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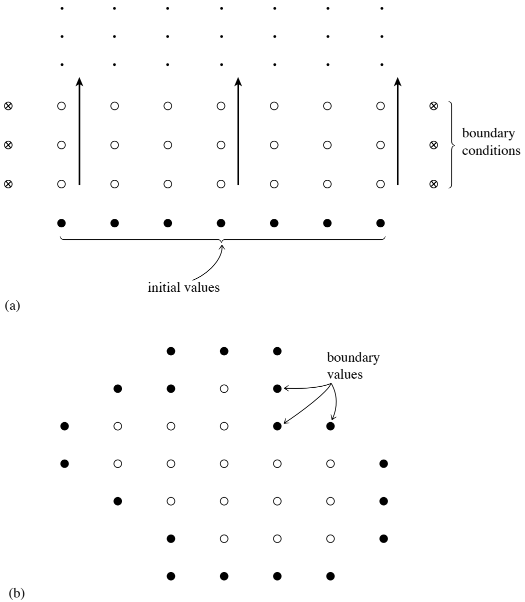
- Of course these are supplemented by appropriate initial/boundary conditions.

Initial & Boundary value problems



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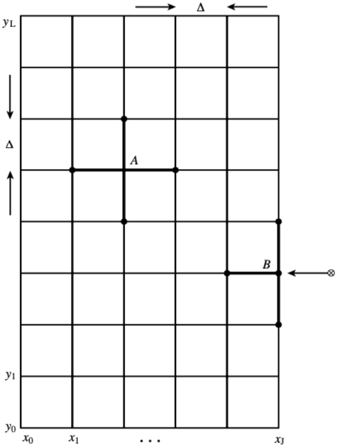
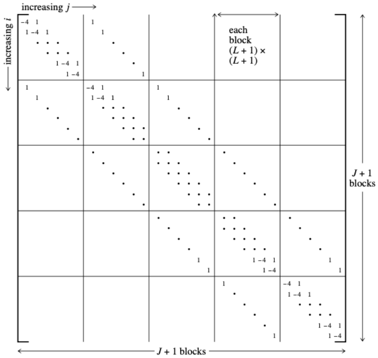
- can translate it into a matrix equation $\mathbf{A} \cdot \mathbf{u} = \mathbf{b}$; boundary terms taken to RHS



- Matrix structure



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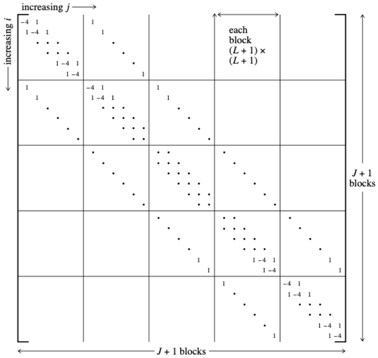

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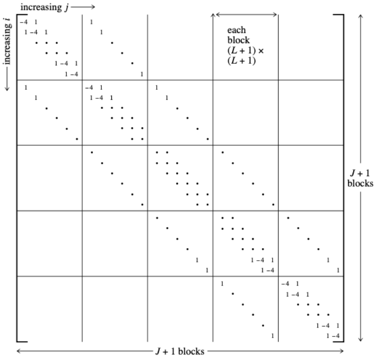

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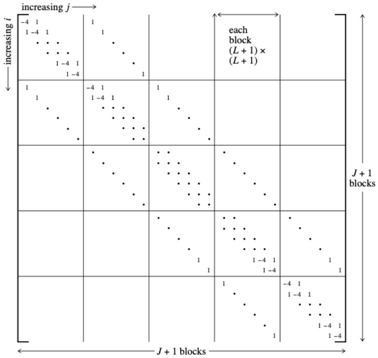

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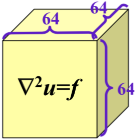
- Fourier methods for periodic boundary conditions $\mathcal{O}[N^d \ln N]$)

The power of optimal algorithms

- Advances in algorithmic efficiency can rival advances in hardware architecture
- Consider Poisson's equation on a cube of size $N=n^3$

Year	*Method*	*Reference*	*Storage*	*Flops*
1947	GE (banded)	Von Neumann & Goldstine	n^5	n^7
1950	Optimal SOR	Young	n^3	$n^4 \log n$
1971	CG	Reid Conjugate Gradients w/ Gustaffson's modified ILU preconditioner	n^3	$n^{3.5} \log n$
1984	Full MG	Brandt Multigrid	n^3	n^3



- If n=64, this implies an overall reduction in flops of ~16 million *

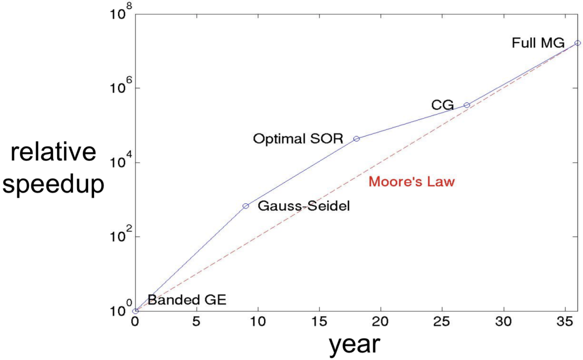
more recently: FMM Fast Multipole Method

*Six-months is reduced to 1 s

PPPL Colloquium, 25 Jan 2006
David Keyes, Columbia Univ.

