

MTH 655/659
**Large scale scientific computing
methods**

Instructor:

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Mathematics

Oregon State University

Class MTH 655/659 information

- Attendance in labs required:
 - Fridays ~~(8:30-)~~9:00-10:00-~~(10:30)~~ in MLC Kidder 108 computer lab
 - (start 8:30-can leave at 10:30)
 - must complete each lab project
- Individual project: paper and (optional) presentation in March
- Fill out questionnaire
 - must have OSU ID and ONID username
- NO CLASS this Wednesday
 - some other no-class dates TBA
- Reading/review:
 - see http://www.math.oregonstate.edu/~mpesz/teaching/655_W07/index.html

Class MTH 655/659 information

- Algorithms and theory
 - nonlinear problems: Newton-based for $F(U)=0$
 - linear solvers: Jacobi family, Krylov family (CG,PCG,GMRES)
 - parallel implementation theory
 - domain decomposition
 - multigrid
 - primer on optimization (nonlinear, continuous, unconstrained)
- Implementation
 - MATLAB prototypes for testing properties of algorithms and applications
 - Fortran (C for geeks) for REAL scientific computing
 - overview of Unix will be given
 - Fortran+MPI for parallel implementation on a cluster

Solution of nonlinear equations $F(U)=0$

- Ex.: find x :

$$e^{-x} = x^2$$

- solution:

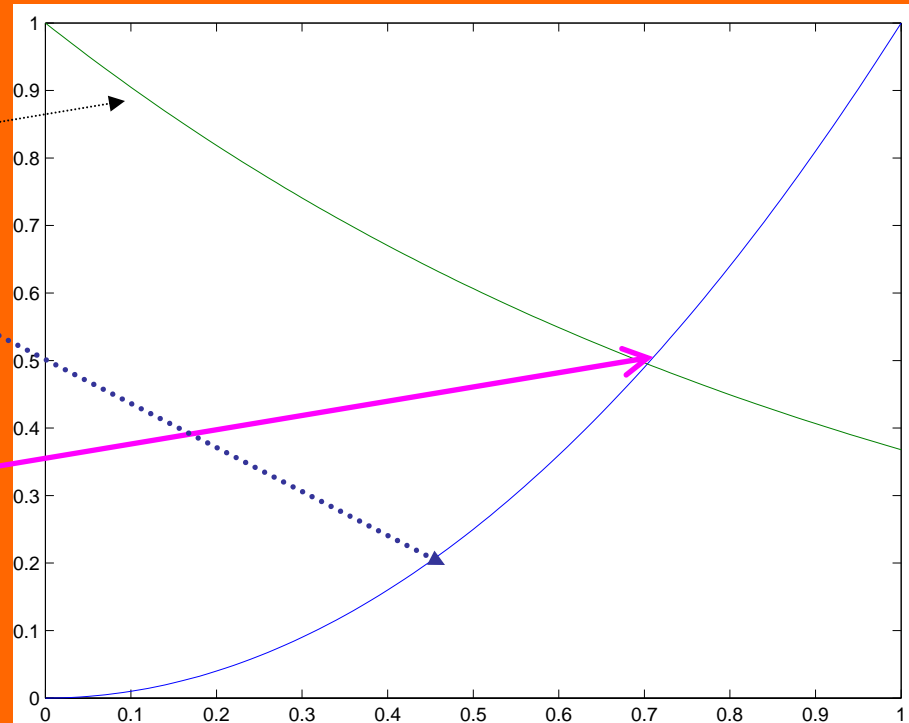
$$x \approx 0.7$$

- set-up

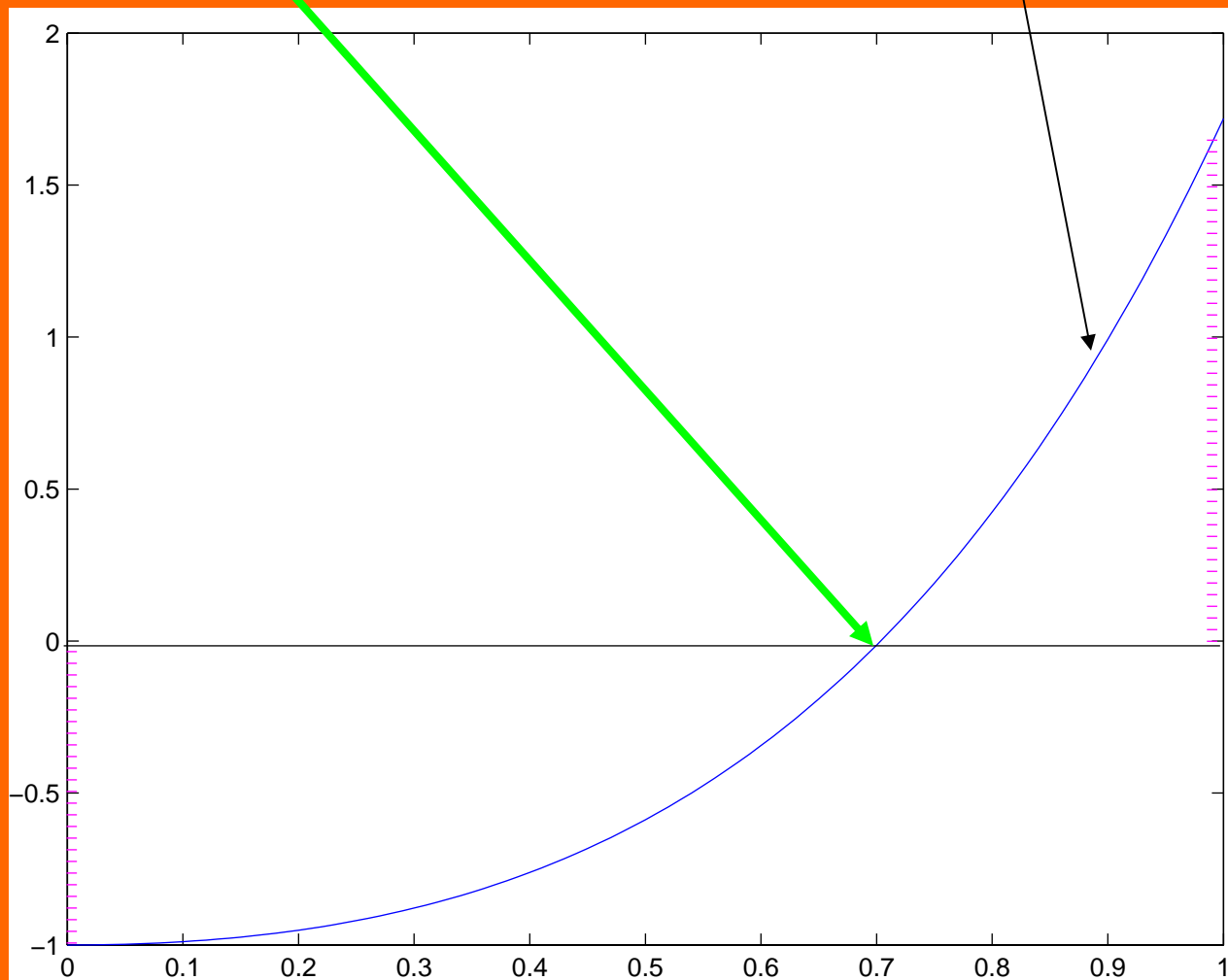
$$f(x) = e^x x^2 - 1$$

- solve

$$f(x) = 0$$

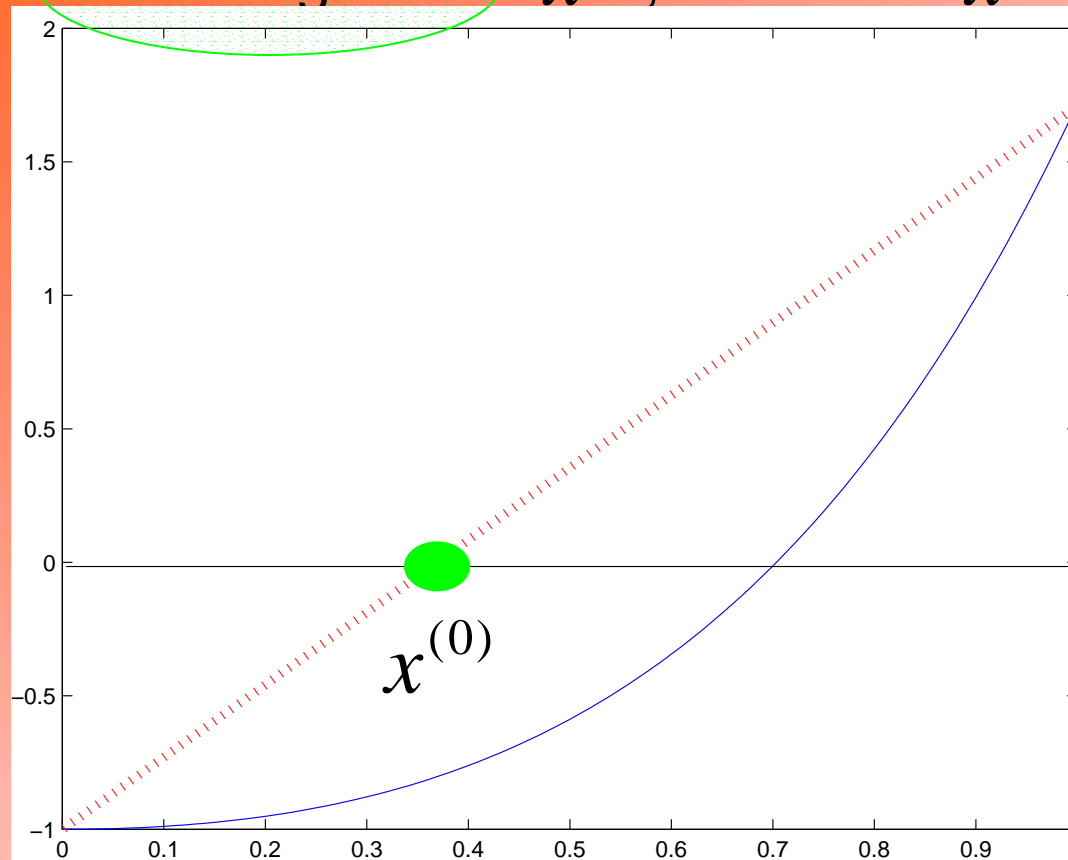


Find $x \in (a, b)$: $f(x) = 0$



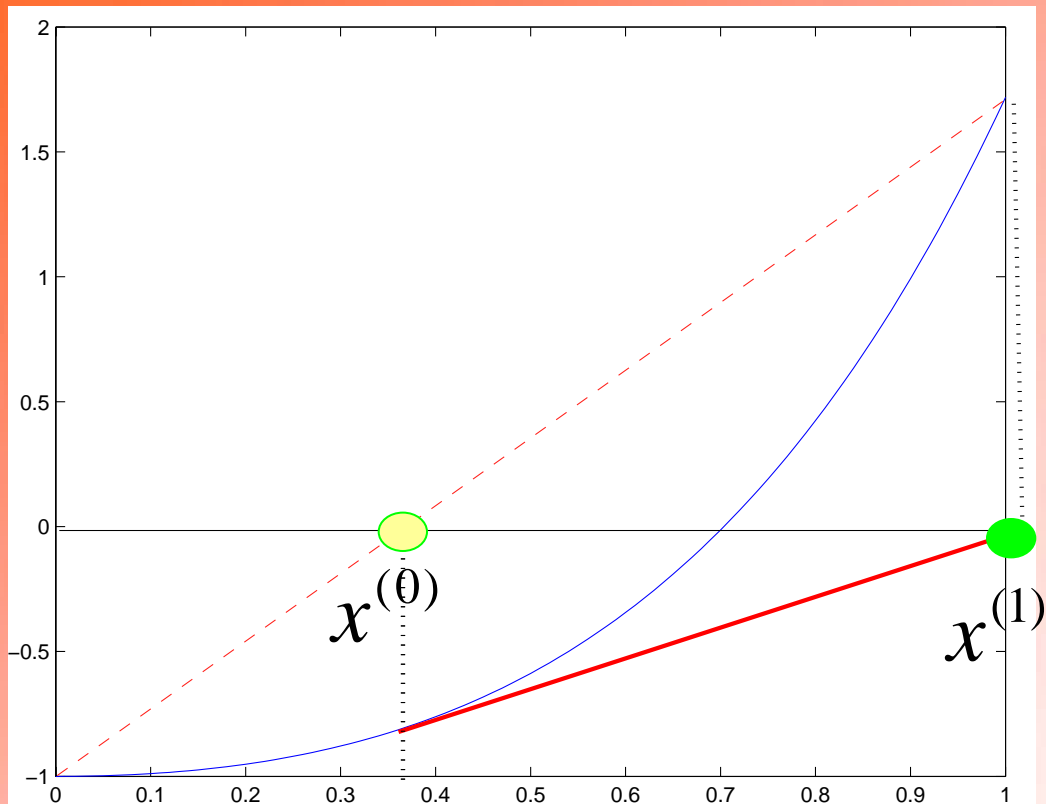
Use Newton's method

- given an initial guess $x^{(0)}$, iterate ... $x^{(1)}$, $x^{(2)}$, $x^{(3)}$, ...



