

# Compressed Row Storage

Thursday, August 27, 2020 4:06 PM

## Compressed Row Storage

$$\begin{bmatrix} 0 & 2 & 3 \\ 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 4 & 5 & 6 & 0 \\ 0 & 7 & 0 & 0 \end{bmatrix}$$

$$values = [0, 1, 1, 2, 3, 4]$$

$$columns = [1, 1, 2, 3, 2]$$

$$Row\ start = [0, 1, 1, 4] [5]$$

{ look up row i directly}

what column  
each entry is

for row = 0 : n-1

    for idx = row\_start[row], ..., row\_start[row+1]-1.

        A(row, columns[idx]) = values[idx]

        otherwise A(i,j) = 0

    end

end

Need one  
extra value in  
so stop next  
value in

## Sparse Matrix-Vector product:

Compute  $y = A \cdot x$

$$y_i = \sum_j a_{ij} x_j, \quad i = 0, 1, \dots, n-1$$

for i = 0, ..., n-1

$$y[i] = 0$$

    for idx = row\_start[i], ..., row\_start[i+1]-1

$$y[i] = y[i] + values[idx] \cdot x[columns[idx]]$$

"random" access,  
indirect addressing

```

for idx = row -> start + 1 to row + 1
    |   y[i] = y[i] + values[idx] * x[column[idx]]
    |   values num. <-->
    |   sequentially accessed O(n)
end
end

```

# FEM Review

Tuesday, September 1, 2020 3:51 PM

## Finite Element Method

$V_h = \{\phi_1, \dots, \phi_n\}$ , how to define basis?

$$u_h(x) = \sum u_i \phi_i(x)$$

### Ciarlet's definition of a Finite Element

$$(\Omega, P, \Sigma)$$

1.)  $\Omega \subseteq \mathbb{R}^d$  domain: connected, compact, non-empty, boundary  $\partial\Omega$   
piecewise linear or Lipschitz

2.)  $P \subseteq V(\Omega) = \{v: \Omega \rightarrow \mathbb{R}\}$  vector space of functions

3.)  $\Sigma$  set of  $n$  linear forms  $\sigma_1, \dots, \sigma_n$ , called degrees of freedom

$$\sigma_i: P \rightarrow \mathbb{R}$$

They form a basis of all  $L(P; \mathbb{R})$

example:  $\sigma_i(x) = v(x_i)$ , evaluate  $v$  at  $x_i$

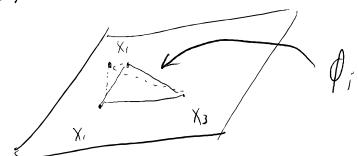
$x_i$ : support points  $\{x_1, \dots, x_n\}, x_i \in \Omega$

$\Rightarrow$  nodal FE space

$\Rightarrow$  There exists a basis  $\{\phi_1, \dots, \phi_n\}$  of  $P$

$$\text{with } \sigma_i(\phi_j) = \delta_{ij}$$

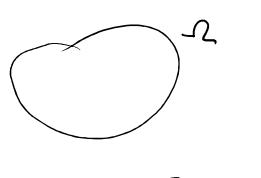
example:



more details

1.) Subdivide  $\Omega \subseteq \mathbb{R}^d$  into mesh

$$T_h = \{K_i\}, K_i: \text{cell}$$



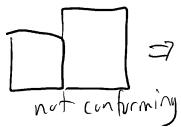
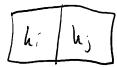
$\left( \begin{array}{l} T_h \text{ is conforming iff } (\forall i, j) \\ \bar{K}_i \cap \bar{K}_j \text{ is } \emptyset \text{ or a vertex} \end{array} \right)$



$$\Omega_h = \bigcup \bar{k}_i \approx \Omega$$

$k_i$ : simplices (triangles or tetrahedra)  
or  
 $k_i$ : quadrilaterals

The  $\bar{k}_i$  is continuous  
 $\bar{k}_i \cap \bar{k}_j$  is  $\emptyset$  or a vertex  
or a face  
(line in 3D)



$\Rightarrow$  makes  $V_h$  not continuous

## 2.) Reference Cell $\hat{k}$

$$\hat{k} = [0, 1]^d \text{ for quads}$$



$$\hat{k} = \left\{ \sum x_i \leq 1 \right\} \text{ simplices}$$

$x_i \geq 0$



Later: allow non-conforming meshes  
w/ hanging nodes

## 3.) Mapping from reference cell



$$F_{k_i}: \hat{k} \rightarrow k_i$$

## 4.) Define Local basis on $\hat{k}$ with

local support points  $\hat{x}_i \in \hat{k}$ :

$$\text{basis } \{\hat{\phi}_i\}, \hat{\phi}_i: \hat{k} \rightarrow \mathbb{R}$$

$$\mathcal{Q}_1 = \text{span}\{1, x, y, xy\}$$



$$\mathcal{P} = \text{span}\{1, x, y\}$$

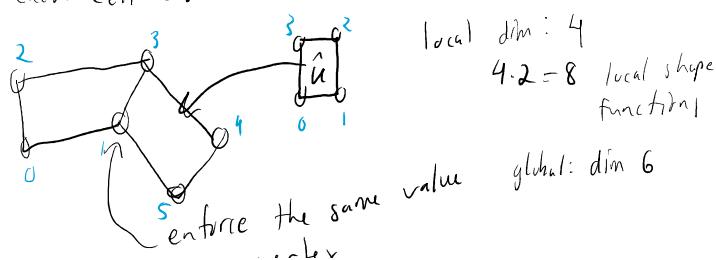


## 5.) Number degree of freedom to create

Global basis  $\phi_1, \dots, \phi_n$  tensor-product  
degree  $k$ , FEM space

$$\mathcal{Q}_h(\Gamma_h) = \{v \in C(\Gamma_h), v|_{k_i} \circ F_{k_i} \in \mathcal{Q}_n\}$$

on each cell use  $\mathcal{Q}_n$  from  $\hat{k}$ , make continuous

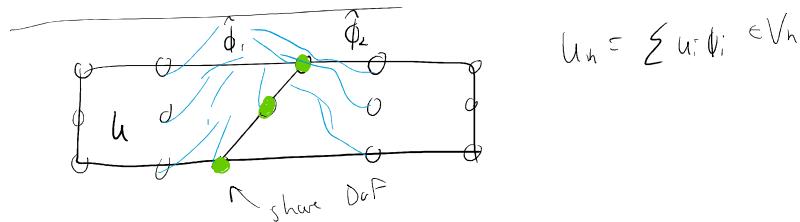


0  enforce the same value  
in vertex

$$h_1: [0, 1, 2, 3] \rightarrow [1, 5, 3, 4]$$

local Dof's      global Dof's

$$h_2: [0, 1, 2, 3] \rightarrow [0, 2, 3, 1]$$



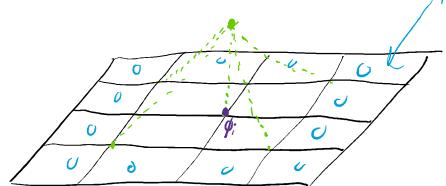
$\phi_i$  need to be continuous

$\Rightarrow$  combine the local  $\hat{\phi}_i$  to be continuous

$$\Rightarrow \phi_i(x)|_{k_j} = \begin{cases} \hat{\phi}_j & \exists j: D_u(j) = i \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \phi_i(x) \in C(\Omega_h), \quad \therefore \Rightarrow V_h \subseteq C(\Omega_h)$$

$\Rightarrow \text{Support}(\phi_i)$  is small (one layer of cells!)



$\Rightarrow$  Tensor-product polynomials on each cell.

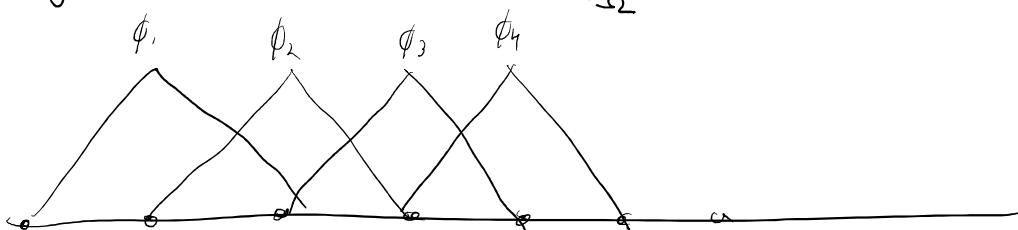
glued together continuously

basis: local support

## More FEM review

Thursday, September 3, 2020 4:37 PM

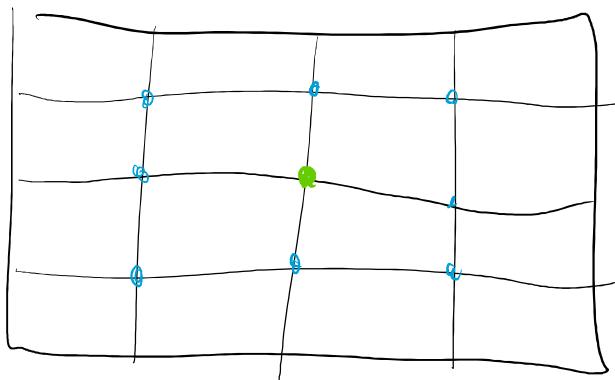
$$A_{ij} = (\nabla \phi_i, \nabla \phi_j) = \int_{\Omega} \nabla \phi_i(x) \cdot \nabla \phi_j(x) dx$$



