## Divide and...

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MIM Colloquium 2017/11/9
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## System of linear equations

## Problem

Given nonsingular $L \in \mathbb{R}^{N \times N}$ and $b \in \mathbb{R}^{N}$, find $x \in \mathbb{R}^{N}$ satisfying

$$
\left\{\begin{array}{cc}
L_{11} x_{1}+L_{12} x_{2}+\ldots L_{1 N} x_{N} & =b_{1} \\
L_{21} x_{1}+L_{22} x_{2}+\ldots L_{2 N x_{N}} & =b_{2} \\
\vdots & \\
L_{N 1} x_{1}+L_{N 2} x_{2}+\ldots L_{N N} x_{N} & =b_{N}
\end{array}\right.
$$

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\end{array}\right.
$$

Can anything be more boring?

## A solved problem

Find $x \in \mathbb{R}^{N}$ such that

$$
L x=b
$$

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- Gaussian elimination known for about 2000 years; costs $O\left(N^{3}\right)$
- Cramer's rule (much) more costly: $O(N!)$
- Complexity: still an open question
- We know $O\left(N^{\omega}\right)$ algorithms exist with $\omega<3$.


## Strassen's matrix multiply

- Matrix-matrix multiplication $X=L \cdot B$ as complex as solving $L x=b$


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- Divide and...

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\left[\begin{array}{ll}
X_{11} & X_{12} \\
X_{21} & X_{22}
\end{array}\right]=\left[\begin{array}{ll}
L_{11} & L_{12} \\
L_{21} & L_{22}
\end{array}\right] \cdot\left[\begin{array}{ll}
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## Strassen's matrix multiply

- Divide and...

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B_{11} & B_{12} \\
B_{21} & B_{22}
\end{array}\right]
$$

Naively,

$$
\begin{aligned}
& X_{11}=L_{11} B_{11}+L_{12} B_{21} \\
& X_{12}=L_{11} B_{12}+L_{12} B_{22} \\
& X_{21}=L_{21} B_{11}+L_{22} B_{21} \\
& X_{22}=L_{21} B_{12}+L_{22} B_{22} .
\end{aligned}
$$

gives a recursive "divide-and-conquer" algorithm.

- Complexity: still $O\left(N^{3}\right)$.


## Strassen's matrix multiply

- Divide and... think again:

$$
\left[\begin{array}{ll}
X_{11} & X_{12} \\
X_{21} & X_{22}
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L_{21} & L_{22}
\end{array}\right] \cdot\left[\begin{array}{ll}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{array}\right]
$$

Reduce number of matrix multiplications to seven!

$$
\begin{array}{lc}
X_{11}=P_{1}+P_{4}-P_{5}+P_{7} & P_{1}=\left(L_{11}+L_{22}\right)\left(B_{11}+B_{22}\right), \\
X_{12}=P_{3}+P_{5} & P_{2}=\left(L_{21}+L_{22}\right) B_{11} \\
X_{21}=P_{2}+P_{4} & \vdots \\
X_{22}=P_{1}+P_{3}-P_{2}+P_{6}, & P_{7}=\left(L_{12}-L_{22}\right)\left(B_{21}+B_{22}\right)
\end{array}
$$

Complexity: $O\left(N^{\log _{2} 7}\right) \approx O\left(N^{2.808 \ldots}\right)$

[^0]Find $x \in \mathbb{R}^{N}$ such that

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If $N=10^{6}$, a PC would have

- computed the solution after $10^{9}$ seconds
if straightforward Gaussian elimination (e.g. LAPACK's DGESV) was used.

Find $x \in \mathbb{R}^{N}$ such that

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If $N=10^{6}$, a PC would have

- computed the solution after $10^{9}$ seconds i.e. $\approx 32$ years
if straightforward Gaussian elimination (e.g. LAPACK's DGESV) was used.


## Large systems are intractable for simple Gaussian elimination

Find $x \in \mathbb{R}^{N}$ such that

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If $N=10^{6}$, a PC would have

- computed the solution after $10^{9}$ seconds i.e. $\approx 32$ years
- needed $10^{13}$ bytes of memory i.e. $\approx \mathbf{9 , 0 0 0} \mathbf{G B}$
if straightforward Gaussian elimination (e.g. LAPACK's DGESV) was used.


## Outline

1. Large systems of linear equations: where do they come from?
2. Systems with (lots of) structure: finite elements for PDEs
3. Solving large sparse systems
4. A sidenote: another class of structured sparse matrices
5. Domain decomposition for PDEs
6. Splitting equations
7. Summing up

Large systems of linear equations: where do they come from?

## The beauty of sparse matrices



Davis, Hu (2011) ACM Trans. Math. Softw.