Newton: step1

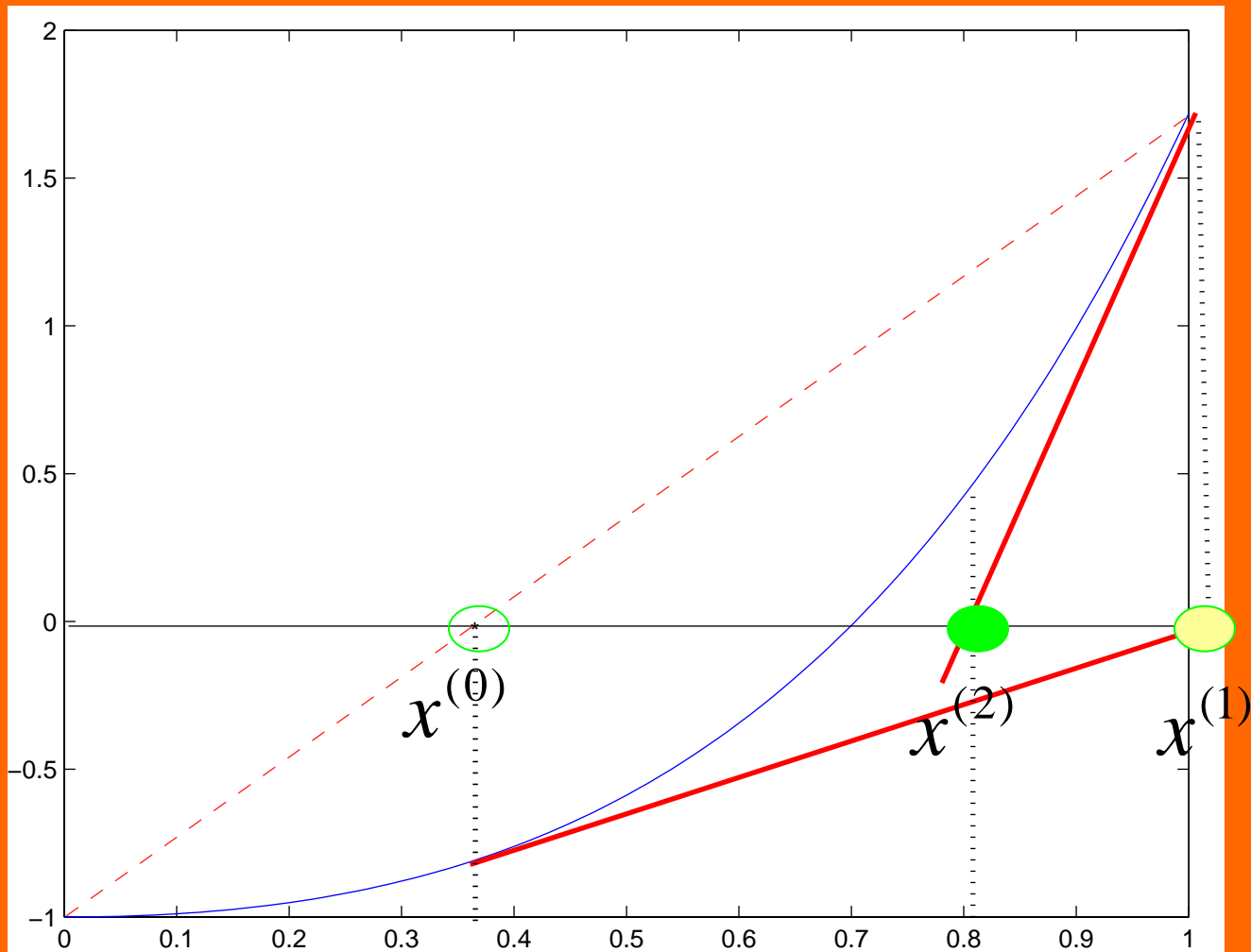
also known as method of tangents



- the next guess (iterate) is found by

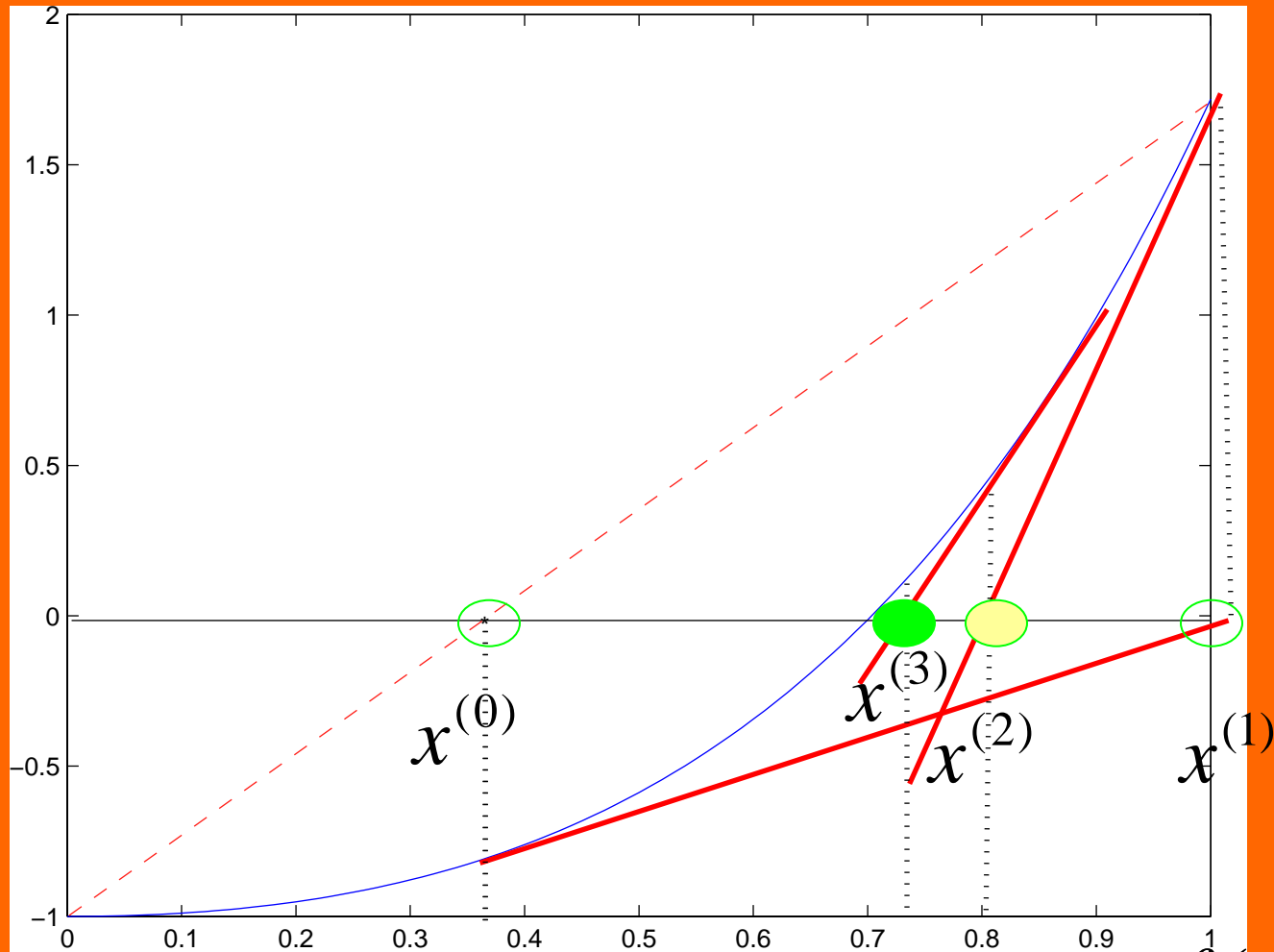
$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

