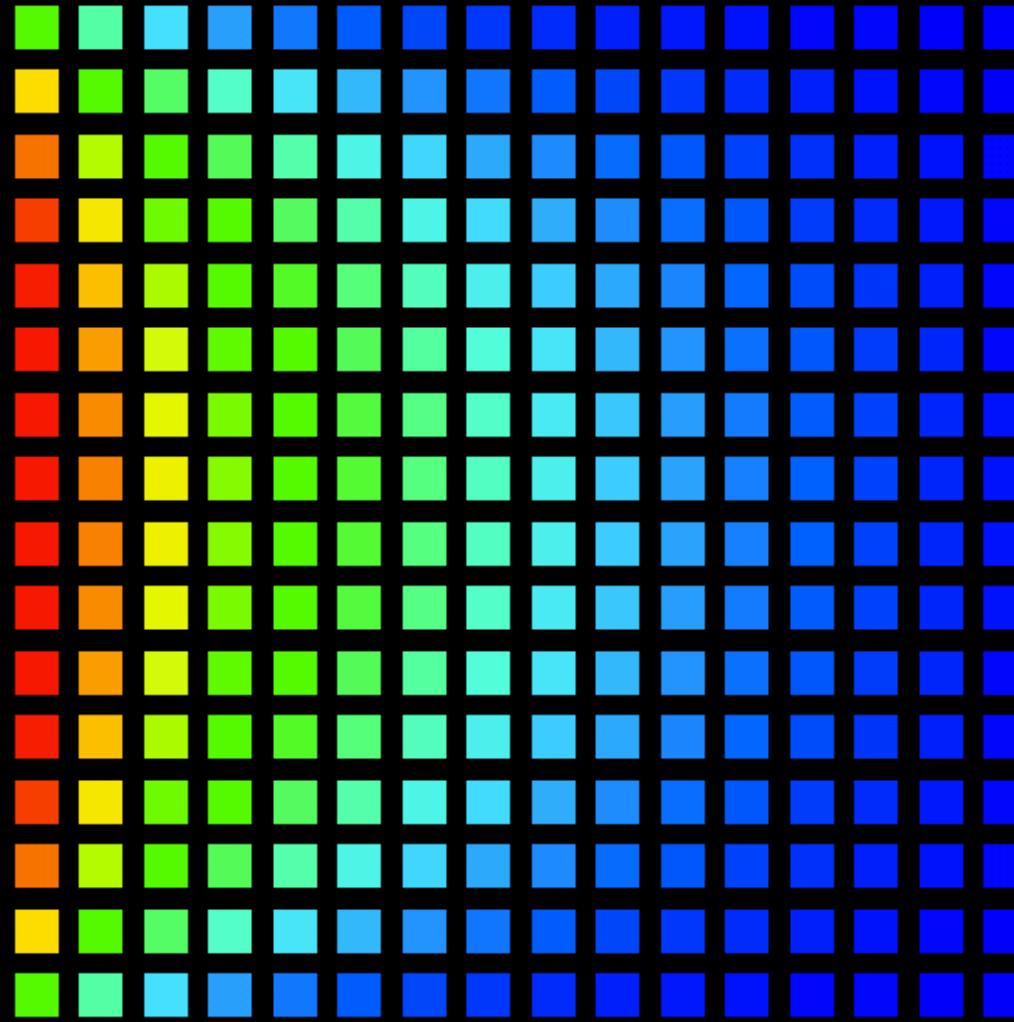
```
cout << endl << "\n\nBuilding a Laplacian:" << endl;
for(int i=0;i<nx*ny;i++){
    for(int j=0;j<nx*ny;j++){
        if(fabs(pot[i][j])>0){
            cout << "{\color{red}" << pot[i][j] << " }";
        }
        else{
            cout << pot[i][j] ;
        }
        if(j<nx*ny-1) {
            cout << " & ";
        }
        else {
            cout << " ";
        }
    }
    if(i<nx*ny-1) cout << " \\ " << "\\ " << endl;
}
cout << endl;
}
```