## Economic problem


$N=15,575$

## Quantum chromodynamics


$N=3,072$

Macroeconomic problem


Wiliams@mac_econ_fwd500. 413000 nodes, 1273389 edges.


$$
N=206,500
$$

## KKT system, nonconvex optimization



$N=16,554$

## Financial portfolio optimization



$$
N=74,752
$$

## Structural engineering, finite element



$N=15,449$

## Structural engineering, finite element


$N=15,449$


## Structural engineering, finite element

This is how a sparse matrix really looks like:

|  | 63929 |  | 444 |  | 10024 |  | 53461 |  | 0 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| rsa |  |  |  | 875 |  | 75 | 1603 | 383 |  |  |
| (11I7) | (16I5) |  |  | (3E23.15) |  |  |  |  |  |  |
| 1 | 25 | 48 | 70 | 103 | 135 | 166 | 199 | 231 | 262 | 295 |
| 327 | 358 | 391 | 423 | 454 | 487 | 519 | 550 | 583 | 615 | 646 |
| 679 | 711 | 742 | 775 | 807 | 838 | 871 | 903 | 934 | 967 | 999 |
| 1030 | 1063 | 1095 | 1126 | 1147 | 1167 | 1186 | 1216 | 1245 | 1273 | 1315 |
| 1356 | 1396 | 1438 | 1479 | 1519 | 1561 | 1602 | 1642 | 1684 | 1725 | 1765 |
| 1807 | 1848 | 1888 | 1930 | 1971 | 2011 | 2053 | 2094 | 2134 | 2176 | 2217 |
| 2257 | 2299 | 2340 | 2380 | 2422 | 2463 | 2503 | 2545 | 2586 | 2626 | 2653 |
| 2679 | 2704 | 2734 | 2763 | 2791 | 2833 | 2874 | 2914 | 2956 | 2997 | 3037 |

$$
\begin{array}{llll}
0.409672687144694 \mathrm{E}-14 & -0.270324344694379 \mathrm{E}-11 & 0.462322806286147 \mathrm{E}-14 \\
-0.125103474334186 \mathrm{E}-15 & -0.157968969372661 \mathrm{E}-11 & 0.120545535566847 \mathrm{E}-14 \\
-0.415025707341799 \mathrm{E}-14 & -0.518149596242225 \mathrm{E}-12 & 0.850962616131678 \mathrm{E}-13 \\
-0.209551074847814 \mathrm{E}-12 & -0.107421047460559 \mathrm{E}-11 & 0.340867474174134 \mathrm{E}-12 \\
-0.371312672815900 \mathrm{E}-13 & -0.562016116896941 \mathrm{E}-12 & 0.811101830369373 \mathrm{E}-13 \\
0.198413464034039 \mathrm{E}-12 & -0.375360224439469 \mathrm{E}-12 & 0.141281556760829 \mathrm{E}-13 \\
-0.805393690795621 \mathrm{E}-12 & 0.267683729453480 \mathrm{E}-11 & 0.861749802483021 \mathrm{E}-16 \\
-0.113997243532461 \mathrm{E}-15 & -0.423020243608237 \mathrm{E}-12 & -0.143670337428612 \mathrm{E}-13 \\
0.830097314588988 \mathrm{E}-12 & -0.580299367504821 \mathrm{E}-12 & -0.811121342725180 \mathrm{E}-13 & \\
-0.198394255770204 \mathrm{E}-12 & -0.107673095703232 \mathrm{E}-11 & -0.340570288494983 \mathrm{E}-12 & 13 \\
0.124288644083145 \mathrm{E}-13 & -0.501209266056193 \mathrm{E}-12 & -0.852387929702163 \mathrm{E}-13 & 1 \\
0.209644642907451 \mathrm{E}-12 & 0.454179546572026 \mathrm{E}-10 & 0.256700564221894 \mathrm{E}-11 & \\
0.248365328762197 \mathrm{E}-16 & 0.885615735926505 \mathrm{E}-11 & 0.482064121963914 \mathrm{E}-13 & \\
0.109981819279385 \mathrm{E}-14 & -0.598541997591639 \mathrm{E}-11 & -0.124576307872633 \mathrm{E}-11 & \\
0.463130261987941 \mathrm{E}-14 & -0.198244879116781 \mathrm{E}-10 & -0.708476661679811 \mathrm{E}-12 &
\end{array}
$$

## Parabolic diffusion-convection-reaction, finite element



Wissgott@parabolic_fem. 525825 nodes, 1574400 edges.

$N=525,825$

Fluid dynamics, finite element

$N=2,017,169$

## Systems with (lots of) structure: finite elements for PDEs

## A model PDE: diffusion equation

Find $u: \mathbb{R}^{d} \supset \Omega \rightarrow R$ satisfying

$$
\begin{aligned}
-\operatorname{div}(\rho(x) \nabla u(x)) & =f(x) \quad \forall x \in \Omega, \\
u(x) & =0 \quad \forall x \in \partial \Omega .
\end{aligned}
$$

For example: $u$ - temperature, $\rho$ - thermal conductivity, $f$ - external heating

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For example: $u$ - temperature, $\rho$ - thermal conductivity, $f$ - external heating

Assume $\rho(x)=1$.