Newton: step2



$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

Newton: step3



$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

Newton: steps 4,5

$x^{(1)}$

- until convergence

– residual is small $|f(x^{(k)})| \leq \tau$

– subsequent iterates do not differ much $|x^{(k)} - x^{(k-1)}| \leq \beta$

Properties of Newton's method

- Iteration

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

written as

$$\begin{cases} \partial^{(k+1)} = (f'(x^{(k)}))^{-1} f(x^{(k)}) \\ x^{(k+1)} = x^{(k)} - \partial^{(k+1)} \end{cases}$$

- Convergence: what conditions ?
 - local convergence: for what initial guess ?
 - conditions ?
 - global: (for any initial guess) how ?
 - line search, trust regions, and other

- Use in optimization

$$\min_x J(x)$$

$$f(x) = J'(x)$$

Newton's method in N-dimensions

- 1D variant for $f(x)=0$ $f : R \mapsto R, x \in R$

$$\begin{cases} \partial^{(k+1)} = (f'(x^{(k)}))^{-1} f(x^{(k)}) \\ x^{(k+1)} = x^{(k)} - \partial^{(k+1)} \end{cases}$$

- N-D Variant for $\mathbf{F}(\mathbf{U}) = \mathbf{0}$

$$\mathbf{F} : R^{Nx1} \mapsto R^{Nx1}, \mathbf{U} \in R^{Nx1}$$

$$\begin{cases} \partial^{(k+1)} = (\mathbf{DF}(\mathbf{U}^{(k)}))^{-1} \mathbf{F}(\mathbf{U}^{(k)}) \\ \mathbf{U}^{(k+1)} = \mathbf{U}^{(k)} - \partial^{(k+1)} \end{cases}$$

$$\mathbf{DF} \in R^{NxN}$$

Newton's method efficiency and scaling

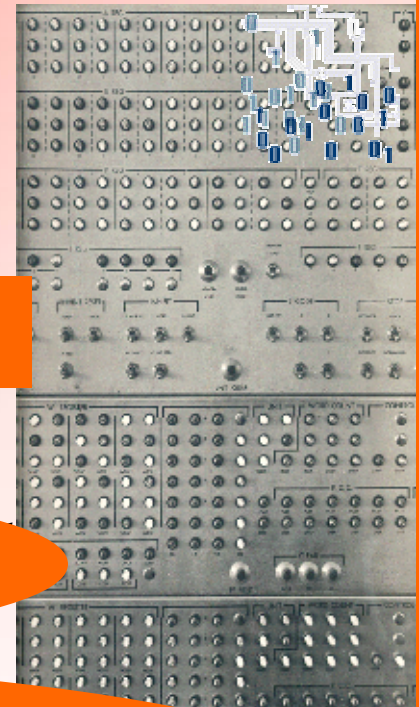
- Solve an N-dimensional problem $\mathbf{F}(\mathbf{U}) = \mathbf{0}$

$$\mathbf{F} : \mathbb{R}^{N \times 1} \mapsto \mathbb{R}^{N \times 1}, \mathbf{U} \in \mathbb{R}^{N \times 1}$$

- using Newton's method:

$$\left[\begin{array}{l} \text{find} \\ \mathbf{F}(\mathbf{U}^{(k)}), \mathbf{DF}(\mathbf{U}^{(k)}) \end{array} \right.$$

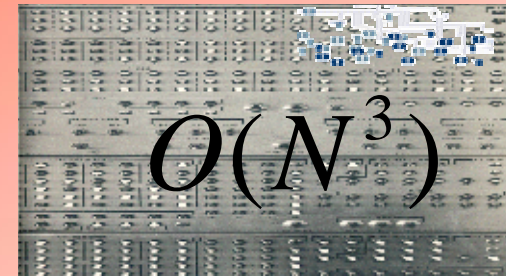
$$\left[\begin{array}{l} \text{update} \\ \mathbf{U}^{(k+1)} = \mathbf{U}^{(k)} - \partial^{(k+1)} \end{array} \right.$$



How to solve most accurately/efficiently

- a linear problem ?

$$\mathbf{AU} = \mathbf{b}$$



- a nonlinear problem ?

$$\mathbf{F}(\mathbf{U}) = \mathbf{0}$$



The answer depends ...

- on the underlying application
- on properties of \mathbf{A} , \mathbf{F}

Linear solvers: how to solve $\mathbf{AU} = \mathbf{b}$

- Problem: solve

$$\mathbf{AU} = \mathbf{b}$$

$$\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{U} \in \mathbb{R}^{N \times 1}, \mathbf{b} \in \mathbb{R}^{N \times 1}$$

- How large is N ?
 - does A fit in computer memory ? (8 bytes x NxN = ?)
 - is A full (dense) / sparse ?
 - how does the speed of the method (number of FLOPs) scale with N ? What is the exponent in $O(N^\alpha)$
- Two main classes of methods
 - direct
 - iterative

Linear solvers:

direct

versus

iterative

- Ex.: Gauss-Jordan elimination (or QR decomposition)

$$\mathbf{A} = \begin{bmatrix} * & 0 & 0 \\ * & * & 0 \\ * & * & * \end{bmatrix} \begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix}$$

- requires storage $O(N^2)$
- scales $O(N^3)$
- do not preserve sparsity
- special variants ILU, ICCL
 - band direct solvers exist $O(N^2)$

- IDEA: $\mathbf{AU} = \mathbf{b}$

iterate $\mathbf{U}^{(k)} \mapsto \mathbf{U}^{(k+1)}$

$k = 1, 2, \dots$ until convergence

requires only product $\mathbf{Y} = \mathbf{AV}$

- no storage necessary
- stationary methods: $O(N^2 \log N)$
 - Jacobi, G-S, SOR
- non-stationary methods $O(N^{1.17})$
 - Krylov family:
 - CG, PCG, GMRES
- multigrid $O(N^1)$

All scaling information for 3D linear PDE models, optimal parameters [Heath'97]

Motivation: solving large systems of nonlinear PDEs

- PDEs = partial differential equations
- PDEs are mathematical models of
 - continuum mechanics
 - fluid flow in subsurface and surface waters
 - gas dynamics
 - heat conduction
 - transport of contaminants
 - and more
- Let us call a generic system of (coupled nonlinear) PDEs

$$F(U) = 0$$

Steps of solving large systems of nonlinear PDEs

- Coupled nonlinear PDEs
 - PDEs imposed over a region D in space and time interval $(0, T)$
 - boundary conditions on boundary of D
 - initial conditions at $t=0$
- Numerical discretization of DEs/PDEs
 - discretize in space: grid over D
 - finite differences, elements, volumes
 - discretize in time, use time step Δt
 - finite differences
 - ANALYSIS of schemes: MTH 552, 553, 654, 655 (FE)
 - Error $U - U_h$
 - for accuracy we must have MANY grid points in D , small Δt
- Solve the system $F_h(U_h) = 0$ as fast as possible
 - solving general linear systems: MTH 551