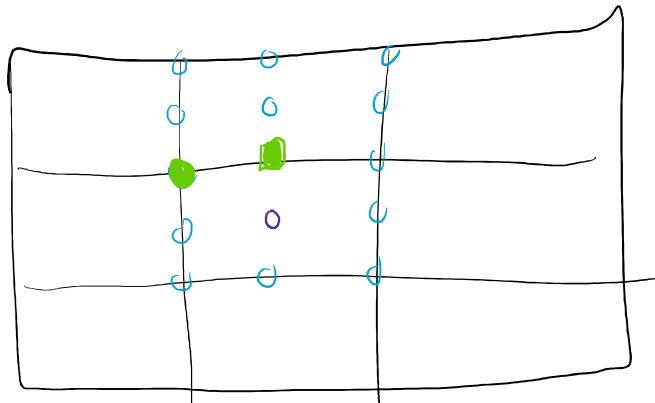
Support  $\phi_i$

Support  $\nabla \phi_i$

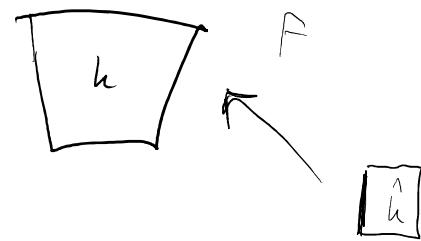
$\Rightarrow A$  is sparse



Q is regular:  
q entries / row



$$A_{ij} = \int_{\Omega_h} \nabla \phi_i(x) \cdot \nabla \phi_j(x) dx$$



$$= \sum_{h \in \mathcal{T}_h} \int_h \nabla \phi_i(x) \cdot \nabla \phi_j(x) dx$$

$$= \sum_h \int_{\hat{h}} (\nabla \phi_i)(F(\hat{x})) \cdot (\nabla \phi_j)(F(\hat{x})) |\det(J(\hat{x}))| d\hat{x}$$

Define  $\hat{\phi}_i = \phi_i(F(\hat{x}))$

$$\begin{aligned} \nabla \hat{\phi}_i(\hat{x}) &= \nabla[\phi_i(F(\hat{x}))] \\ &= (\nabla \phi_i)(F(\hat{x})) \cdot \underbrace{\nabla F(\hat{x})}_{=J(\hat{x})} \end{aligned}$$

$$= \sum_h \int_{\hat{h}} J^{-1}(\hat{x}) \nabla \hat{\phi}_i(\hat{x}) \cdot J^{-1}(\hat{x}) \nabla \phi_j(\hat{x}) |\det(J(\hat{x}))| d\hat{x}$$

$$\approx \sum_h \sum_{g=1}^m J^{-1}(x_g) \nabla \hat{\phi}_i(x_g) \cdot J^{-1}(x_g) \nabla \phi_j(x_g) |\det(J(x_g))| w_g$$

$\underbrace{J^{-1}(x_g) \nabla \hat{\phi}_i(x_g)}_{\text{shape\_grad}(i,g)} \quad \underbrace{J^{-1}(x_g) \nabla \phi_j(x_g)}_{\text{shape\_grad}(j,g)} \quad = J_x w(g)$

quad rule

See step-3

Naive way to assemble:

```
for i = 1:N
    for j = 1:N
        for h ∈ Th
            for q = 1:nq
                Ai,j += shape-grad(i,q)
```

$O(N^3)$  bad

better  
for h ∈ Th ↗ local indices!

$M = 0$

for  $\hat{i} = 1 : n_{\text{local\_dofs}}$   
    for  $\hat{j} = 1 : n_{\text{local\_dofs}}$   
        for  $q = 1 : n_q$   
             $M(\hat{i}, \hat{j}) = \text{shape-grad}(\hat{i}, q)$

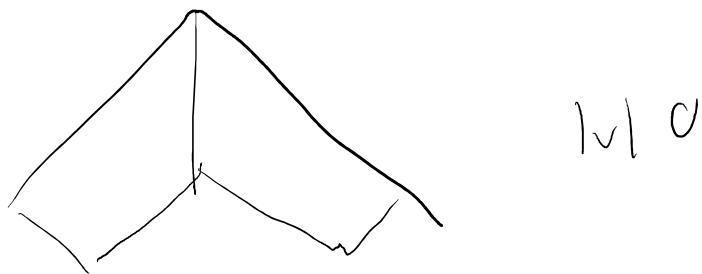
$A_{i,j} += M(\hat{i}, \hat{j})$  where  $i = \alpha(\hat{i})$  ↗ dof indices  
 $j = \beta(\hat{j})$  ↗ local → global

copy local  
to global

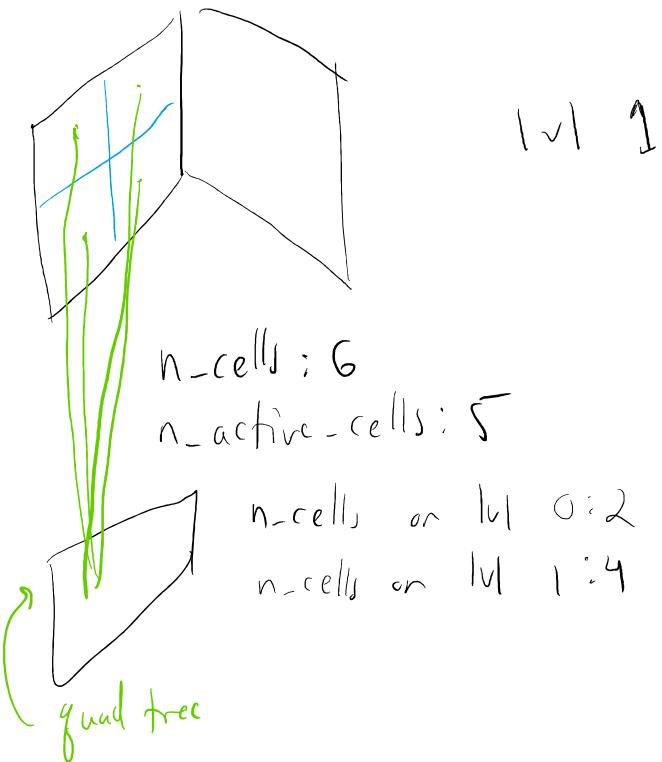
$\Rightarrow O(N)$

# Mesh refinement

Thursday, September 10, 2020 3:38 PM



↓  
refine  
global



A cell without children is called  
active

Computation is done on active cells

# Quadrature

Thursday, September 10, 2020 4:07 PM

$$\int_a^b f(x) dx \approx \sum_q f(x_q) w_q$$

eval pts  $\downarrow$  weight

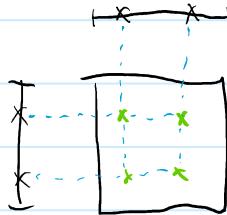
$\Rightarrow$  Gauss most common with  $n$  points

\*  $\Rightarrow$  Exact for polynomials of degree  $2n-1$   
(optimal for fixed  $n$ )

in 2D or 3D?

Tensor product quadrature:

$$G_n(f, [0,1]^2) = \sum_{q,p} f(x_q) w_p w_q$$



$$G_n(f, [0,1]^2) = \sum_{p,q} f\left(\begin{bmatrix} x_p \\ x_q \end{bmatrix}\right) w_p w_q$$

$\Rightarrow$  for any quadrature, any degree  
(very difficult on triangles)

What order do I need?

$$\text{degree } \rightarrow \int \nabla \phi_i \cdot \nabla \phi_j dx$$

$\underbrace{\phantom{\int}_{\text{fe degree}}}_{\text{fe degree}}$

$\nabla \phi_i$  still is at most fe degree  
(due to  $J^{-1}$  transform)

$\nabla \phi_i \cdot \nabla \phi_j$  is 2·fe degree

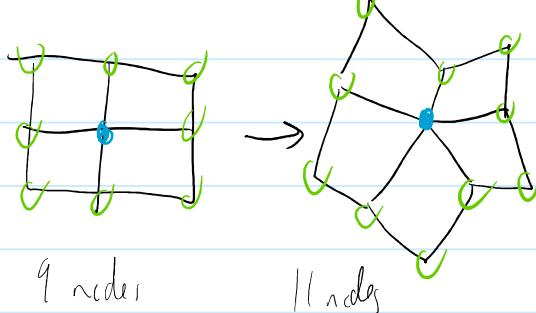
$$\text{So } 2n-1 = \text{fe degree} \Rightarrow n = \text{fe degree} + \frac{1}{2}$$

$\uparrow \text{fe degree} + 1$

Ex.)  $G_2$  in 3D

Ex.) Q<sub>2</sub> in 3D  
 $3 \cdot 3 \cdot 3 = 27$

For Lub 3, Pnb 4



Prob 6.)  $A_{ij} = (\nabla \phi_i, \nabla \phi_j)$  are sparsity pattern symmetric?

$A_{ij} \neq 0$  iff  $\phi_i$  and  $\phi_j$  have support on some cell  $k$ .