## A model PDE: diffusion equation

Find $u: \mathbb{R}^{d} \supset \Omega \rightarrow R$ satisfying

$$
\begin{aligned}
-\Delta u(x) & =f(x) \quad \forall x \in \Omega, \\
u(x) & =0 \quad \forall x \in \partial \Omega .
\end{aligned}
$$

## Problem

Find $u \in H_{0}^{1}(\Omega)$ such that

$$
\int_{\Omega} \nabla u \cdot \nabla v d x=\int_{\Omega} f v d x \quad \forall v \in H_{0}^{1}(\Omega) .
$$

## Finite element approximation

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$$

## Problem (discrete)

Find $u_{h} \in V_{h} \subset H_{0}^{1}(\Omega)$ such that

$$
\int_{\Omega} \nabla u_{h} \cdot \nabla v_{h} d x=\int_{\Omega} f v_{h} d x \quad \forall v_{h} \in V_{h} .
$$

Here $V_{h}$ is finite dimensional. How to choose it?

## Finite element approximation

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$$
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$$

Here $V_{h}$ is finite dimensional. How to choose it?
Divide and... approximate wisely.

## Finite elements



Divide $\Omega$ into smaller elements:

- Triangulation $\mathcal{T}_{h}$ consisting of elements $\kappa$.


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- Triangulation $\mathcal{T}_{h}$ consisting of elements $\kappa$.

$$
V_{h}=\left\{v \in C(\Omega) \cap H_{0}^{1}(\Omega): v_{\left.\right|_{\kappa}} \in P_{1}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \subset H_{0}^{1}(\Omega)
$$

## Finite elements



- Triangulation $\mathcal{T}_{h}$ consisting of elements $\kappa$.

$$
V_{h}=\left\{v \in C(\Omega) \cap H_{0}^{1}(\Omega): v_{\left.\right|_{\kappa}} \in P_{1}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \subset H_{0}^{1}(\Omega)
$$

More generally,

$$
V_{h}^{p}=\left\{v \in C(\Omega) \cap H_{0}^{1}(\Omega): v_{l_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} .
$$

## Experiment: h-approximation vs p-approximation

Consider true solution to $-\Delta u=f$ :

## Experiment: $h$-approximation vs $p$-approximation

Consider true solution to $-\Delta u=f$ :

How well can it be approximated by the finite element method?

## Finite element $h$-approximation vs $p$-approximation

fixed $p=1$
decrease $h$
fixed $h=1 / 2$
increase $p$

$$
\begin{gathered}
h=1 / 2 \\
\mathrm{~N}=9
\end{gathered}
$$

$$
p=1
$$

$$
\mathrm{N}=9
$$

## $h$-approximation vs $p$-approximation

$$
\begin{gathered}
h=1 / 2 \\
\mathrm{~N}=9
\end{gathered}
$$

$$
p=1
$$

$$
N=9
$$

## $h$-approximation vs $p$-approximation

$$
\text { fixed } p=1
$$

$$
\text { fixed } h=1 / 2
$$

$$
\begin{gathered}
h=1 / 2^{2} \\
\mathrm{~N}=25
\end{gathered}
$$

$$
p=2
$$

$$
N=25
$$

## $h$-approximation vs $p$-approximation

$$
\text { fixed } p=1
$$

$$
\text { fixed } h=1 / 2
$$

$h=1 / 2^{3}$
$p=3$
$\mathrm{N}=81$
$\mathrm{N}=49$

## $h$-approximation vs $p$-approximation

$$
\text { fixed } p=1
$$

$$
\text { fixed } h=1 / 2
$$

$$
\begin{gathered}
h=1 / 2^{4} \\
\mathrm{~N}=289
\end{gathered}
$$

$$
p=4
$$

$$
N=81
$$

## $h$-approximation vs $p$-approximation

$$
\text { fixed } p=1
$$

$$
\text { fixed } h=1 / 2
$$

$\begin{array}{cr}h=1 / 2^{5} & p=5 \\ \mathrm{~N}=1089 & \mathrm{~N}=121\end{array}$

## More finite elements...

## Periodic Table of the Finite Elements


A.

...


Arnold, Logg (2014) SIAM News

## What are discontinuous finite elements?

'Continuous' finite elements:


$$
V_{h}=\left\{v \in C(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \subset H_{0}^{1}(\Omega)
$$

## Discontinuous finite elements

'Discontinuous' finite elements:


$$
V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \nsubseteq H_{0}^{1}(\Omega)
$$

...allow for using discontinuous basis functions.

## Discontinuous finite elements

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$$
V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \nsubseteq H_{0}^{1}(\Omega)
$$

...allow for using discontinuous basis functions.
More degrees of freedom, but: easy $h$-refinement and $p$-refinement (nonconforming elements allowed by design)

## DGFEM approximation of the model problem

## Problem

Find $u \in H_{0}^{1}(\Omega)$ such that

$$
\int_{\Omega} \nabla u \cdot \nabla v d x=\int_{\Omega} f v d x \quad \forall v \in H_{0}^{1}(\Omega) .
$$

Problem (DGFEM approximation)

$$
\begin{gathered}
u_{h}, v_{h} \in V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} \\
\sum_{\kappa \in \mathcal{T}_{h}} \int_{\kappa} \nabla u_{h} \cdot \nabla v_{h} d x
\end{gathered}
$$

$$
=\left(f, v_{h}\right)_{\Omega}
$$

Divide and... reconnect (weakly).