Algorithms and Moore's Law

- This advance took place over a span of about 36 years, or 24 doubling times for Moore's Law
- $2^{24} \approx 16$ million $\Rightarrow$ the same as the factor from algorithms alone!



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- no variables from previous iteration; just use current value

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- **error** $\mathbf{e}^n = \mathbf{x} - \mathbf{x}^n$; **residual** $\mathbf{r}^n = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}^n$;
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Analysis of 1-D Poisson equation

- Jacobi: $\phi_i^{n+1} = (\phi_{i-1}^n + \phi_{i+1}^n)/2 - \Delta^2 \rho_i/2$
- matrix form: $P = I - \frac{1}{2}A$ with

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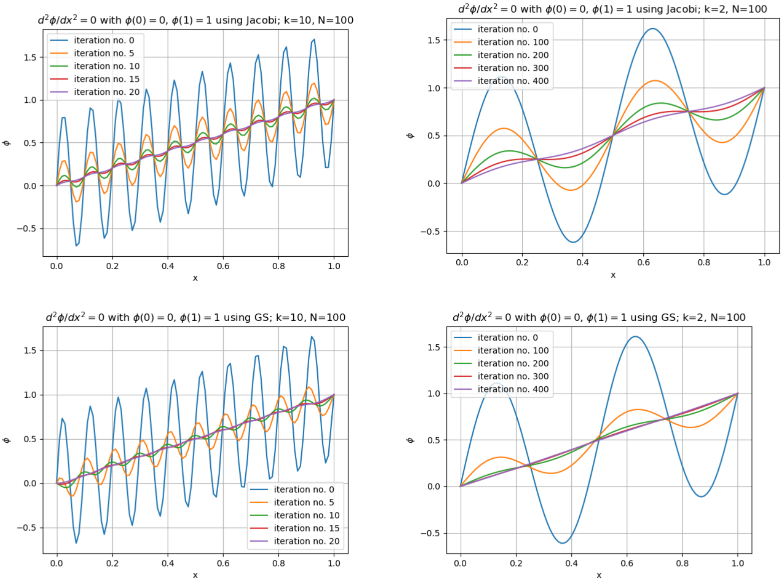
- lowest k converge slowest, worse for large N; key idea of MG methods

1-D Poisson equation: numerical experiments



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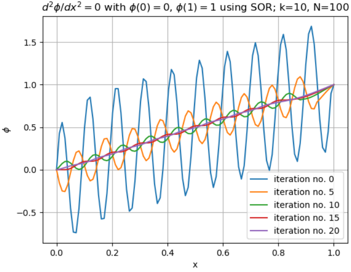
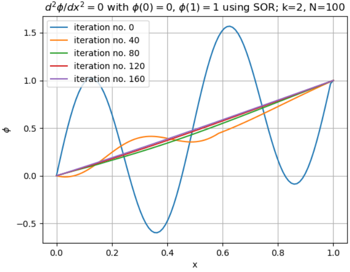
- optimum $\omega = \frac{2}{1+\sqrt{1-\rho_J^2}}$
- for Poisson eq. $\rho_{\mathrm{SOR}} \simeq 1-2\pi/N$ for large N
- much faster than GS with $\rho_{\mathrm{GS}} \simeq 1-\pi^2/N^2$

1-D Poisson equation: numerical experiments





- note faster convergence, especially for low k
- here we used optimum ω for a given k
- worse performance for non-optimum ω
- ω determined by trial and error, local approximation

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  $u_{j,l}^{n} + \frac{\Delta t}{\Delta^2}(u_{j+1,l}^{n} + u_{j-1,l}^{n} + u_{j,l+l}^{n} + u_{j,l-1}^{n} - 4u_{j,l}^{n}) - \rho_{j,l}\Delta t$
- FTCS stability condition in 2-D: $\Delta t \leq \Delta^2/4$; choosing largest stable step in above,
- $u_{j,l}^{n+1} = \frac{1}{4}(u_{j+1,l}^{n} + u_{j-1,l}^{n} + u_{j,l+l}^{n} + u_{j,l-1}^{n}) - \frac{\Delta^2}{4}\rho_{j,l}$ Jacobi!
- **Multigrid methods** are the most sophisticated schemes for BVPs, go back and forth between coarse and fine grids