$\Rightarrow$  For a scalar PDE, the SP is symmetric

5) For each cell

for each  $i, j$

$d\_s\_p\_add(\text{global\_}i, \text{global\_}j)$

Sparsity Pattern :: iterator  $it = s\_p.\text{begin}(42)$

gives iterator

while ( $it \neq s\_p.\text{end}(42)$ )

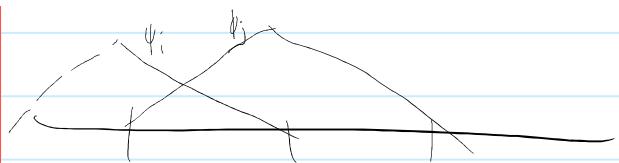
{

$\text{std::cout} \ll it \rightarrow \text{column}() \ll \text{std::endl};$

$it++$

}





$(\phi_i, \phi_j)$       support is  
 $(\phi_j, \phi_i)$       symmetric

## For Lab

To get Gaus points

Point (x) & int = f-e-values. quadrature point (g-index)

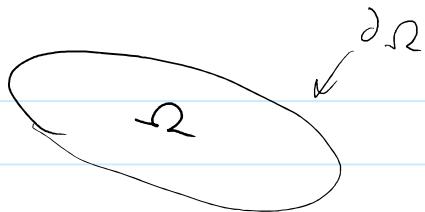
const

# Boundary Conditions

Thursday, September 17, 2020 3:59 PM

Example:  $-\Delta u = f$

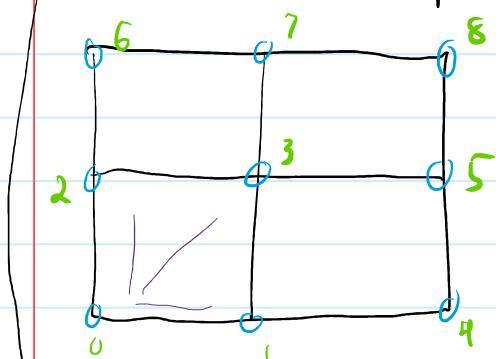
$$u|_{\partial\Omega} = 0$$



↑ required for unique solutions

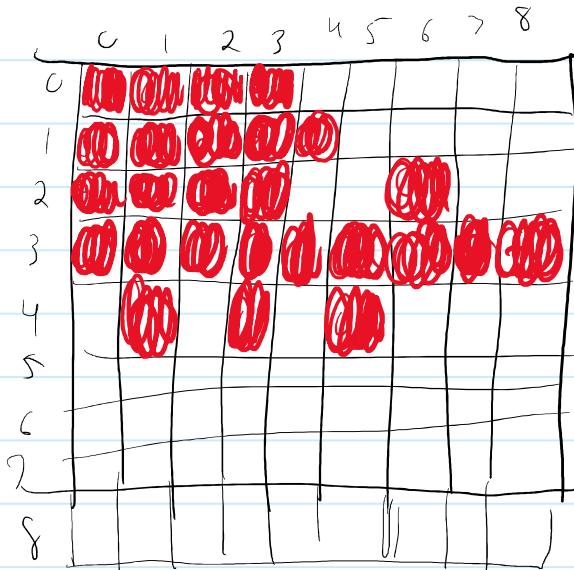
$$V = H_0^1(\Omega)$$

$$V_h \subseteq V, V_h = \text{span}\{\phi_i\}$$



$$\hookrightarrow u = \sum u_i \phi_i$$

$$\Rightarrow u_0 = 0, u_1 = 0, \dots$$



option A: do not include  $\phi_0, \phi_1, \dots$

⇒ a cell can have fewer shape functions

⇒ Not a good solution

option B: 1.) include  $\phi_j$  on the boundary

2.) Fix the boundary values by enforcing  $u_0 = 0, u_1 = 0, \dots$

3.) Remove these lines from linear system

⇒ not  $u \in \begin{bmatrix} u_0 \\ \vdots \\ u_8 \end{bmatrix}$ , but just for leftover unknowns

not ideal:  $\dim V_h \neq \text{size}(u)$

option C: Like B but we store 0 entries  
how to enforce  $u_j=0$ ? ( $j \in \partial\Omega$ )

$\Rightarrow$  replace row j by  $A_{jj}=1, f_j=0$

$\Rightarrow$  Matrix is no longer symmetric even if PDE

is symmetric

optional: eliminate column j using row j  
• advantage: A SPD

Cost: how many columns?  $\sim \sqrt{N}$

cost for one column?

if S.P. is symmetric, only check row

check row j  $\Rightarrow O(1)$  ok ✓

if not:  $O(N)$  😐

$\Rightarrow$  only do this if you require symmetry

But: Matrix full :: apply

⋮  
⋮

better: local elimination (step 6)

$$\begin{bmatrix} * & * & * & \dots & * \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \downarrow & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} \quad | F$$

until now:  $u|_{\partial\Omega} = 0, H_0^1(\Omega)$

How to extend to  $u|_{\partial\Omega} = g$ ?

(non-homogeneous Dirichlet b.c.)

$$u_i = g(x_i)$$

support point of  $\phi_i$

done in  `interpolate_boundary_values()`

## Boundary conditions 2

Tuesday, September 22, 2020 3:35 PM

Example:



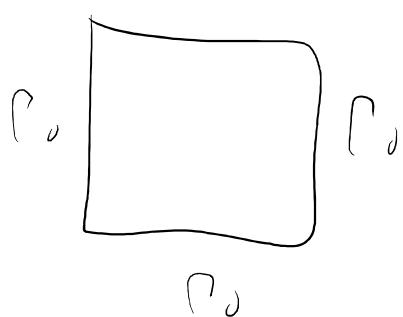
$$\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{wall}} \cup \Gamma_{\text{out}} \cup \Gamma_c$$

$$\Gamma_0 \quad \Gamma_1 \quad \Gamma_2 \quad \Gamma_3$$

↑  
boundary id

default hyper-cube: all faces have id 0

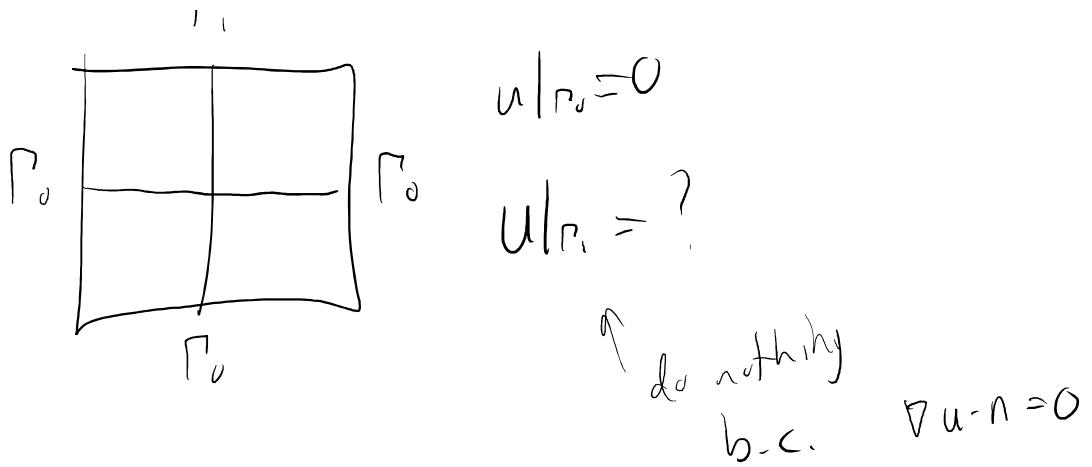
$$\Gamma_0$$



$$\Gamma_1$$



$$u|_{\Gamma_1} = 0$$



### On Lab 4 : Prob 6

The discontinuous point prioritizes the boundary that is last defined, in the example the boundary is changed after, so that "gets" the point.

### Natural Boundary Conditions

$$-\Delta u = f, \quad u|_{\partial\Omega} = g$$

$$\int_{\Omega} V(-\Delta u) = \int_{\Omega} Vf$$

$$\int_{\Omega} \nabla v \cdot \nabla u - \int_{\partial\Omega} v (\nabla u \cdot n) = \int_{\Omega} vf$$

||

0 if  $v \in H_0^1$

$$\Rightarrow (\nabla v, \nabla u) = (v, f) \Rightarrow \text{step-3}$$

if "do nothing" on  $\Gamma_1$ , then I have  $v \neq 0$  on  $\Gamma_1$   
 and this integral doesn't vanish.

if I have solution  $u_h$  of weak form

$$\Rightarrow \int_{\Omega} v(-\Delta u) + \int_{\partial\Omega} v(\nabla u \cdot n) = \int_{\Omega} vf$$

Test w/  $v=0$  on  $\partial\Omega$

$$-\Delta u = f$$

Test w/  $v=1$  on  $\partial\Omega$ ,  $v=0$  interior

$$\Rightarrow \nabla u \cdot n = 0 \text{ on } \partial\Omega$$

$\Rightarrow$  that is why "do nothing" means  $\boxed{\nabla u \cdot n = 0}$

# Manufactured solutions

Thursday, September 24, 2020 3:34 PM

Goal: Validation of a FE code

Example:  $-\Delta u = f$ ,  $u|_{\partial\Omega} = g$

- steps.)
  - 1: pick any function  $u$  as your solution
  - 2: Compute RHS  $f$  for given  $u$
  - 3: Solve numerically  $-\Delta u_n = f$ ,  $u_n|_{\partial\Omega} = g$
  - 4: Compute errors  $\|u - u_n\|_1$ ,  $\|u - u_n\|_{L^2}$   
 $| \text{mean}(u_n) - \text{mean}(u) |, \dots$
- goal: verify theory

Note: Pick something where you can pick  $f = -\Delta u$

- what about  $u \in V_h$ ? bad idea, small error
- careful w/ polynomials b/c polynomial space  $Q_h$
- Better use trig functions
- Choose difficult enough  $u$  s.t.  $u - u_n$  is not close to zero  
otherwise
  - quadrature error
  - floating point arithmetic
  - linear solve tolerance

-  $u$  smooth enough for theory to hold

- step 4 contains approximation error

$$\text{mean}(u_n) = \frac{1}{|\Omega|} \int_{\Omega} u_n \, dx$$

$$\approx \sum_n \sum_g u_n(x_g) w_g$$

$$\|u - u_n\|_{L^2}^2 = \int_{\Omega} (u - u_n)^2 \, dx$$

$$\text{infty-difference} \approx \sum_n \sum_g \underbrace{(u(x_g) - u_n(x_g))^2}_{w_g} w_g$$

$$\text{in trapz - difference} \approx \sum_{i=1}^n \underbrace{(u(x_i) - u_n(x_i))^2}_{\text{exact, but quadrature}} w_i$$

introduces error

Note: good idea to use higher degree quadrature

## Manufactured solutions pt. 2

Tuesday, September 29, 2020 4:18 PM

$$\text{ex.) } -\nabla u = f$$

$$(\nabla v, \nabla u) = (v, f) \text{ weak form}$$

$$a(u, v) = (\nabla u, \nabla v) \text{ bilinear form}$$

$$f(v) = (f, v) \text{ linear form}$$

$$\text{Find } u \in V : a(u, v) = f(v) \quad (*)$$

Lax Milgram:  $\exists$  unique  $u \in V$  s.t.  $(*)$  holds

Assume:  $V_h \subseteq V$ ,  $V_h = Q_h$  or  $V_h = P_h$  uniform

w/ mesh size  $h$

discrete weak form:  $a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h$

$$\begin{aligned} \text{Cea's Lemma: } \|u - u_h\|_{H^1} &\leq C \inf_{v_h \in V_h} \|u - v_h\|_{H^1}, \\ (\text{Assume } u \in H^2(\Omega)) & \quad \swarrow \text{interpolator} \\ &\leq C \|u - \tilde{u}\|_{H^1} \\ &\leq C \cdot h^4 |u|_{H^5} \end{aligned}$$

$$\text{Note: } \text{FE-Q}(u) \Rightarrow \|u - u_h\|_1 \leq C \cdot h^4$$

What about  $\|u - u_h\|_2$ ?