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Problem (DGFEM approximation)

$$
u_{h}, v_{h} \in V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\}
$$

$$
\sum_{\kappa \in \mathcal{T}_{h}} \int_{\kappa} \nabla u_{h} \cdot \nabla v_{h} d x+\sum_{e \in \mathcal{E}_{h}} \int_{e} \frac{\gamma p^{2}}{h}\left[u_{h}\right] \cdot\left[v_{h}\right] d \sigma
$$

$$
=\left(f, v_{h}\right)_{\Omega}
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Divide and... reconnect (weakly).

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$$

$$
\begin{aligned}
& \sum_{\kappa \in \mathcal{T}_{h}} \int_{\kappa} \nabla u_{h} \cdot \nabla v_{h} d x+\sum_{e \in \mathcal{E}_{h}} \int_{e} \frac{\gamma p^{2}}{h}\left[u_{h}\right] \cdot\left[v_{h}\right] d \sigma \\
&-\sum_{e \in \mathcal{E}_{h}} \int_{e}\left\{\nabla u_{h}\right\}_{\omega} \cdot\left[v_{h}\right] d \sigma \\
&=\left(f, v_{h}\right)_{\Omega}
\end{aligned}
$$

Divide and... reconnect (weakly).

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Divide and... reconnect (weakly).

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$$

Problem (DGFEM approximation)

$$
\begin{aligned}
u_{h}, v_{h} \in V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}}\right. & \left.\in P_{p}(\kappa) \forall \kappa \in \mathcal{T}_{h}\right\} \\
\mathcal{A}_{h}\left(u_{h}, v_{h}\right) \equiv \sum_{\kappa \in \mathcal{T}_{h}} & \int_{\kappa} \nabla u_{h} \cdot \nabla v_{h} d x+\sum_{e \in \mathcal{E}_{h}} \int_{e} \frac{\gamma p^{2}}{h}\left[u_{h}\right] \cdot\left[v_{h}\right] d \sigma \\
& -\sum_{e \in \mathcal{E}_{h}} \int_{e}\left\{\nabla u_{h}\right\}_{\omega} \cdot\left[v_{h}\right] d \sigma \\
& -\sum_{e \in \mathcal{E}_{h}} \int_{e}\left\{\nabla v_{h}\right\}_{\omega} \cdot\left[u_{h}\right] d \sigma=\left(f, v_{h}\right)_{\Omega}
\end{aligned}
$$

Divide and... reconnect (weakly).

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## Problem (DGFEM approximation)

$u_{h}, v_{h} \in V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\}$

$$
\mathcal{A}_{h}\left(u_{h}, v_{h}\right) \equiv \sum_{\kappa \in \mathcal{T}_{h}} \int_{\kappa} \nabla u_{h} \cdot \nabla v_{h} d x+\ldots \text { iterface terms... }=\left(f, v_{h}\right)_{\Omega}
$$

Divide and... reconnect (weakly).

[^1]
## FEM/DGFEM stiffness matrix

Find $u_{h} \in V_{h}^{p}$ such that

$$
\mathcal{A}_{h}\left(u_{h}, v_{h}\right)=\left(f, v_{h}\right)_{\Omega} \quad \forall v_{h} \in V_{h}^{p}
$$

Let $V_{h}^{p}=\operatorname{span}\left\{\phi_{1}, \ldots, \phi_{N}\right\}$ and expand $u_{h}=\sum_{i} u_{i} \phi_{i}$.

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$$

Let $V_{h}^{p}=\operatorname{span}\left\{\phi_{1}, \ldots, \phi_{N}\right\}$ and expand $u_{h}=\sum_{i} u_{i} \phi_{i}$.
Then $u=\left[u_{1}, \ldots, u_{N}\right] \in \mathbb{R}^{N}$ satisfies

$$
L u=b
$$

where

$$
L_{i j}=\mathcal{A}_{h}\left(\phi_{i}, \phi_{j}\right), \quad i, j=1, \ldots, N .
$$

## FEM/DGFEM stiffness matrix

Find $u_{h} \in V_{h}^{p}$ such that

$$
\mathcal{A}_{h}\left(u_{h}, v_{h}\right)=\left(f, v_{h}\right)_{\Omega} \quad \forall v_{h} \in V_{h}^{p}
$$

Let $V_{h}^{p}=\operatorname{span}\left\{\phi_{1}, \ldots, \phi_{N}\right\}$ and expand $u_{h}=\sum_{i} u_{i} \phi_{i}$.
Then $u=\left[u_{1}, \ldots, u_{N}\right] \in \mathbb{R}^{N}$ satisfies

$$
L u=b
$$

where

$$
L_{i j}=\mathcal{A}_{h}\left(\phi_{i}, \phi_{j}\right), \quad i, j=1, \ldots, N
$$

Properties of stiffness matrix $L$ :

- symmetric and positive definite: $L=L^{T}>0$
- $N$ can be as large as one can afford ( $h \searrow 0, p \nearrow$ large)
- sparse: each row has only a few nonzero elements


## Solving large sparse systems

## No need for Gaussian elimination

Approximate solution to $L x=b$ is a reasonable choice.