8×8



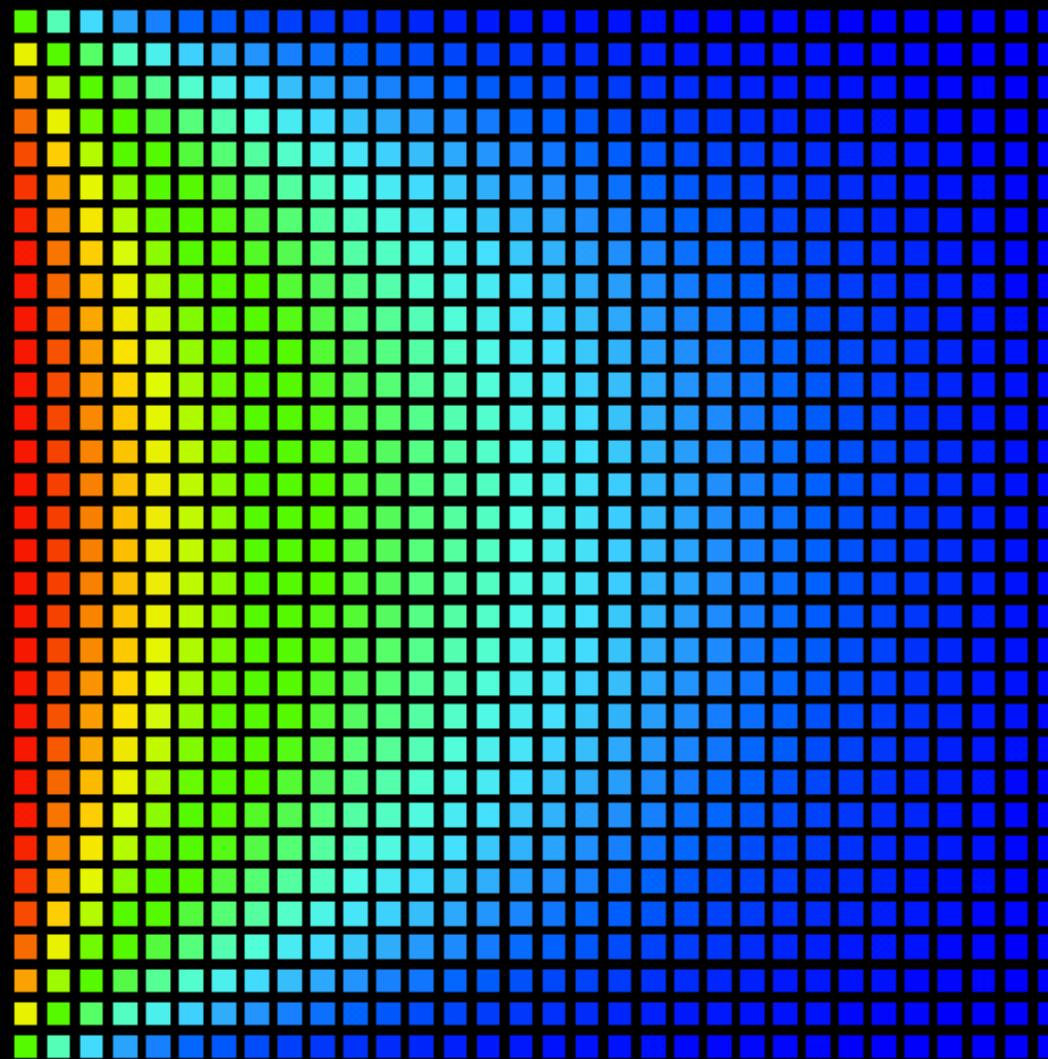
$t = 2\text{ms (LU)}, 4\text{ms(sparse)}, 5\text{ms(GJ)}$

16 X 16



t=66ms (LU), 19ms(sp), 251ms(GJ)

32X32



t=3966ms (LU), 167ms(sp), 17347 ms(GJ)