"Nitsche trick", Aubin-Nitsche Lemma

Needs regularity of the domain,  $u \in H^{1+\frac{1}{2}}(\Omega)$

$$\Rightarrow \|u - u_h\|_2 \leq C \cdot h \cdot \|u\|_1$$

How to compute  $\|u - u_h\|_{L^2}^2$

$$\begin{aligned} &= \int_{\Omega} (u - u_h)(u - u_h) = \sum_i \int_{\Omega} (u - u_h)(u - u_h) \\ &\quad \text{integrate-difference} \approx \sum_i \sum_j (u - u_h)(u - u_h) w_j \\ &\quad \text{error-per-cell} \end{aligned}$$

$$\Rightarrow \|u - u_h\|_{L^2} = \sqrt{\sum_T \text{error-per-cell}(T)}$$

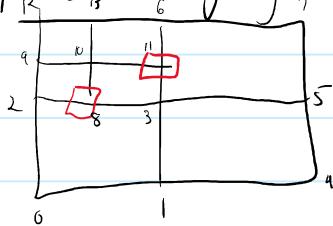
compute-global-error

# Why adaptivity?

Thursday, October 1, 2020 3:40 PM

- Error is not distributed equally, especially with non-smooth solutions
- Represents features in geometry

Example.) hanging nodes



$$u_8 = \frac{1}{2}(u_2 + u_3)$$

$$u_{11} = \frac{1}{2}(u_3 + u_6)$$

$$\Rightarrow u_n \in H_1(\Omega)$$

apply these constraints to  
make-hanging-node-constraint

$$2u_2 + 10u_8 + 3u_3 = 0$$

add a line

constraint-add-line(8)

$$u_8 = -\frac{2}{10}u_2 - \frac{3}{10}u_3$$

constraint-add-entry  $(8, 2, -\frac{1}{5})$

" "  $(8, 3, -\frac{3}{10})$

Need to write the constraint

$$a_i = \sum_j a_{ij} u_j + b$$

$\nearrow$  Dirichlet B.C.  
 $j \in [0, N], N \neq F$

$$\begin{aligned} j \in [0, N], \quad & N \text{ DoFs} \\ i \in \mathcal{I} \quad & (\text{constraint}) \end{aligned}$$

Most  $a_{ij} = 0$   
-  $O(1)$  constrained entries

Logically: Sparse matrix  $C_m$   
RHS  $C_R$

$$C_m \begin{bmatrix} u_0 \\ \vdots \\ u_{N-1} \end{bmatrix} = C_R$$

$$V_h = \left\{ u = \left\{ u_i \right\}_{i \in \mathcal{I}} : C_m \begin{bmatrix} u_0 \\ \vdots \\ u_{N-1} \end{bmatrix} = C_R \right\}$$

### Affine Constraints <double>

$$x_i = \sum_j a_{ij} x_j + c_i$$

used for

1.) hanging nodes

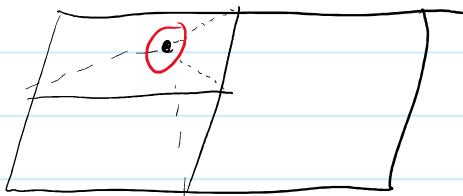
2.) boundary conditions:  $u_i = c_i = g(x_i)$

3.) other boundary conditions:

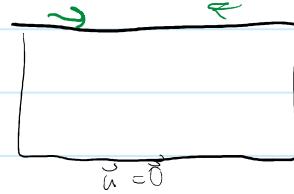
for example Stokes

velocity  $\vec{u}$

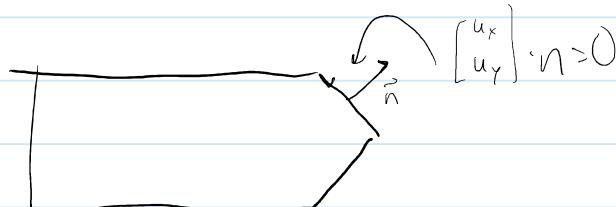
$$\vec{u} \cdot \vec{n} = 0 \quad \text{"free slip"}$$



$$\vec{u} \cdot \vec{n} = 0 \Rightarrow u_x = 0$$



no slip



no slip

periodic B.C.:  $\Gamma_L$   $\Gamma_R$



$$u \left( \begin{pmatrix} 0 \\ y \end{pmatrix} \right) = u \left( \begin{pmatrix} l \\ y \end{pmatrix} \right)$$

$$u(\cdot) = u(\cdot)$$

4.) other things:

mean value constraint

for example

$$-\Delta u = f, \int_{\Omega} u = 0$$

$$\text{b.c.: } \nabla u \cdot n = 0$$

Step-6:

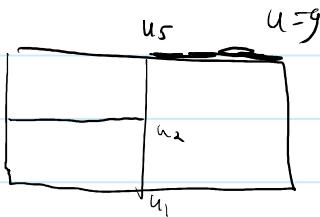
constraint closure

simplifies representation

resolves chains

$$u_2 = \frac{1}{2}u_1 + \frac{1}{2}u_5$$

$$u_5 = 42$$



$$\Rightarrow u_2 = \frac{1}{2}u_1 + 21$$

distribute\_local\_to\_global():

copies local matrix/RHS to global one

and applies constraints

distribute(): ?

# Chapter 2: parallel computing

Tuesday, October 6, 2020 4:27 PM

example: 1 workstation

2 cpus

16 cores

2 processing units (hyper-threading)

⇒ 64 processing units

⇒ concurrently

important: parallel computing doesn't happen automatically!

/proc/cpuinfo

Linux command to see specs on CPU

past: task switching (even on one processing unit) gives illusion of switching

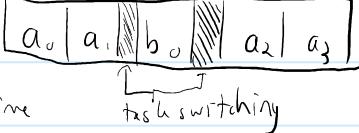
ex.) task a



task b



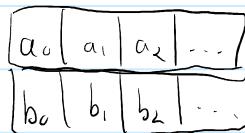
1 pu :



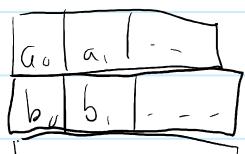
→ time

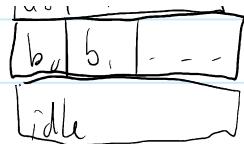
task switching

2 pu :



3 pu :

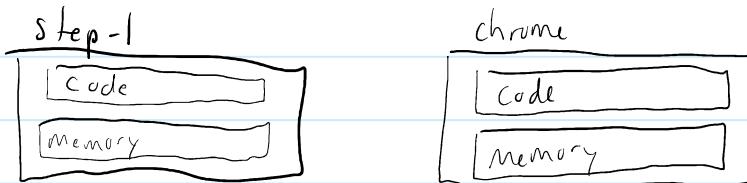




- pu: processing units  
 → hyperthreading / SMT  
 OS thinks you have  $\times 2$  cores  
 → about 0 - 20% extra performance  
 over 1 task per core

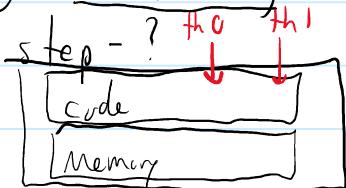
## Processes VS Threads

Processes:



- all processes have separate memory
- isolated
- scheduled by OS to run on PU

### (A) Multithreading



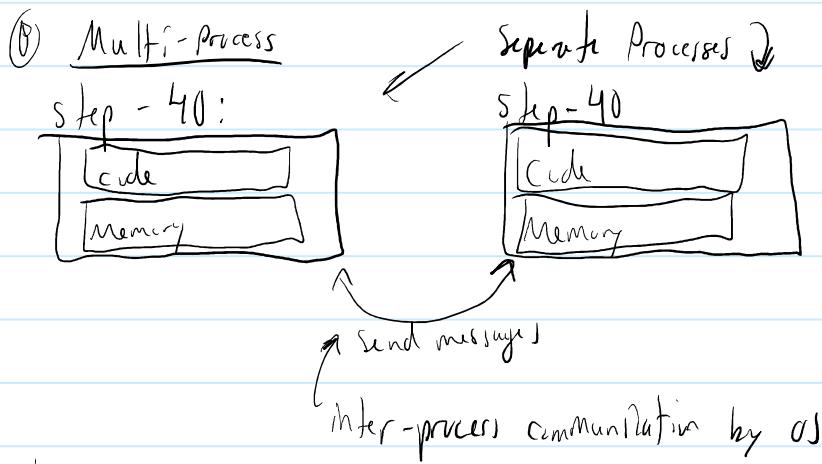
- create thread (ask OS)
- $\Rightarrow$  2 concurrent threads of execution
- memory is shared (!)
- low overhead
- arbitrary number of threads
- data is accessed concurrently?
- data races/corruption possible
- invalid data