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Model iteration:

$$
x_{n+1}=x_{n}+\tau D^{-1}\left(b-L x_{n}\right) \quad \text { (damped Jacobi iteration) }
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$$
L=D-A, \quad(D \text { is the diagonal of } L)
$$

Divide and... be patient: for $L=L^{T}>0$,

- with optimal damping $\tau$, convergence driven by the condition number

$$
\kappa=\frac{\lambda_{\max }\left(D^{-1} L\right)}{\lambda_{\min }\left(D^{-1} L\right)}
$$

- error reduction:

$$
\left\|x_{n+1}-x\right\| \lesssim \underbrace{\frac{\kappa-1}{\kappa+1}}_{=\gamma}\left\|x_{n}-x\right\|
$$

## Iterative solution of $L x=b$

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Our L from finite element method is ill-conditioned: $p \nearrow \infty, h \searrow 0$ and

$$
\kappa(L)=O\left(p^{4} / h^{2}\right)
$$

$D^{-1} L$ is ill-conditioned, too.

## Iterative solution of $L x=b$

- Model iterative method:

$$
x_{n+1}=x_{n}+\tau P^{-1}\left(b-L x_{n}\right)
$$

- error reduction factor $\gamma=\frac{\kappa-1}{\kappa+1}$ depends on $\kappa=\frac{\lambda_{\max }\left(P^{-1} L\right)}{\lambda_{\min }\left(P^{-1} L\right)}$


## Problem

If $P^{-1} L$ is ill-conditioned: $\kappa \gg 1 \quad \Longrightarrow \quad \gamma \approx 1$.
Our L from finite element method is ill-conditioned: $p \nearrow \infty, h \searrow 0$ and

$$
\kappa(L)=O\left(p^{4} / h^{2}\right)
$$

$D^{-1} L$ is ill-conditioned, too.
Divide and... use a good preconditioner $P$.
If $P^{-1} L$ is well-conditioned: $\kappa \approx 1 \quad \Longrightarrow \quad \gamma \ll 1$.

## What makes a good preconditioner?

Simple preconditioned iteration:

$$
x_{n+1}=x_{n}+P^{-1}\left(b-L x_{n}\right)
$$

Ideally, $P$ should:

- be easy to construct,
- be easy to invert (i.e. solving a system with $P$ is cheap),
- reduce the condition number: $\kappa\left(P^{-1} L\right) \ll \kappa(L)$.

These rules apply when simple iteration is replaced with a better method (e.g. Conjugate Gradients).

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Extreme case: $P=L$ does not satisfy all requirements as well.

## Guidelines for choosing efficient $P$

$L=L^{T}>0$, so choose $P=P^{T}>0$.

- Impose spectral equivalence: if exist $C_{0}, C_{1}>0$ independent of $h, p, \ldots$, such that

$$
C_{0} x^{\top} P x \leq x^{\top} L x \leq C_{1} x^{\top} P x \quad \Longrightarrow \quad \kappa\left(P^{-1} L\right) \leq \frac{C_{1}}{C_{0}} .
$$

$\rightarrow$ This makes the number of iterations independent of problem size.

- Think globally, act locally: embrace parallelism.
$\rightarrow$ This makes each iteration fast.

A sidenote: another class of structured sparse matrices

## Pretty drawing graphs



Spider's messy net: how to draw it nicely?

## Graph Laplacians: pretty drawing graphs



- Assume edges are elastic threads, obeying (linear!) Hooke's law


## Graph Laplacians: pretty drawing graphs



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- Solve for other positions:



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## Graph Laplacian

Simple, unidirected, weighted graph $(V, E)$
(e.g. social network, transport network, electric circuit, ...)

- Vertices $V=\{1, \ldots, N\}$
- Edge between $i, j \in V$ denoted $(i, j)$; the set of all edges: $E$;
- Degree of vertex $i$ is

$$
D_{i i}=\sum_{j:(i, j) \in E} w_{i j}
$$



- Adjacency matrix: $A_{i j}=w_{i j}$ if $(i, j) \in E$; zero otherwise.
- Graph Laplacian: $L=D-A$; equivalently

$$
L=L^{T} \geq 0
$$

$$
x^{T} L x=\sum_{(i, j) \in E} w_{i j}\left(x_{i}-x_{j}\right)^{2}
$$

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Reasons to solve systems $L x=b$ with graph Laplacian:

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- finding voltages in a resistor network, with some input/output voltages fixed
- finding Fiedler vector of the graph (using inverse power iteration) (e.g. for mesh partitioning)

Some graphs have very large number of vertices $N$. But then usually every node is connected to only a few others: the graph is sparse:

$$
\forall i \quad L_{i j} \neq 0 \quad \text { only for several } \mathrm{j}
$$

We experienced this browsing through the Sparse Matrix Collection!