Example: linear PDE on a simple domain

- model

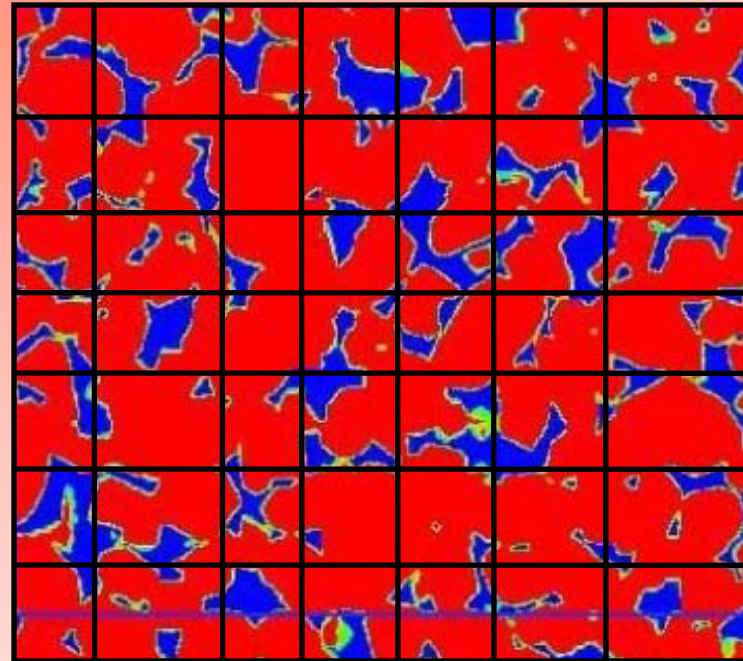
$$F(U) = 0$$

is Poisson equation

$$-\Delta U = b$$

- discretized model

$$-\Delta_h U_h = b_h$$



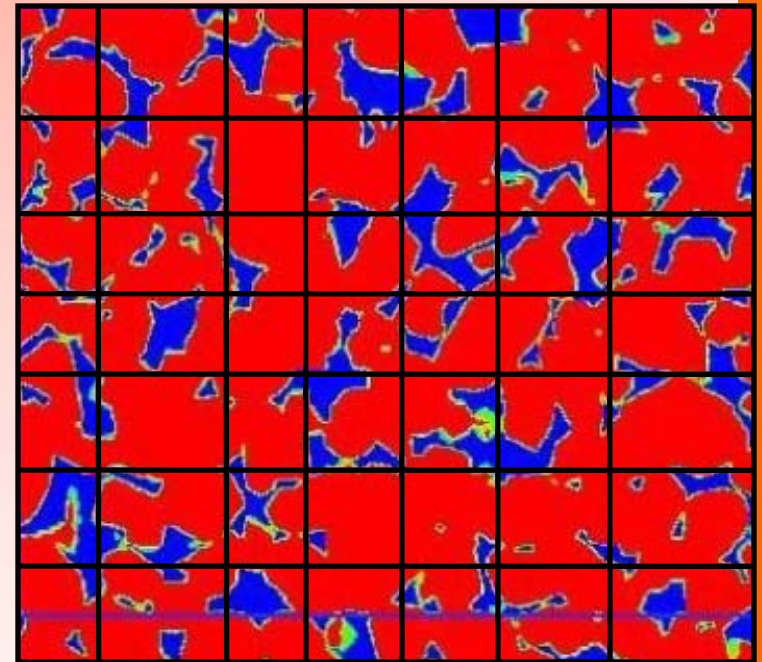
Discrete (linear) model

- linear discrete model $F_h(U_h) = 0$

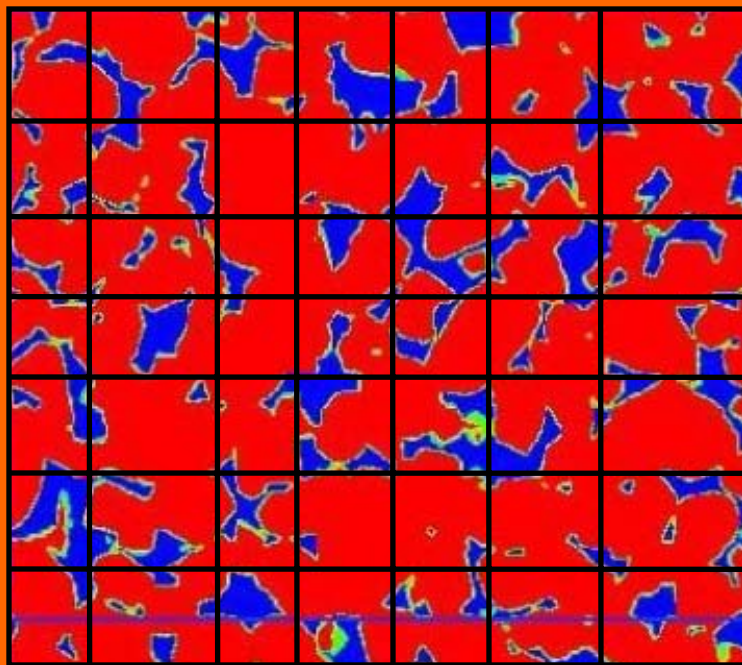
or

$$-\Delta_h U_h = b_h \quad \text{or} \quad \mathbf{A}\mathbf{U} = \mathbf{b}$$

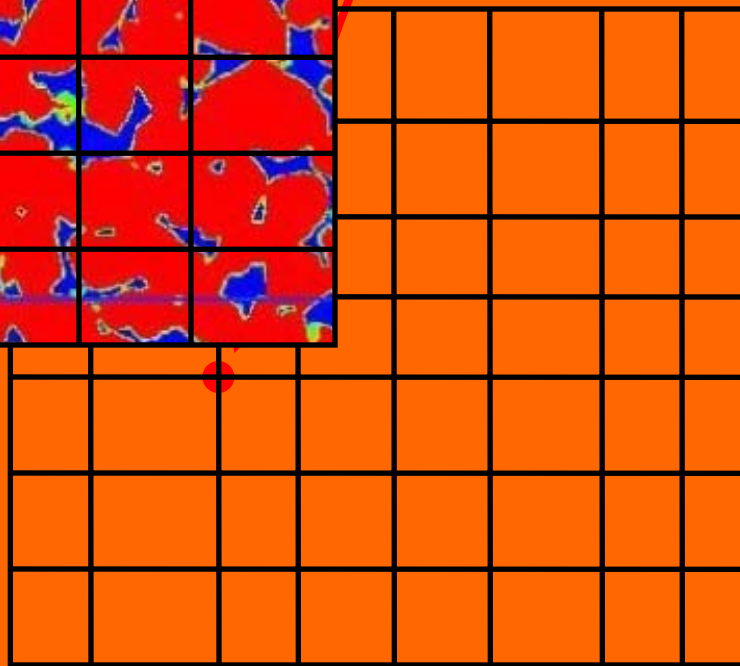
$$U_h \equiv \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ \dots \\ u_{9,7} \\ u_{9,8} \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \\ \dots \\ U_{71} \\ U_{72} \end{bmatrix} = \mathbf{U}$$