SUMMARY

- Solving $Ax=b$ is a difficult task to perform numerically, especially for very large systems
- Choosing the “right solver” for a given problem with specific symmetry property is key
- Many modern research codes rely heavily on the use of optimal solvers
- In fact, the time used to run such solvers is usually the basis for supercomputer ranking

ADVANCED TOPICS

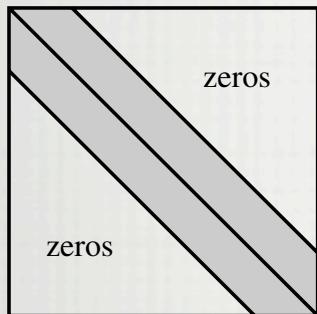
ADVANCED TOPIC

SINGULAR VALUE DECOMPOSITION

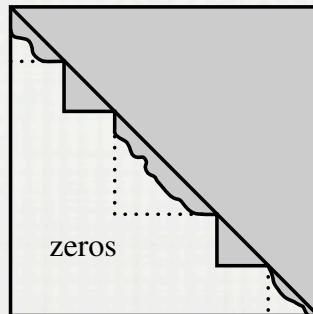
- When problems are too close to singularity
- SVD will **DIAGNOSE** the problem and even provide a **SOLUTION** to it
- SVD also solve linear **LEAST-SQUARE** problems (**overdetermined problems**)
- This is an advanced topic that could be covered in depth in a project

ADVANCED TOPIC

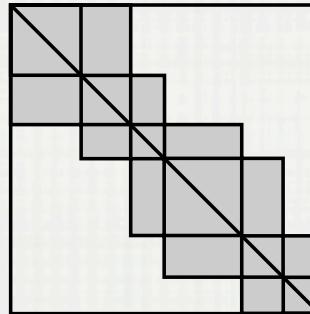
SPARSE MATRICES



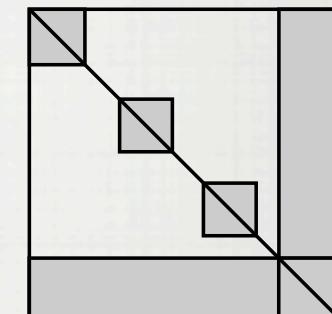
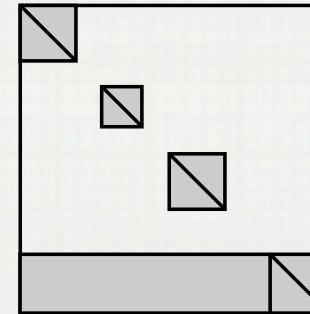
Band-diagonal



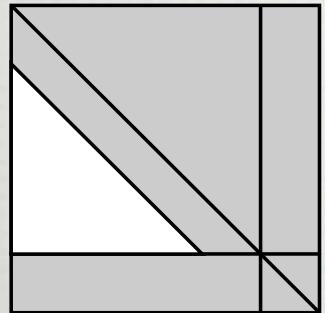
Block triangular



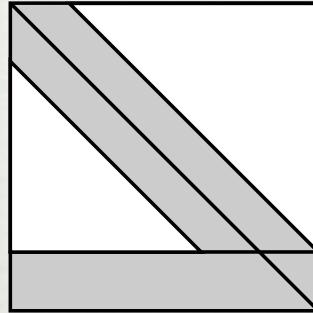
Block tridiagonal
**singly bordered
block diagonal**



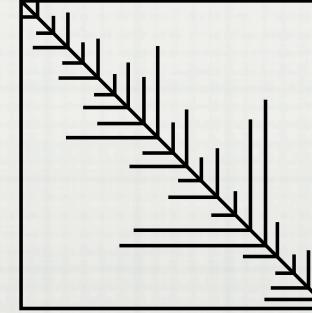
**doubly bordered
block diagonal**



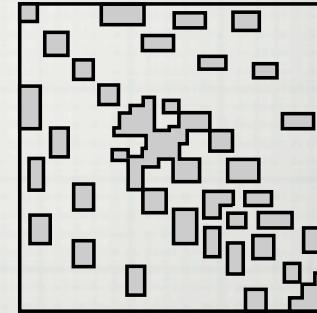
**bordered
band-triangular**



singly and doubly bordered band-diagonal



OTHERS



INDEXED STORAGE COMPRESSED COLUMN STORAGE

ADVANCED TOPIC

3.0	0.0	1.0	2.0	0.0
0.0	4.0	0.0	0.0	0.0
0.0	7.0	5.0	9.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	6.0	5.0