# Domain decomposition for PDEs 

## What makes a good preconditioner?

We are solving

$$
L x=b
$$

with $L=L^{T}>0$.
Simple preconditioned iteration:

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$P$ must:

- be easy to construct,
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$$

- Use full processing power: embrace parallelism.


## Domain decomposition



Source: MSC/PARASOL

Divide and... solve smaller problems in parallel.
Then ,,glue" them together.

## Additive Schwarz method

## Problem

Find $u_{h} \in V_{h}$ such that

$$
\mathcal{A}_{h}\left(u_{h}, v_{h}\right)=\left(f, v_{h}\right) \quad \forall v_{h} \in V_{h}
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$$

Divide and... add:

- Space decomposition:

$$
V_{h}=V_{0}+V_{1}+\ldots+V_{N}
$$

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\mathcal{A}_{h}\left(u_{h}, v_{h}\right)=\left(f, v_{h}\right) \quad \forall v_{h} \in V_{h} .
$$

Divide and... add, and solve in parallel.

- Space decomposition:

$$
V_{h}=V_{0}+V_{1}+\ldots+V_{N}
$$

- Local solution operators $T_{i}: V_{h} \rightarrow V_{i}$ such that

$$
A_{h}\left(T_{i} u_{i}, v_{i}\right)=\mathcal{A}_{h}\left(u_{i}, v_{i}\right) \quad \forall v_{i} \in V_{i}
$$

## Additive Schwarz method

## Theorem (Divide and... maintain stability)

Let $T=T_{0}+T_{1}+\ldots+T_{N}$. Suppose that the following hold:
Stable decomposition: $\exists C>0 \quad \exists u_{i} \in V_{i}, u=\sum_{i} u_{i}$

$$
\sum_{i} A_{h}\left(u_{i}, u_{i}\right) \leq C \mathcal{A}_{h}(u, u) \quad \forall u \in V_{h}
$$

Strengthened Cauchy-Schwarz ineq.: $\exists 0 \leq \mathcal{E}_{i j} \leq 1 \forall 1 \leq i, j \leq N$

$$
\mathcal{A}_{h}\left(u_{i}, u_{j}\right) \leq \mathcal{E}_{i j} \cdot \mathcal{A}_{h}\left(u_{i}, u_{i}\right)^{1 / 2} \cdot \mathcal{A}_{h}\left(u_{j}, u_{j}\right)^{1 / 2} \quad \forall u_{i} \in V_{i}, u_{j} \in V_{j},
$$

Local stability: $\exists \omega>0 \forall 0 \leq i \leq N$

$$
\mathcal{A}_{h}\left(u_{i}, u_{i}\right) \leq \omega A_{h}\left(u_{i}, u_{i}\right) \quad \forall u_{i} \in V_{i}
$$

Then

$$
\kappa(T) \leq C \omega(\rho(\mathcal{E})+1) .
$$

Dryja, Widlund (1990) "Towards a unified theory of domain decomposition algorithms for elliptic problems"

## Additive/Multiplicative Schwarz method

30 years of successful applications:

- overlapping domain decomposition
- substructuring domain decomposition
- multigrid
- building block of PETSc parallel linear solvers library

[^2]
## ACM Gordon Bell prize 2016

"Chinese Research Team that Employs High Performance Computing to Understand Weather Patterns Wins 2016 ACM Gordon Bell Prize"

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[^3]
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- "In the solver, we propose a highly efficient domain-decomposed multigrid preconditioner that can greatly accelerate the convergence rate at the extreme scale. For solving the overlapped subdomain problems, a geometry-based pipelined incomplete LU factorization method is designed to further exploit the on-chip fine-grained concurrency."

[^4]
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- Additive Schwarz at the core of computation

[^5]
## Non-overlapping domain decomposition for DGFEM

$$
V_{h}^{p}=\left\{v \in L^{2}(\Omega): v_{\left.\right|_{\kappa}} \in P_{p}(\kappa) \quad \forall \kappa \in \mathcal{T}_{h}\right\} .
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V_{h}^{p}=\sum_{i=1}^{N} V_{i}
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where

$$
V_{i}=\left\{v \in V_{h}^{p}: v=0 \text { on } \Omega_{j}, \quad j \neq i\right\}
$$

Divide and... aggregate.


Is there no overlap between subdomains?

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$$
\mathcal{A}_{h}(u, v) \equiv \sum_{\kappa \in \mathcal{T}_{h}} \int_{\kappa} \nabla u \cdot \nabla v d x+\int_{\Gamma} \frac{\gamma p^{2}}{h}[u][v] d \sigma+\ldots \text { etc. }
$$

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$$

Coarse space:

$$
V_{0}=V_{\mathcal{H}}^{q}, \quad \text { where } \mathcal{H} \geq H, \quad q \leq p .
$$

Divide and... aggregate.

$N$ subdomains, $\mathcal{M}$ coarse space cells.