Structure of Δ_h



$$u_{3,4} \equiv U_{30}$$

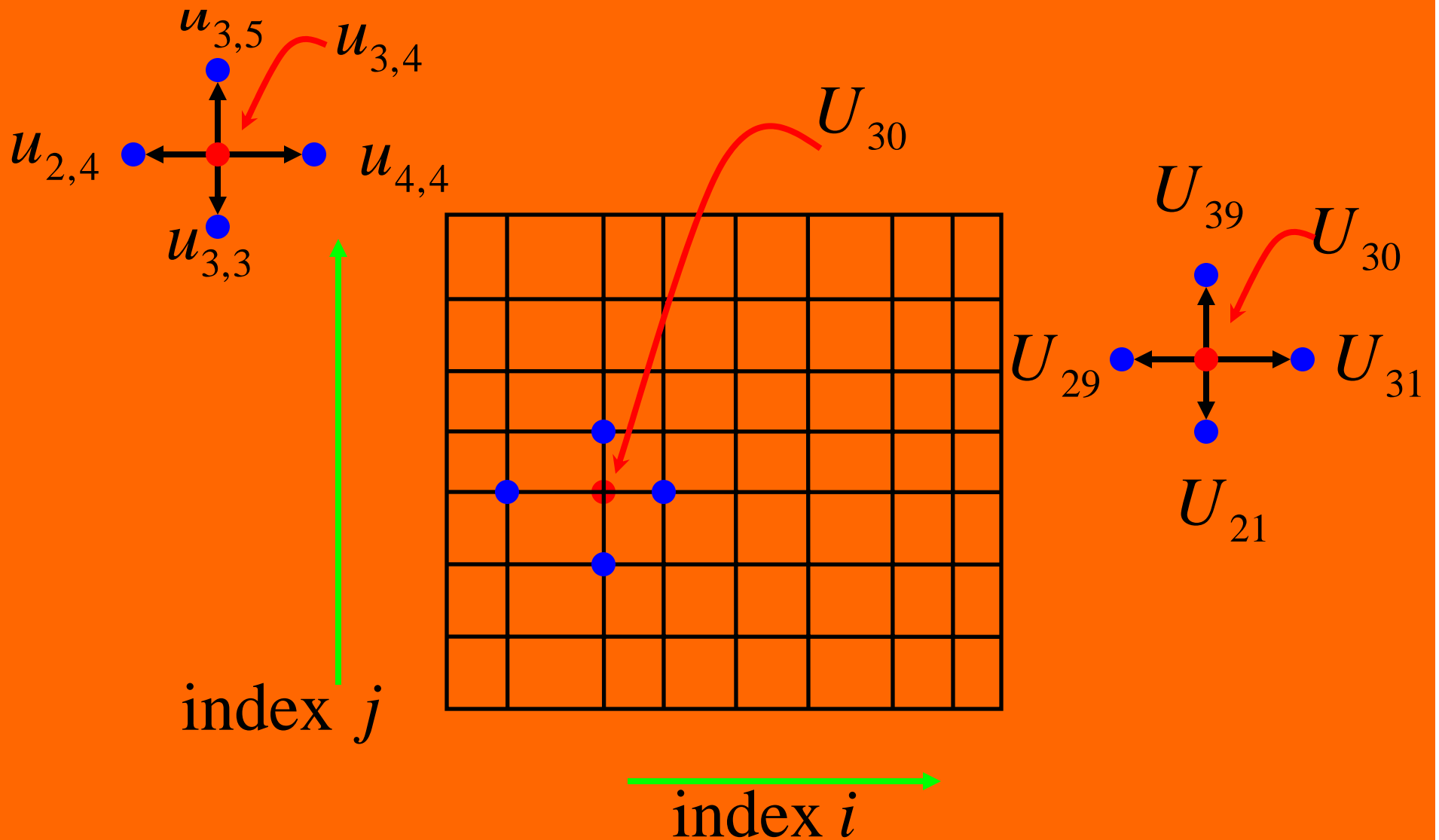


index j

index i

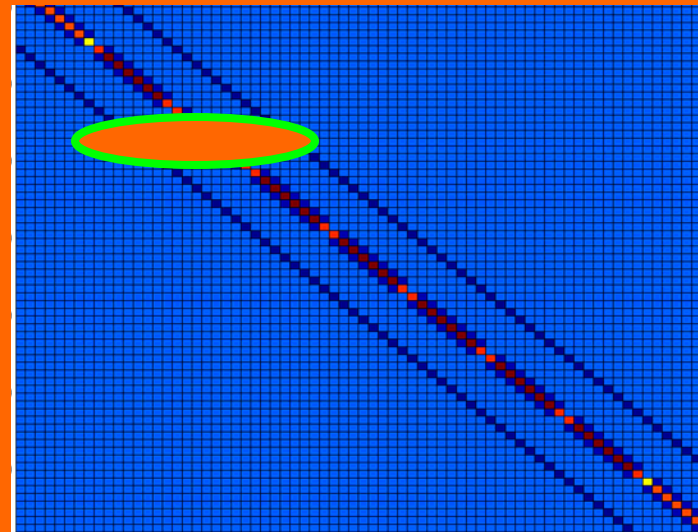
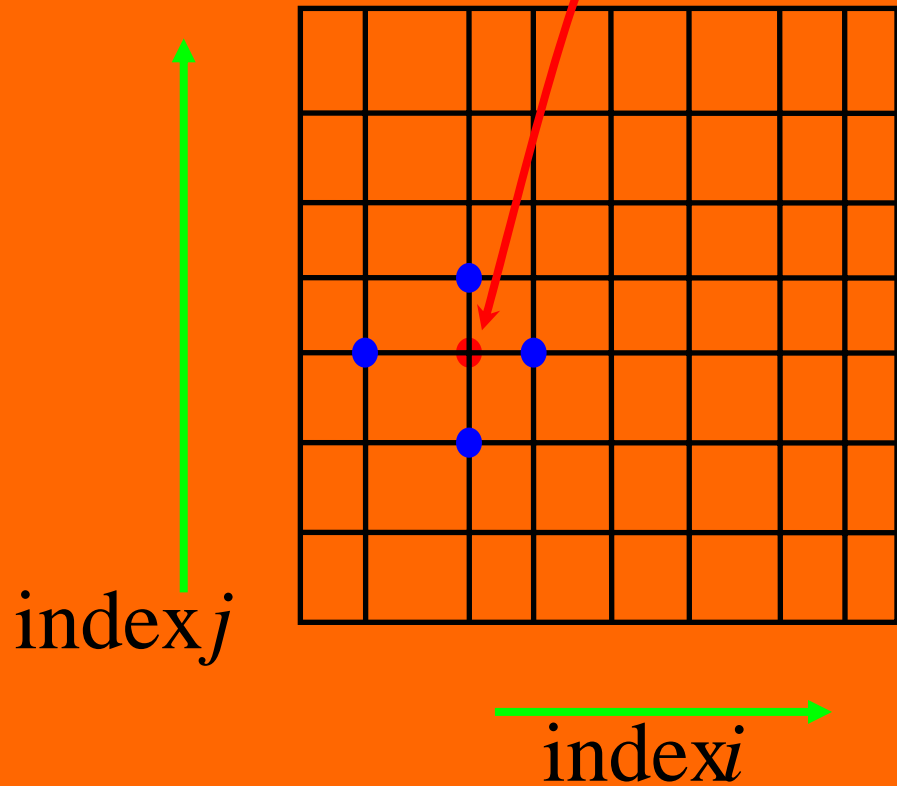
$$U_h = \begin{bmatrix} u_{1,1} \\ u_{2,1} \\ \dots \\ u_{9,7} \\ u_{9,8} \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \\ \dots \\ U_{71} \\ U_{72} \end{bmatrix}$$