index k	0	1	2	3	4	5	6	7	8
val[k]	3.0	4.0	7.0	1.0	5.0	2.0	9.0	6.0	5.0
row_ind[k]	0	1	2	0	2	0	2	4	4

index i	0	1	2	3	4	5
col_ptr[i]	0	1	3	5	8	9

ADVANCED TOPIC

HARWELL-BOEING FORMAT

- 3 vectors are used
- val : non zero-values
- row_ind: row index
- col_ptr: column index ***
 - col_ptr[0]=0;
 - col_ptr[ncol+1]=nsparse
 - col_ptr[i] =>
 - the first nonzero in column i is in col_ptr[i]; the last is at col_ptr[i+1]-1
 - [[answers the question: *How many non-zero elements have we encountered in previous column?*]]

$$\begin{bmatrix} 3.0 & 0.0 & 1.0 & 2.0 & 0.0 \\ 0.0 & 4.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 7.0 & 5.0 & 9.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 6.0 & 5.0 \end{bmatrix}$$

index k	0	1	2	3	4	5	6	7	8
val[k]	3.0	4.0	7.0	1.0	5.0	2.0	9.0	6.0	5.0
row_ind[k]	0	1	2	0	2	0	2	4	4

index i	0	1	2	3	4	5
col_ptr[i]	0	1	3	5	8	9

3.0	0.0	1.0	2.0	0.0
0.0	4.0	0.0	0.0	0.0
0.0	7.0	5.0	9.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	6.0	5.0

index k	0	1	2	3	4	5	6	7	8
val[k]	3.0	4.0	7.0	1.0	5.0	2.0	9.0	6.0	5.0
row_ind[k]	0	1	2	0	2	0	2	4	4

index i	0	1	2	3	4	5
col_ptr[i]	0	1	3	5	8	9

```

/* in this first example I explicitely define the variables
to be used later to build a sparse matrix */
NRsparseMat A(5,5,9);

//the following should not be needed since they have been
given above
A.nrows=5;
A.ncols=5;
A.nvals=9;

// column index (see lecture notes)
A.col_ptr[0]=0;
A.col_ptr[1]=1;
A.col_ptr[2]=3;
A.col_ptr[3]=5;
A.col_ptr[4]=8;
A.col_ptr[5]=9;

// rows where sparse elements will be located
A.row_ind[0]=0;
A.row_ind[1]=1;
A.row_ind[2]=2;
A.row_ind[3]=0;
A.row_ind[4]=2;
A.row_ind[5]=0;
A.row_ind[6]=2;
A.row_ind[7]=4;
A.row_ind[8]=3; //this is modified compared to NR book
par.2.7 since the matrix there is singular

//now the values themselves
A.val[0] = 3.;
A.val[1] = 4.;
A.val[2] = 7.;
A.val[3] = 1.;
A.val[4] = 5.;
A.val[5] = 2.;
A.val[6] = 9.;
A.val[7] = 6.;
A.val[8] = 5.;
```