- data races/corruption possible
  - invalid data
- ⇒ explicit synchronization needed

### O3 - threads\_race:

problem: concurrent reading and writing in  
one memory location

solution: explicit synchronization



Library: Message Passing Interface (MPI)

↳ same machine (OS function)

or over network (super computer)

⇒ - memory is separate

- explicit communication

Ex.) 8 Cu (laptop, 4 cores x2 HT)

a.) 1 process, 8 threads /step-7

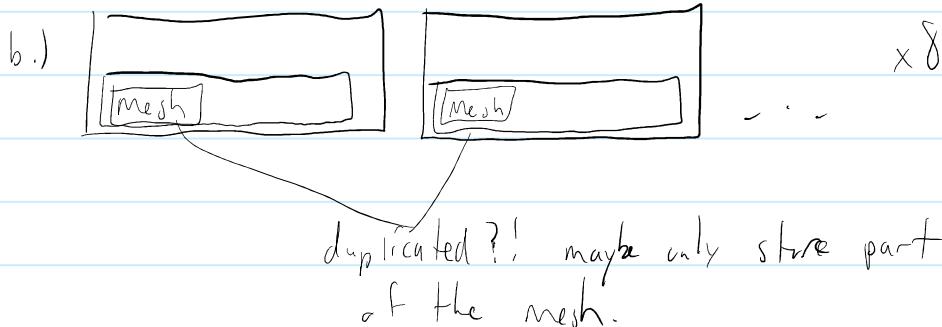
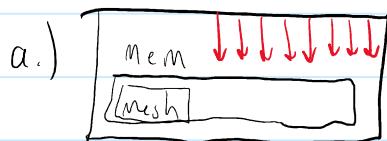
b.) 8 processes, 1 thread each mpirun -n8

(hyperthreaded)

4 processes, 2 threads each

2 processes, 4 threads

⇒ complicated, probably not useful



Concurrency example:

fixed work,  $N$  workers

ideal situation:  $N$  times faster than 1 worker

but:

- don't split up work evenly

- communication

- limited resource

- sequential part of the code

(fraction)

let  $0 \leq s \leq 1$  sequential part of the work

$p = 1 - s$  parallel part/fraction

$T(1)$  time w/ 1 worker

$T(N) = s \cdot T(1) + p \frac{T(1)}{N}$ , Amdahl's Law

Speed up:  $\frac{T(1)}{T(N)}$

max?  $\xrightarrow{N \rightarrow \infty} \frac{1}{s}$

80% parallel  $\Rightarrow$  max. speed up is 5

reality: - There is no  $N = \infty$

- can you split up work evenly for large  $N$ ?  
(limits  $N$ )

- communication (often takes more time) does not

(limits  $N$ )

- communication (often takes more time) does not scale, gets slower with large  $N$

$$T(N) = sT(1) + p\left(\frac{T(1)}{N}\right) + aN + bN^2 + c\log(N)$$

↑  
reduction (think  
binary tree!)

## Threads in C++:

- 1.) Passing objects by reference makes (unnecessary?) copies  
⇒ avoid this by doing  
`std::thread(func, std::ref(x));`  
note:  $x$  needs to be valid until thread ends

## 2.) std::thread::hardware\_concurrency()

⇒ int = no. of PUs

$$\left[ \begin{array}{c} \\ \end{array} \right] = \left[ \begin{array}{c} \\ \end{array} \right] + \left[ \begin{array}{c} \\ \end{array} \right] \text{ ↗ thread 1}$$

$\vec{z}$        $\vec{x}$        $\vec{y}$

$\text{↗ thread 2}$   
⋮

## 3.) Synchronization

- necessary if a.) 2+ writers  
b.) 1 writer, 1 reader

to the same memory address

### A.) Locking using mutex

times recorded in test code

int (incorrect) .045

atomic<int> .255

mutex 1.15

`atomic<T> x`

`x.compare_exchange_weak(T & expected,  
T desired)`

returns bool

if `x` currently contains "expected" ] atomic

1.) replace `x` by "desired"

2.) returns true // success

else :

1.) puts current value into expected

2.) return false

### Multi-threading

create threads, split up work

⇒ concurrent computation

danger: synchronization

⇒ lock-based (mutex, ...)

or lock-free (atomic operations, exchange or ref) )

Numerical linear algebra library:

- vectors, sparse matrices

- operations ( $x+y$ ,  $A \cdot x$ ,  $\|x\|$ ,  $x \cdot y$ ,  $x^T A$ )

- Solvers: CG, GMRES, ...

- concurrent implementation of operations

⇒ the user does not need to know that things happen concurrently (includes CG)

Note:

- deal.II does this (`Vector<double>::norm()`)

- only create threads if it's worth doing

- only create threads if it's worth doing  
(overhead to create threads)

vs

time to run concurrently)

issue: how do you know how many threads to create?

what if n things are already running?

⇒ maybe "tasks" is a better abstraction than threads?

⇒ tasking frameworks

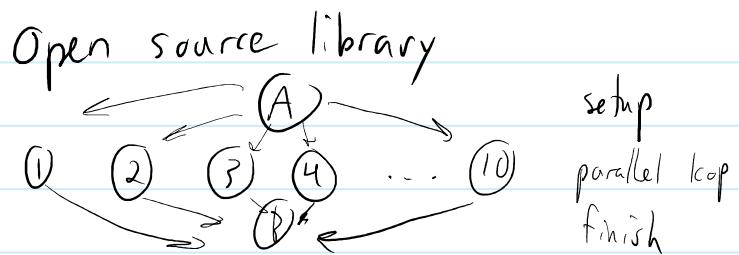
(create 100-thousands of tasks, let the runtime schedule them)

"Intel TBB"

↳ "taskflow"

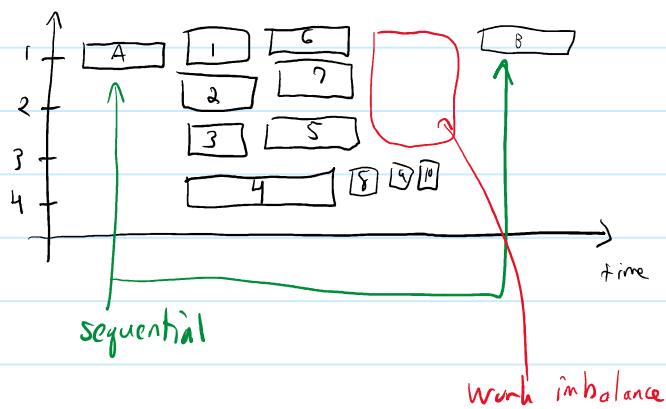
# Taskflow

Thursday, October 22, 2020 3:36 PM



Dependency  $A \rightarrow B$  means A needs to finish before B starts

Maybe schedule like this:



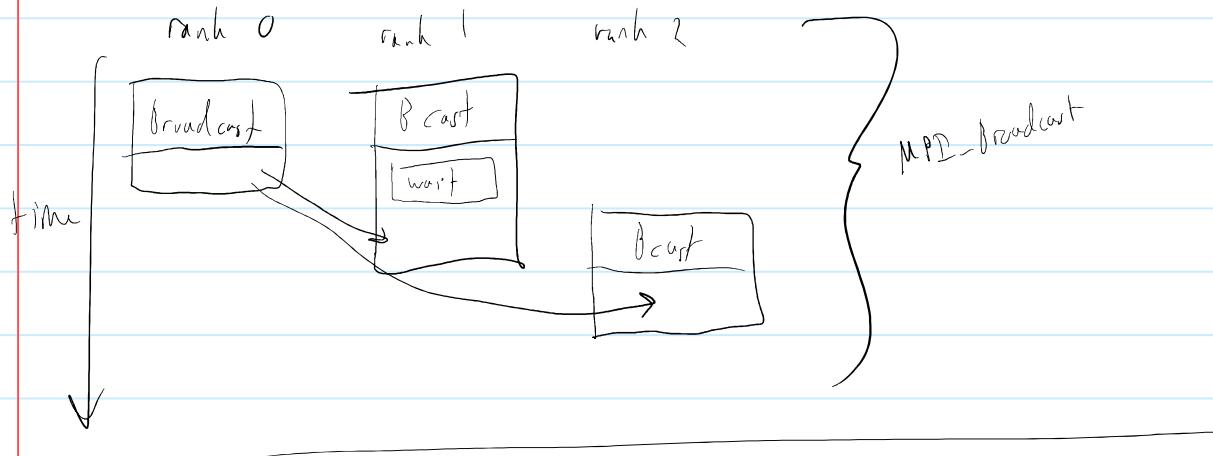
Tasking:

- Do not worry about # of threads
- Remove sequential steps if no dependency exists  
↳ better performance!

# MPI and linear algebra

Thursday, October 22, 2020 4:01 PM

- 1.) MPI\_Recv - send
- 2.) MPI\_BARRIER() - wait until everybody gets to this line  
(rarely necessary)  
use to sync. text output
- 3.) MPI\_Probe()  
- checks for a waiting message
- 4.) Collective operations (>2 participants)



## Linear Algebra

ingredients:  
- Sparse Matrix, Vector  
- operations:  $Ax$ ,  $x+y$ ,  $x \cdot y$ ,  $\|x\|$ ,  $\alpha x$   
- algorithms: GMRES, CG

Multithreading: Break up work and run on different threads

MPI: Split up the data!  
⇒ afterwards: aka split the work

why?  
- faster  
- larger problem

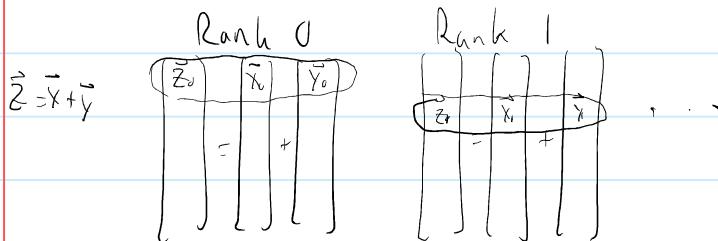
$\Rightarrow$  afterwards: aka split the work

- larger problem

$$\text{Vector } \vec{x} = \begin{cases} \#0 & [x_0] \\ \#1 & [ ] \\ \#2 & [ ] \\ \#3 & [x_{n-1}] \end{cases} \in \mathbb{R}^n$$

each rank stores a subset of all entries

each entry has a single owner



$\Rightarrow$  no communication

Assume rank  $m$  owns  $I_m \subseteq [0, N-1]$

for example  $[0, N-1] = \underbrace{I_0}_{0-10} \cup \underbrace{I_1}_{11-20} \cup \underbrace{I_2}_{21-30} \cup \underbrace{I_3}_{31-40}$

Index Set

$$\|x\| = \sqrt{\sum x_i^2}$$

1.) local part  $= \sum_{i \in I_m} x_i^2$

2.) MPI\_Reduce (... sum ...)