Details on the stencil in Δ_h



Matrix of the system $\mathbf{AU} = \mathbf{b}$

U_{30}



row 30

[... $\textcircled{-1}$ 0 0 0 0 0 0 $\textcircled{-1}$ $\textcircled{4}$ $\textcircled{-1}$ 0 0 0 0 0 0 0 0 $\textcircled{-1}$..]

21 29 30 31 39

How to best solve $\mathbf{AU} = \mathbf{b}$

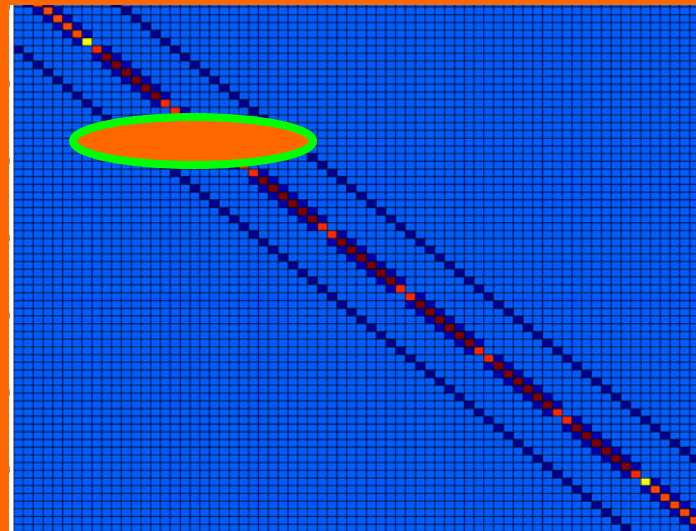
- **Exploit**

-

-

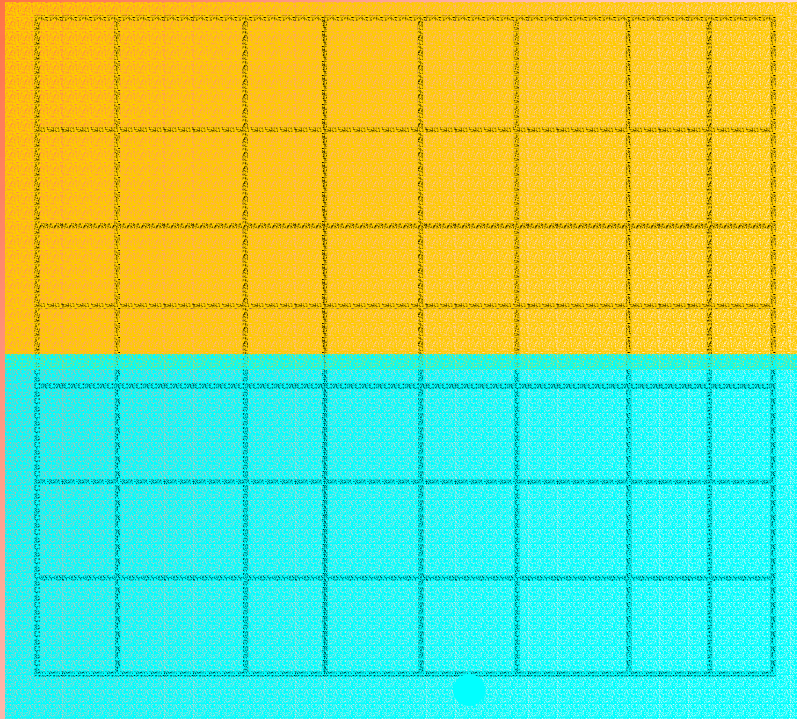
- **Modern methods:**

- multigrid
- domain decomposition
- parallel algorithms



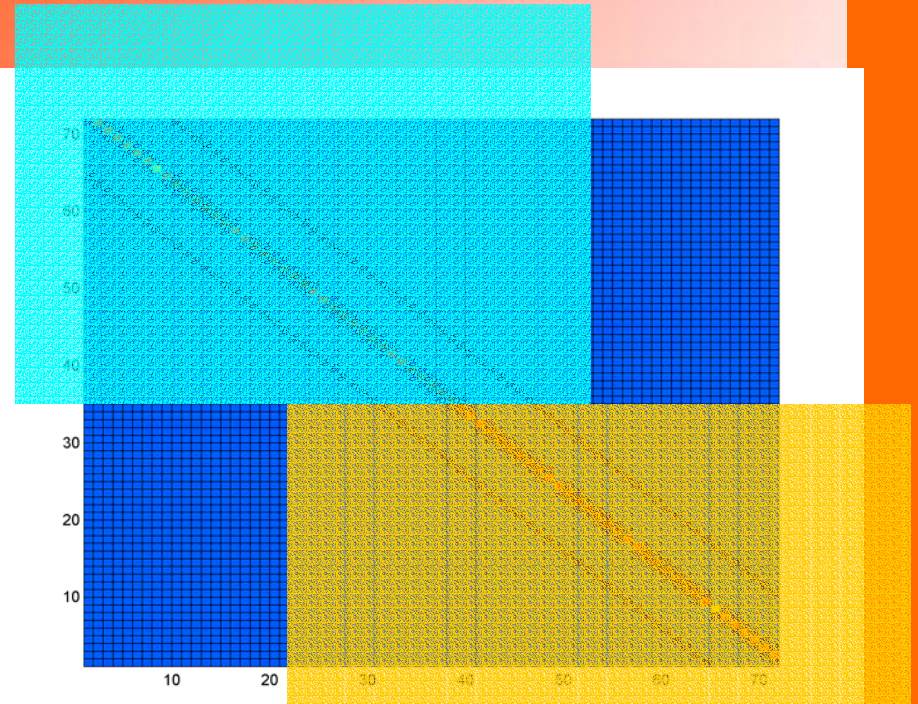
Divide D and conquer $AU = b$