## DGFEM additive Schwarz condition estimate

## Theorem

Let $T=T_{0}+\sum_{i=1}^{N} T_{i}$ be the preconditioned operator. Then

$$
\kappa(T)=O\left(\frac{\mathcal{H}^{2}}{h H} \cdot \frac{p^{2}}{\max \{q, 1\}}\right)
$$

Bound independent of discontinuities in the coefficient, extended to nonconforming meshes and varying polynomial degree.

[^6]
## DGFEM additive Schwarz condition estimate

Key condition for the coarse space $V_{0}$ :
Divide and... maintain approximation:
$\forall u \in V_{h} \quad \exists u_{0} \in V_{0}:$

$$
\sum_{n=1}^{\mathcal{M}}\left(\frac{q_{n}^{2}}{\mathcal{H}_{n}^{2}}\left\|u-u_{0}\right\|_{0, D_{n}}^{2}+\left\|u-u_{0}\right\|_{D_{n}}^{2}\right) \leq \text { Const } \cdot \mathcal{A}_{h}(u, u) .
$$

K. (2016) Num. Meth. PDEs

Antonietti, Houston, Smears (2016) Int. J. Numer. Anal. Model.

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$$

## Open questions:

- Optimal balance between $\mathcal{H}$ and $H$ ? $p$ and $q$ ?
- How does it depend on the computer architecture?

[^7]
## What kind of parallelism?


( 24 cores, $2.6 \mathrm{GHz}, 128 \mathrm{~GB}$ ) $\times 1084$ nodes (Cray XC40, at ICM UW)
or...

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( 24 cores, $2.6 \mathrm{GHz}, 128 \mathrm{~GB}$ ) $\times 1084$ nodes (Cray XC40, at ICM UW)
or...


2560 cores, 1.6 GHz, 8 GB (NVIDIA GTX 1080, in your PC)

## Extreme parallelism

Suppose subdomain $=$ single finite element.
Then \# parallel tasks $=\#$ subdomains $=\#$ finite elements $=N$.

## Theorem

Let $T=T_{0}+\sum_{i=1}^{N} T_{i}$ be the preconditioned operator. Then

$$
\kappa(T) \lesssim \max _{n=1, \ldots, \mathcal{M}}\left\{\frac{\mathcal{H}_{n}^{2}}{\min _{\kappa \in \mathcal{T}_{h}\left(D_{n}\right)} h_{\kappa}^{2}}\right\}
$$

Bound independent of discontinuities in the coefficient (under certain assumptions).

[^8]
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$$

Bound independent of discontinuities in the coefficient (under certain assumptions).

Dryja, K. (2015) Num. Math.

## Splitting equations

## Block systems

System with nonsinglar, symmetric $2 \times 2$ block matrix:

$$
\mathcal{L}\left[\begin{array}{l}
u \\
p
\end{array}\right] \equiv\left[\begin{array}{cc}
A & B^{T} \\
B & -C
\end{array}\right]\left[\begin{array}{l}
u \\
p
\end{array}\right]=\left[\begin{array}{l}
f \\
g
\end{array}\right] .
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$$

Examples of "natural" block decomposition:

- $A>0, C=0$
- Stokes equations,
- mixed methods for elliptic PDEs,
- $A>0, C<0$
- structured methods for elliptic PDEs:
- $A>0, C>0$
- linear elasticity mixed discretization
- stabilized mixed methods
- $A$ indefinite, $C>0$
- time harmonic Maxwell equations


## A family of preconditioners

For ill-conditioned $\mathcal{L}$, use preconditioner $\mathcal{P}$, and solve iteratively

$$
\mathcal{P}^{-1}\left[\begin{array}{ll}
A & B^{T} \\
B & -C
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Benzi, Golub, Liesen (2005) Acta Numer.
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u \\
p
\end{array}\right]=\mathcal{P}^{-1}\left[\begin{array}{l}
F \\
G
\end{array}\right]
$$

Divide and... follow this decomposition!

$$
\mathcal{P}_{1}=\left[\begin{array}{cc}
I & \\
c B A_{0}^{-1} & I
\end{array}\right]\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right]\left[\begin{array}{cc}
I & d A_{0}^{-1} B^{T} \\
& I
\end{array}\right]
$$

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$$
\mathcal{P}^{-1}\left[\begin{array}{ll}
A & B^{T} \\
B & -C
\end{array}\right]\left[\begin{array}{l}
u \\
p
\end{array}\right]=\mathcal{P}^{-1}\left[\begin{array}{l}
F \\
G
\end{array}\right]
$$

Divide and... follow this decomposition!

$$
\mathcal{P}_{1}=\left[\begin{array}{cc}
I & \\
c B A_{0}^{-1} & I
\end{array}\right]\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right]\left[\begin{array}{cc}
I & d A_{0}^{-1} B^{T} \\
& I
\end{array}\right]
$$

or

$$
\mathcal{P}_{2}=\left[\begin{array}{cc}
I & d B^{T} S_{0}^{-1} \\
& I
\end{array}\right]\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right]\left[\begin{array}{cc}
I & \\
c S_{0}^{-1} B & I
\end{array}\right],
$$

Benzi, Golub, Liesen (2005) Acta Numer.
K. (2011) Efficient preconditioned [...] PDEs

Brown (2012) Intl. Symp. Para. Distr. Comp.