3.) sqrt(value) and return

$\vec{x} \cdot \vec{y}$  works the same

$$\vec{y} = A \vec{x}$$

$$\begin{cases} 0 & \left[ \vec{y}_0 \right] \\ 1 & \left[ \vec{y}_1 \right] \\ 2 & \left[ \vec{y}_2 \right] \\ 3 & \left[ \vec{y}_3 \right] \end{cases} = \begin{cases} A_{00} & A_{01} & A_{02} & 0 \\ 0 & A_{11} & 0 & 0 \\ 0 & 0 & A_{22} & 0 \\ 0 & 0 & 0 & A_{33} \end{cases} \begin{cases} \vec{x}_0 \\ \vec{x}_1 \\ \vec{x}_2 \\ \vec{x}_3 \end{cases} \stackrel{\#0}{=}$$

$\Rightarrow$  store matrix blocked by row in the

same way

$$\vec{y}_3 = \underbrace{A_{32}}_{\text{local}} \vec{x}_2 + \underbrace{A_{33} \cdot \vec{x}_3}_{\text{local}}$$

Import  $\vec{x}_2$  from rank 2

$\Rightarrow$  do not transfer matrix entries instead.

import entries from  $\vec{x}$  as needed

do not import all of  $\vec{x}$  (too expensive)  
as a pre-process (just with sparsity pattern)

compute  $\{j \mid A_{ij} \neq 0, i \in I_m\}$   
indices I need to import

1.) Find owner  $m$  of each index  $j$  ( $j \in I_m$ )

2.) For each rank listed in 1.), send them

the list of indices I will need

3.) Receive list of indices from certain ranks

### Implementation of $A\vec{x}$

1.) Send out parts of  $\vec{x}$  to others (based on setup above)

optimization: MPI\_Isend()

2.) Compute local part:

$$\vec{y}_m = A_{m,m} \cdot \vec{x}_m$$

3.) For each message from rank s:

grab  $\vec{x}_j$ , compute

$$\vec{y}_m^+ = A_{s,m} \vec{x}_s$$

4.) Wait for all sends to complete

Note: send early, receive as late as possible  
(do as much computation as possible)

$\Rightarrow$  hides the latency (time to send messages)

$\Rightarrow$  better parallel scaling!

$\therefore - L - L - \Rightarrow h.. L .. \therefore L$

⇒ better parallel scaling!

in contrast:  $\bar{x} \cdot \bar{y}$  has to wait.

## Preconditioner:

This is difficult & problem dependent.

Only multigrid (potentially) gives you  $\mathcal{O}(N)$  time

Given a preconditioner, solving  $Ax=b$   
 in  $O(\frac{N}{p})$  time ( $N = \# \text{ of DoFs}$ ,  $p = \# \text{ of ranks}$ )  
 is possible

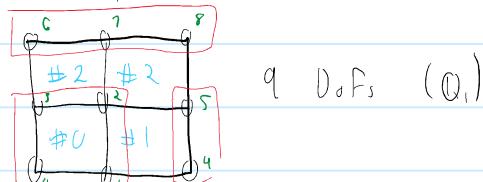
With these operations ( $Ax, xy, \dots$ ) GMRES/CG is equivalent to a sequential algorithm

missing: how to compute  $A \circ b$ ?

$\Rightarrow$  parallel F.E. assembly

$\Rightarrow$  rank  $m$  does not know the whole mesh

$\Rightarrow$  can only compute part of A.



1.) distribute the mesh (1 owner per cell)

$$\left( \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \right) \quad \#0$$

$$\left( \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \right) \quad \#1$$

$$\left( \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \right) \quad \#2$$

2.) assign DoFs to ranks:

if internal to a rank, assign to rank

if an interface: decide somehow

(deal. II assign for lower rank)

(deal.II assign to lower rank)

3.) Sort/number the unknowns so that they  
are consecutive by rank.

4.) assemble own cells

$A_{i,j}$  where  $i \neq I_m$  (non-local entries)  
 $\Rightarrow$  send this to owner of  $i$

(matrix.compress())

5.) done

# Running on palmetto

Thursday, November 5, 2020 3:46 PM

Tim has a page on how to do this

- Don't compute on the login node
- login node might be different than compute nodes  
I know this already
- Pay attention to large I/O
  - ⇒ 1.) be careful (not wasteful!)
  - 2.) special file system for large files  
(/scratch1 / USERNAME)

# Vector-values problems

Thursday, November 5, 2020 4:20 PM

Step 8: elasticity

20: mixed Laplace

22: Stokes

Instead of  $u: \Omega \rightarrow \mathbb{R}$

we solve for  $u: \Omega \rightarrow \mathbb{R}^n$

Stokes equation

Find  $\vec{u}, p$  s.t.  $-D\vec{u} + \nabla p = \vec{f}$   
 $\nabla \cdot \vec{u} = 0$

$\vec{u}(x) \in \mathbb{R}^d, p(x) \in \mathbb{R}$

$$D = \nabla \cdot \nabla$$

$$\vec{D} = \begin{bmatrix} 0 & \\ & 0 \end{bmatrix} \quad (d=2)$$

$$-\int \vec{v} \cdot (\vec{D}\vec{u}) + \int \vec{v} \cdot (\nabla p) = \int \vec{v} \cdot \vec{f} \quad \forall v \in V$$

$$\int q \cdot \nabla \cdot \vec{u} = 0 \quad \forall q \in Q$$

$$\Rightarrow (\nabla \vec{v}, \vec{D}\vec{u}) - (\nabla \cdot \vec{v}, p) = (\vec{v}, \vec{f}) \quad \forall v \in V$$

$$(q, \nabla \cdot \vec{u}) = 0$$

How do I get  $Ax=b$ ?

$\Rightarrow$  number all unknowns as  $\{\vec{\phi}_i\}$

$\vec{\phi}_i$  is a vector-valued basis function

$$u = \begin{bmatrix} u_x \\ u_y \\ p \end{bmatrix} \in X \subseteq \{f: \Omega \rightarrow \mathbb{R}^{d+1}\}$$

$$\int_{\Omega} \vec{\Phi}^T \begin{bmatrix} -\vec{D} & : & \nabla \\ : & \ddots & : \\ \vec{D} & : & 0 \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ p \end{bmatrix} = \int_{\Omega} \vec{\Phi}^T \cdot \vec{f}$$
$$\dots + \begin{bmatrix} \vec{\phi}_x^T \\ \dots \\ \vec{\phi}_y^T \end{bmatrix} \begin{bmatrix} \vec{f} \\ \dots \\ \vec{f} \end{bmatrix} \checkmark$$

$$\forall \underline{\Phi} = \begin{bmatrix} \phi_x^u \\ \phi_y^u \\ \phi_p \end{bmatrix} = \begin{bmatrix} \vec{\phi}^u \\ \phi_p \end{bmatrix} \in X$$

$$(\vec{\phi}^u, -\nabla \vec{u} + \nabla p) + (\phi^r, \nabla \cdot \vec{u}) = (\vec{\phi}^u, \vec{f})$$

$$\Rightarrow (\nabla \vec{\phi}^u, \nabla \vec{u}) - (\nabla \cdot \vec{\phi}^u, p) + (\vec{\phi}^r, \nabla \cdot \vec{u}) = (\vec{\phi}^u, \vec{f})$$

1 equation

$$X_h = \text{span} \left\{ \underline{\Phi}_i : \Omega \rightarrow \mathbb{R}^{d+1} \right\}$$

$$\sum_j \left[ (\nabla \phi_i^u, \nabla \phi_j^u) + (\nabla \cdot \phi_i^u, \phi_j^r) + (\phi_i^r, \nabla \cdot \phi_j^u) \right] \cdot u_j = (\phi_i^u, f)$$

$= A_{i,j}$

$$\Rightarrow A u = f$$

Specify  $X_h$ ?