ADVANCED TOPIC

```

#include <iostream>
#include "nr3.h"
#include "sort.h"
#include "sparse.h"

int main (int argc, char * const argv[]) {

    int nsparse=0;
    int i, j;
    double eps=0.00001;

    //example from lecture notes
    int n=5;
    MatDoub Full(n,n,0.0);

    Full[0][0]=3.0;
    Full[0][2]=1.0;
    Full[0][3]=2.0;
    Full[1][1]=4.0;
    Full[2][1]=7.0;
    Full[2][2]=5.0;
    Full[2][3]=9.0;
    Full[4][3]=6.0;
    Full[4][4]=5.0;

    //first we need to find out how many non-zero elements we have
    //we store that information in "nsparse"
    for (i= 0; i<n; i++){
        for (j = 0; j<n; j++){
            if(fabs((Full[i][j]))>eps) {
                nsparse++;
            }
        }
    }
    //now we can create a sparse object
    NRsparseMat Sparse(n,n,nsparse);

    nsparse=0;
    for (j = 0; j<n; j++){
        if(j>0) {
            Sparse.col_ptr[j+1]=Sparse.col_ptr[j];
        }
        else
        {
            Sparse.col_ptr[0]=0;
        }
        for (i = 0; i<n; i++){
            if(fabs(Full[i][j])>eps) {
                Sparse.row_ind[nsparse]=i;
                Sparse.val[nsparse]=Full[i][j];
                Sparse.col_ptr[j+1]++;
                nsparse++;
            }
        }
    }
}

```

```

COUT << "NSPARSE=" << NSPARSE << endl;
COUT << "I= \t";
FOR(I=0;I<NSPARSE;I++){
    COUT << I << " \t" ;
}
COUT << endl;
COUT << "VAL= \t";
FOR(I=0;I<NSPARSE;I++){
    COUT << SPARSE.VAL[I] << " \t";
}
COUT << endl;
COUT << "ROW= \t";
FOR(I=0;I<NSPARSE;I++){
    COUT << SPARSE.ROW_IND[I] << " \t";
}
COUT << endl;
COUT << endl;
COUT << "I= \t";
FOR(I=0;I<N+1;I++){
    COUT << I << " \t";
}
COUT << endl;
COUT << "COL= \t";
FOR(I=0;I<N+1;I++){
    COUT << SPARSE.COL_PTR[I] << " \t";
}
COUT << endl;

RETURN 0;
}

```

```

Vinces-MacBook-Pro:Debug vml2$ ./Resistors
nsparse=9
i=      0      1      2      3      4      5      6      7      8
val=    3      4      7      1      5      2      9      6      5
row=   0      1      2      0      2      0      2      4      4
i=      0      1      2      3      4      5
col=   0      1      3      5      8      9
Vinces-MacBook-Pro:Debug vml2$ 

```

ADVANCED TOPIC

IN PRACTICE: SPARSE.H

```
struct NRsparseMat
```

Sparse matrix data structure for compressed column storage.

```
{
```

```
    Int nrows;
```

Number of rows.

```
    Int ncols;
```

Number of columns.

```
    Int nnvals;
```

Maximum number of nonzeros.

```
    VecInt col_ptr;
```

Pointers to start of columns. Length is ncols+1.

```
    VecInt row_ind;
```

Row indices of nonzeros.

```
    VecDoub val;
```

Array of nonzero values.

```
    NRsparseMat();
```

Default constructor.

```
    NRsparseMat(Int m, Int n, Int nnvals);
```

Constructor. Initializes vector to zero.

```
    VecDoub ax(const VecDoub &x) const;
```

Multiply \mathbf{A} by a vector $x[0..ncols-1]$.

```
    VecDoub atx(const VecDoub &x) const;
```

Multiply \mathbf{A}^T by a vector $x[0..nrows-1]$.

```
    NRsparseMat transpose() const;
```

Form \mathbf{A}^T .

```
};
```

SPARSE: EXAMPLE (SEE SPARSE.CPP)

ADVANCED TOPIC

```
#include "sparse.h"

#include "linbcg.h"
#include "asolve.h"

NRsparseMat A(5,5,9);

//here we define A

NRsparseLinbcg C(A);

VecDoub x(5,1.0);
VecDoub b(5,0.0);

//here we define x and b

Int itol=1;
Doub tol=1.0E-72;;
Int itmax=10000;
Int iter;
Doub err;

C.solve(b,x,itol,tol,itmax,iter,err);
```

SCALING

- Gaussj -> N^3
- LU -> $N^3/3$
- (Cholesky -> $N^3/6$)
- Sparse -> N^2