## A family of preconditioners

For ill-conditioned $\mathcal{L}$, use preconditioner $\mathcal{P}$, and solve iteratively

$$
\mathcal{P}^{-1}\left[\begin{array}{ll}
A & B^{\top} \\
B & -C
\end{array}\right]\left[\begin{array}{l}
u \\
p
\end{array}\right]=\mathcal{P}^{-1}\left[\begin{array}{l}
F \\
G
\end{array}\right]
$$

Divide and... follow this decomposition!

$$
\mathcal{P}_{1}=\left[\begin{array}{cc}
I & \\
c B A_{0}^{-1} & I
\end{array}\right]\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right]\left[\begin{array}{cc}
I & d A_{0}^{-1} B^{T} \\
& I
\end{array}\right]
$$

or

$$
\mathcal{P}_{2}=\left[\begin{array}{cc}
I & d B^{T} S_{0}^{-1} \\
& I
\end{array}\right]\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right]\left[\begin{array}{cc}
I & \\
c S_{0}^{-1} B & I
\end{array}\right],
$$

Some implemented in PETSc as PCFIELDSPLIT type preconditioners.

Benzi, Golub, Liesen (2005) Acta Numer.
K. (2011) Efficient preconditioned [...] PDEs

Brown (2012) Intl. Symp. Para. Distr. Comp.

## Choosing the ingredients: c,d parameters

| Type | Form of $\mathcal{P}$ | $c$ | $d$ |
| :--- | :---: | :--- | :--- |
| block-diagonal | $\left[\begin{array}{ll}A_{0} & \\ & S_{0}\end{array}\right]$ | 0 | 0 |
| block-triangular | $\left[\begin{array}{ll}A_{0} & \\ B & -S_{0}\end{array}\right]$ | 1 | 0 |
| block symmetric indefinite | $\left[\begin{array}{ccc}A_{0} & B^{T} \\ B & B A_{0}^{-1} B^{T} & -S_{0}\end{array}\right]$ | 1 | 1 |
| primal-based penalty | $\left[\begin{array}{ccc}A_{0}-B^{T} S_{0}^{-1} B & B^{T} \\ B & -S_{0}\end{array}\right]$ | 1 | 1 |

## Choosing the ingredients: $A_{0}, S_{0}$ preconditioners

Let us define a block diagonal matrix and a norm

$$
\begin{aligned}
\mathcal{J}=\left[\begin{array}{ll}
A_{0} & \\
& S_{0}
\end{array}\right], \quad\left\|\left[\begin{array}{l}
u \\
p
\end{array}\right]\right\|_{\mathcal{J}}^{2} & =\|u\|_{A_{0}}^{2}+\|p\|_{S_{0}}^{2} \\
& =u^{T} A_{0} u+p^{T} S_{0} p
\end{aligned}
$$

Divide and... keep balance:
stability and continuity

$$
\exists_{m_{0}, m_{1}>0} \quad m_{0}\|x\|_{\mathcal{J}} \leq\|\mathcal{L} x\|_{\mathcal{J}^{-1}} \leq m_{1}\|x\|_{\mathcal{J}} \quad \forall x
$$

mixed continuity $\exists_{b_{0}>0} \quad\left|p^{\top} B u\right| \leq b_{0}\|u\|_{A_{0}}\|p\|_{s_{0}} \quad \forall u, \forall p$,
inner product definiteness $\mathcal{H}>0$
spectral equivalence $\exists_{h_{0}, h_{1}>0} \quad h_{0}\|x\|_{\mathcal{H}} \leq\|x\|_{\mathcal{J}} \leq h_{1}\|x\|_{\mathcal{H}}, \quad \forall x$.

## Eigenvalue estimates and PCR convergence

It is known that the convergence speed of PCR iteration depends on

$$
\kappa=\frac{\max \left|\lambda\left(\mathcal{P}^{-1} \mathcal{L}\right)\right|}{\min \left|\lambda\left(\mathcal{P}^{-1} \mathcal{L}\right)\right|}
$$

## Theorem

If $\lambda$ is an eigenvalue of $\mathcal{P}^{-1} \mathcal{L}$, then

$$
\frac{1}{2 m_{0}\left(1+b_{0}^{2}\right)} \leq|\lambda| \leq 2 m_{1}\left(1+b_{0}^{2}\right) .
$$

This has direct implications to preconditioning Stokes equation or certain multiphysics systems of PDEs.

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```


## Summing up

- reconnect wisely
- reconnect wisely
- solve parts in parallel
- reconnect wisely
- solve parts in parallel
- keep balance
- reconnect wisely
- solve parts in parallel
- keep balance
- maintain stability or approximation


## Selected active research areas

- preconditioners for nonstandard finite elements
- algorithms for new computer architectures
- communication avoiding parallel methods/preconditioners
- domain decomposition for nonlinear problems
- nonsymmetric/indefinite linear systems
- robust methods for graph Laplacians


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