Specify  $\phi_i^u$

Continuous space  $X$ :  $X = V \times Q$

LBB stability / inf-sup condition

$\Rightarrow V$  (velocity) needs to be "big enough" compared to  $Q$

$$\inf_{v \in V} \sup_{q \in Q} \frac{(\nabla \cdot v, q)}{\|v\|_1 \|q\|_0} \geq c > 0$$

$$V = H_0^1(\Omega), Q = L^2(\Omega) \quad \checkmark$$

discrete: more work (not always true!)

$$V_h = Q_{h+1}^d, Q_h = \mathbb{Q}_h$$

(Taylor-Hood elements)

There are other options

$$X_h = \text{span} \{ \underline{\Phi}_i \} = V_h \times Q_h$$

$$X_h = \text{span}\{\Phi_i\} = V_h \times Q_h$$

$$= Q_{h+1}^d \times Q_h$$

$$(in 2D) = Q_{hn} \times Q_{hn} \times Q_h$$

$$Q_2 = \text{span}\{1, x, y, x^2, y^2, xy, \dots, x^2y^2\}$$

on reference cell

$$Q_2: \Omega \rightarrow \mathbb{R}$$

on ref. cell:

$$X_h = \text{span}\left\{\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} x \\ 0 \end{bmatrix}, \begin{bmatrix} y \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} x^2y^2 \\ 0 \end{bmatrix}, \right.$$

$$\left. \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ x \end{bmatrix}, \dots, \begin{bmatrix} 0 \\ x^2y^2 \end{bmatrix}, \right.$$

$$\left. \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ x \end{bmatrix}, \dots, \begin{bmatrix} 0 \\ x^2y^2 \end{bmatrix} \right\}$$

$\Rightarrow$  extend shape functions to have  $d+1$  components (all but one are nonzero)

primitive FE space

$$X_h = Q_{hn}^d \times Q_h : \text{FESystem}(\text{FE-Q} \langle \dim \rangle(h+1),$$

rel. pres.

$$\dim, // \dim \text{ copies}$$

d+1 components

$$\text{FE-Q} \langle \dim \rangle(h)$$

1)       $\uparrow$        $\uparrow$   
 $\dim$  of ref. cell       $\dim$  of ref. cell

FESystem can be an arbitrary combination of finite elements, including FESystem.

$\Rightarrow$  FE w/ m components

access to components / shape functions?

$$\text{FE Values} :: \text{shape\_grad}(i, q) \quad \nabla \phi_i(x_q)$$

$$\text{shape value}(i, q) \quad \phi_i(x_q)$$

return the gradient / value for the only nonzero component

$\Rightarrow$  not useful

instead shape\\_grad\\_component(i, q, m)

$$\nabla (\Phi_i)_m(x_q) \in \mathbb{R}^d$$

shape\\_value\\_component(i, q, m)

$$\nabla (\Phi_i)_m(x_f) \in \mathbb{R}^n$$

shape-value-component ( $i, y, m$ )

$$(\Phi_i)_m(x_f) \in \mathbb{R}$$


---

even better: "extractors"

stokes 2D

$$\begin{aligned} \operatorname{div} \phi^u & \text{ shape-grad-component } (i, y, 0) [0] \\ \downarrow & + \text{ " } (i, y, 1) [1] \\ \frac{\partial}{\partial x} \phi_i^{ux} + \frac{\partial}{\partial y} \phi_i^{uy} & \Rightarrow \text{annoying, dim-dep} \end{aligned}$$

$\operatorname{div}$  only makes sense if you have  $d$  components

forming a vector in  $d$  dimensions

$$\vec{\Phi} = \begin{bmatrix} \vec{\phi}^u \\ \vec{\phi}^v \end{bmatrix}$$

$$\begin{aligned} \text{PEValues [vector extractor]} &:: \operatorname{divergence}(i, y) \in \mathbb{R} \\ &:: \operatorname{gradient}(i, y) \in \mathbb{R}^{d \times d} \\ &:: \operatorname{value}(i, y) \in \mathbb{R}^d \end{aligned}$$

$$\begin{aligned} \text{PEValues [scalar extractor]} &:: \operatorname{value}(i, y) \in \mathbb{R} \\ &:: \operatorname{gradient}(i, y) \in \mathbb{R}^d \end{aligned}$$

→ step-22

Note: For vector valued problems:

use extractors

or shape-value/grad if you

use component-index

Tim talked about dof numbering for  
the vector  $u$  and  $p$ . Can change that  
with things, DoFRenumbering

# Multigrid methods and step 22

Tuesday, November 10, 2020 3:46 PM

Goal: solve FEM problem in  $O(\frac{N}{p})$  time

$$N = \# \text{ DoFs}$$

$p$  = processors

All ingredients need to be  $O(\frac{N}{p})$

- numbering of DoFs ✓

- sparsity patterns ✓

- assembly ✓

- mat-vecs ✓

- if. solvers (✓)

- preconditioners !

↳ multigrid

$$-\nabla \cdot \boldsymbol{\varepsilon}(\mathbf{u}) + \nabla p = \mathbf{f} \quad \begin{matrix} \text{symmetrized} \\ \text{formulation} \end{matrix}$$

is equivalent to

$$-\Delta \mathbf{u} + \nabla p = \mathbf{f}$$

If:

- viscosity is constant (here  $\equiv 1$ )

- regularity  $\mathbf{u} \in [C^1]^d$

-  $\nabla \cdot \mathbf{u} = 0$

⇒ is this a good assumption in discrete setting?

# Block systems and numbering

Tuesday, November 17, 2020 3:35 PM

By default, `distribute_dofs()` distributes the unknowns by:

- 1.) cell by cell
- 2.) through objects: vertices, faces, cells
- 3.) Component

(ex.)

$$\begin{bmatrix} u_x \\ u_y \\ p \\ u_x \\ u_y \\ \vdots \end{bmatrix} \quad \begin{bmatrix} u_x \\ u_y \\ u_x \\ u_y \\ \vdots \\ \vdots \end{bmatrix}$$

either is ok, sometimes we want to control this however

DofRenumbering : permutation  $[0, N) \rightarrow [0, N)$

component-wise:

for each component  $c$ , specify an index or block  
block-component [ $c$ ]

The reordering first enumerates all Dofs with  
block-component [ $c$ ] = 0, then 1, then 2, ...

$$\begin{bmatrix} u_x \\ u_y \\ p \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix} \quad \text{velocity first, then all pressures}$$
$$\begin{bmatrix} u_x \\ u_y \\ p \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix} \quad \begin{bmatrix} u_x; p \\ u_y; p \\ p \end{bmatrix}$$
$$\begin{bmatrix} u_x \\ u_y \\ p \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix} \quad \begin{array}{l} x \text{ vel, } y \text{ vel, pressure} \\ \begin{bmatrix} u_x; u_y; p \\ \vdots; \vdots; \vdots \end{bmatrix} \end{array}$$

Note: Assembly does not need to know/change hand  
on numbering  
 $\Rightarrow$  only for solves

$\Rightarrow$  only for solvers

Note: combine ordering:

- 1.) Cuthill-McKee
  - 2.) Component-wise
- } step-2

Many other options

### For Block Linear Systems

arbitrary grouping into blocks

$\Rightarrow$  independent of components

$\Rightarrow$   $n \times n$  array of SparseMatrix/SparsePattern

$\Rightarrow$  block

# Debug and release mode

Tuesday, November 17, 2020 4:24 PM

Switch using  
"make debug"  
"make release"

## debug mode

- + can delay using gbb and other tools
- turns off all optimizations ( $\Rightarrow$  slow)
- good for debugging

- deal. II has many consistency checks in the library

to help you find bugs

"defensive programming"

$\Rightarrow$  only in debug mode

$\Rightarrow$  release mode 2-10x faster, not helpful

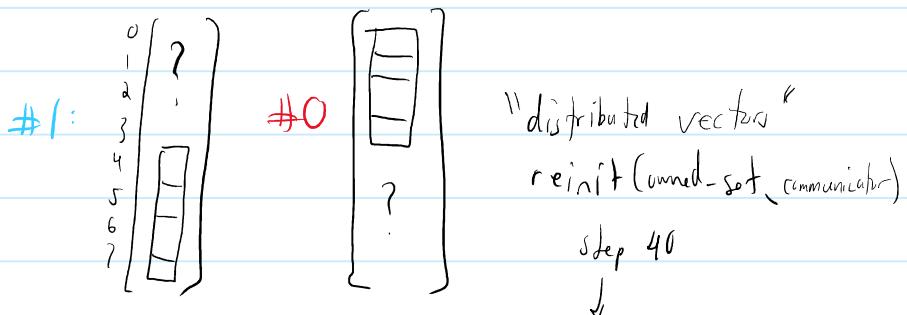
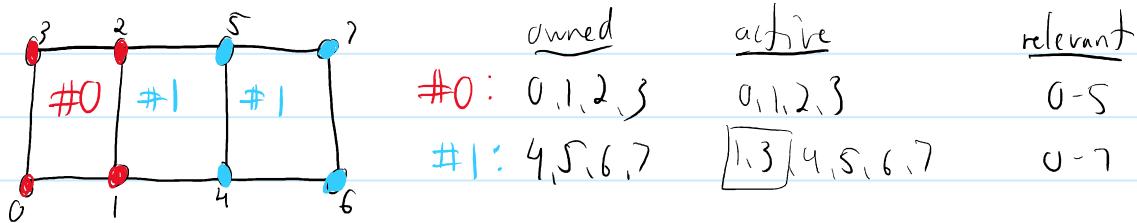
(use only for large computations)

## Distributed/ghosted vectors

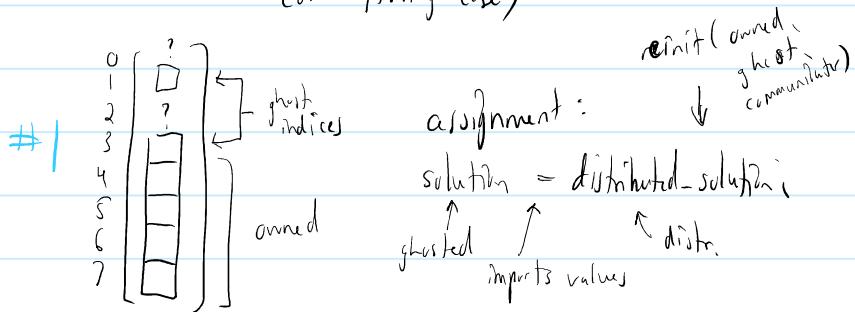
Thursday, November 19, 2020 3

3:50 PM

Index Sets: owned, active, relevant



"ghosted vectors", active or relevant  
(or anything else)



ghosted vectors : dangerous to allow modifications  
(out of date information)

$\Rightarrow$  ghosted vectors are read-only

Create them via assignment from distr. vector

## distributed vectors

## - assembly

### - Solvers

- modified

(constraints, ...)

## ghosted vectors

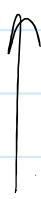
-output (at least "active")

- read values during assembly?

old timestep, nonlinear iteration

- Computing errors (at least)

(constraint,...)



- computing errors (at least active for DG: relevant)
- error estimates  
(at least relevant)



Viewpoint: "linear algebra" Viewpoint: "PDE"

# Time dependent problems

Thursday, November 19, 2020 4:16 PM

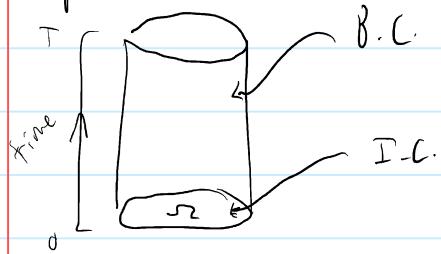
ex.) heat equation:  $\frac{d}{dt}u - \nabla \cdot \kappa \nabla u = f, \forall x \in \Omega, \forall t \in [0, T]$

$$u: \Omega \times [0, T] \rightarrow \mathbb{R}$$

$$u(x, 0) = u_0(x), \forall x \in \Omega$$

$$u(x, t) = u_t, \forall x \in \Omega, t \in (0, T)$$

Space-time cylinder



ex.) Navier-Stokes Equations

$$\frac{d}{dt}u - \nu \Delta u + u \cdot \nabla u + \nabla p = f + I.C., B.C.$$

$$\nabla \cdot u = 0$$

$$u: \Omega \times [0, T] \rightarrow \mathbb{R}^d$$

$$p: \Omega \times [0, T] \rightarrow \mathbb{R}$$

ex.) Wave Equation

$$\frac{d^2}{dt^2}u - \Delta u = f \quad (\text{step-23})$$

need  $u$  &  $\frac{du}{dt}$  at  $t=0$  for I.C.

Spaces?  $u(t): \Omega \rightarrow \mathbb{R} \rightarrow$  appropriate Sobolev spaces

regularity in time?

$$C^1([0, T]; V), \| \cdot \| = \sup_{t \in [0, T]} \left( \|u(t)\|_V + \left\| \frac{d}{dt}u(t) \right\|_V \right)$$

$$L^p([0, T]; V), \| \cdot \| = \left( \int_0^T \|u(t)\|_V^p dt \right)^{1/p}$$

## Theory:

- existence & uniqueness is difficult and problem dependent
- parabolic problems: easy like Lax-Milgram (heat eqn)  
$$(u_t, v) + a(t; u, v) = (f(t), v)$$
a bilinear form + bounded + coercive  
 $\Rightarrow \exists!$  solution

Computing?

### a.) Method of Lines (discretize space then time)

1.) discretize in space

(weak form  $\rightarrow$  Galerkin  $\rightarrow Ax=b$ )

but your  $u_h = \sum \phi_i u_i$  still time-dependent

$$u_h(t) = \sum \phi_i u_i(t) \leftarrow$$

$$\frac{d}{dt} \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} + A \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = b \quad \text{coefficients are functions of time}$$

$\Rightarrow$  system of ODEs

$\Rightarrow$  ODE solver

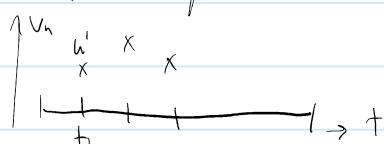
problems

- large Dofs difficult
- cannot change the mesh
- difficult if  $A$  (PDE) depends on  $t$

### b.) Rothe's method (disc. time, then space)

$$0 = t_0 < t_1 < \dots < t_N = T$$

$$u(t_n) \approx u_h^n \in V_h$$



$$\frac{d}{dt} u = f(t, u)$$

$$\text{explicit Euler: } \frac{d}{dt} u = \frac{u^{n+1} - u^n}{\Delta t}$$

$$\text{explicit Euler: } \frac{d}{dt} u = \frac{u^{n+1} - u^n}{\Delta t}$$

$$\frac{u^{n+1} - u^n}{\Delta t} = f(t_n, u^n)$$

implicit Euler (backward)

$$\frac{u^{n+1} - u^n}{\Delta t} = f(t_{n+1}, u^{n+1})$$

BDF (implicit)

Rk (either)

:

when to use explicit vs implicit?

stability (conditional)

explicit methods are (most of the time) only conditionally stable  $\Rightarrow \Delta t < X(h, \text{POE}, \dots)$

generally: implicit methods are unconditionally stable

explicit methods:

$$\frac{1}{\Delta t} u^{n+1} = f(t^n, u^n) + \underbrace{f(\dots) + c_1 u^n + c_2 u^{n-1} + \dots}_{\text{known}}$$

$\Rightarrow$  no PDE solve necessary!

often: weak form

$$\frac{1}{\Delta t} (v, u^{n+1}) = (v, f(t^n, u^n)) + \dots$$

$\nwarrow$  mass matrix  $\Rightarrow$  invert/solve for mass matrix

BDF2: 2nd order, implicit (popular, default choice)

$$\frac{3}{2\Delta t} (u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}) = f(t^{n+1}, u^{n+1})$$

note: initial solve requires 2 old solutions!

how to get  $u^1$ ?

start up method (use implicit Euler for  $u^1$ )

start up method (use implicit Euler for  $u^1$ )  
⇒ could destroy convergence

⇒ stationary PDE solve for  $u^{n+1}$

example: heat equation + BDF2

$$\frac{3}{2\Delta t} u^{n+1} - \nabla \cdot k \nabla u^{n+1} = f + \frac{2}{\Delta t} u^n - \frac{1}{2\Delta t} u^{n-1}$$

⇒ weak form ⇒ assemble & solve for  $u^{n+1}$

# Nonlinear, time-dependent problems

Tuesday, December 1, 2020 4:19 PM

NSE:

$$\frac{d}{dt} u + \nabla \cdot u + u \cdot \nabla u + \nabla p = f$$
$$\nabla \cdot u = 0$$

a) explicit in time

⇒ at most a single mass matrix solve

b) implicit in time:

$$C u^{n+1} - \nabla \cdot u^{n+1} + \underbrace{u^{n+1} \cdot \nabla u^{n+1}}_{\text{nonlinear}} + \nabla \cdot p^{n+1} = f$$
$$\nabla \cdot u^{n+1} = 0$$

options:

(1)  $u^{n+1} \cdot \nabla u^{n+1} \approx u^n \cdot \nabla u^n$  explicit nonlinear term

⇒ PDE does not change over time

⇒ reuse matrix/preconditioner

stability? no longer unconditional?

better: extrapolation or explicit method to

approximate  $u \cdot \nabla u$ .

[IMEX methods]

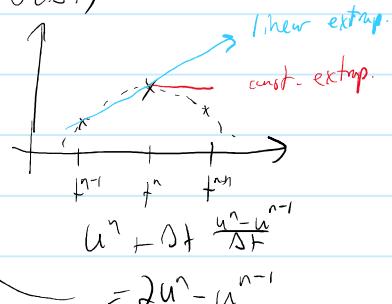
(B2)  $u^{n+1} \cdot \nabla u^{n+1} \approx u^* \cdot \nabla u^{n+1}$  (linearized, implicit)

$u^*$  can be  $u^n \Rightarrow$  error  $\sim O(\Delta t)$

or extrapolation:

$$u^* = 2u^n - u^{n-1}$$

(to be paired with  
2nd order method)



(B3) keep  $u^{n+1} \cdot \nabla u^{n+1}$

⇒ Picard/Newton iteration @ each step  
how expensive?

# Boundary Conditions

Thursday, December 3, 2020 3:58 PM

- Boundary conditions are required for us to think about

- Required for unique solvability,  $\Delta u = f$  is only solvable up to a constant.

Dirichlet,  $u|_{\partial\Omega} = g \rightarrow \text{constraint}$

Neumann  $\nabla u \cdot n = g$

→ 1.) integration by parts

2.) replace  $\nabla u \cdot n$  by  $g$

3.) move  $\int_{\partial\Omega} v \cdot \nabla u \, ds$  to RHS  $\int_{\text{boundary}} v \, ds$

if  $g \neq 0$ : assembly PEFaceValues

$g = 0$ :  $\int_{\partial\Omega} v \cdot g \, ds = 0 \rightarrow \text{do nothing}$

Robin:  $c_1 u + c_2 \nabla u \cdot \hat{n} = g$

$\Rightarrow \nabla u \cdot n = \frac{1}{c_2}(g - c_1 u) \rightarrow \text{assemble}$

No normal flux:  $\hat{u} \cdot n = 0$

"free slip"

compute\_nr\_normal\_flux\_constraints

No tangential flux:  $\hat{u} \times n = \vec{0}$

→ can be combined

# Linear Solvers

Thursday, December 3, 2020 4:15 PM

- small problems / starting out / not parallel:  
⇒ use direct solver, solver Direct UMFPack step 29  
(Matlab backslash)

why?

- hard to beat (for small/medium problems)
- no tolerance to pick (no accuracy problems)
- no convergence issues
- not invertible? → solver will fail

limits:

- 3d (even medium sized)
- 100k + Dofs
- parallelization beyond a single workstation

• Alternative: Krylov solvers

↳ difficult to parallel, often requires PDE knowledge

• Krylov guideline:

SPO  $\rightarrow$  CG

S  $\rightarrow$  MINRES

else  $\rightarrow$  GMRES

$O(n)$

• Preconditioning: want

- 10-50 iterations
- h independent (hard)
- parameter indep. (hard)

• approach

- 1.) decompose PDE on blocks ( $\approx$  components)

1.) decompose PDE on blocks ( $\approx$  components)

2.) block factorization

3.) for each block : by type of PDE term

Laplace  $\rightarrow$  AMG/GMG

mass  $\rightarrow$  ILU