- Iterative solver: must communicate data between yellow and blue zones



- domain decomposition
 - overlapping or nonoverlapping

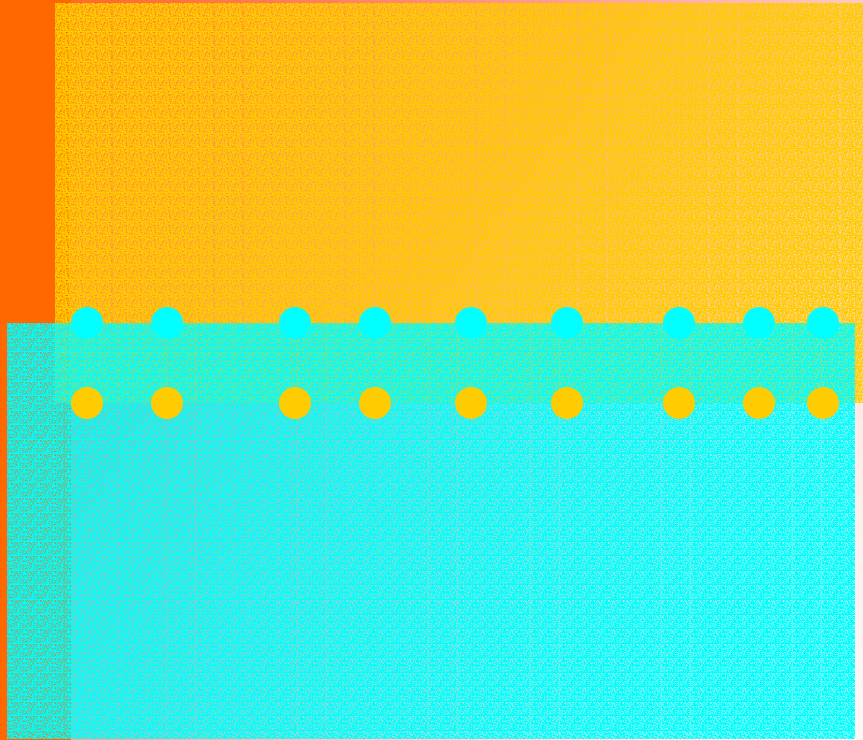
- Matrix/vector view: similar to block decomposition



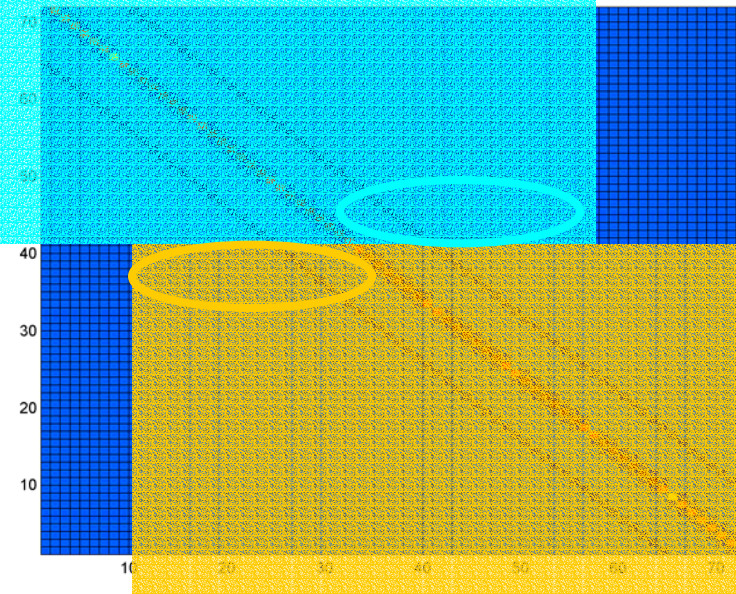
- implement on single processor or multiprocessor computer

Domain decomposition: overlapping

- blue and yellow values lag between iterations

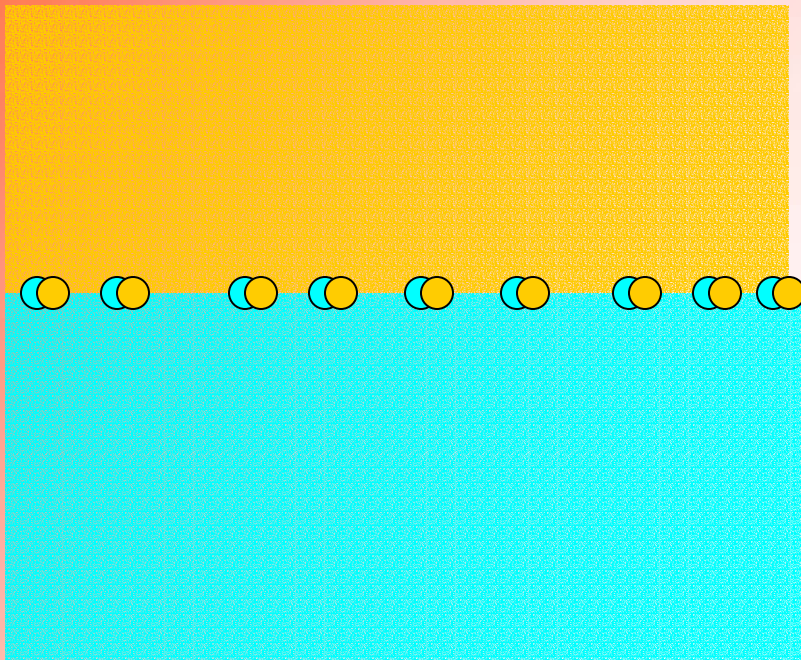


- similar to block Jacobi solver

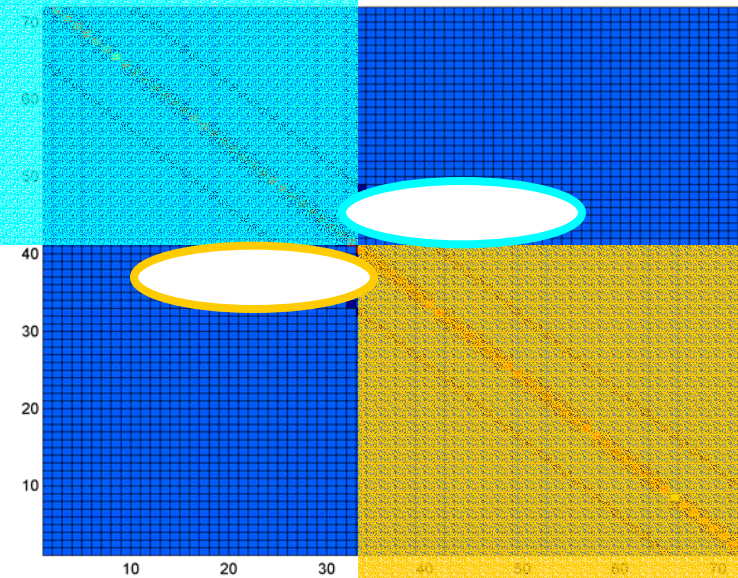


Domain decomposition: non-overlapping

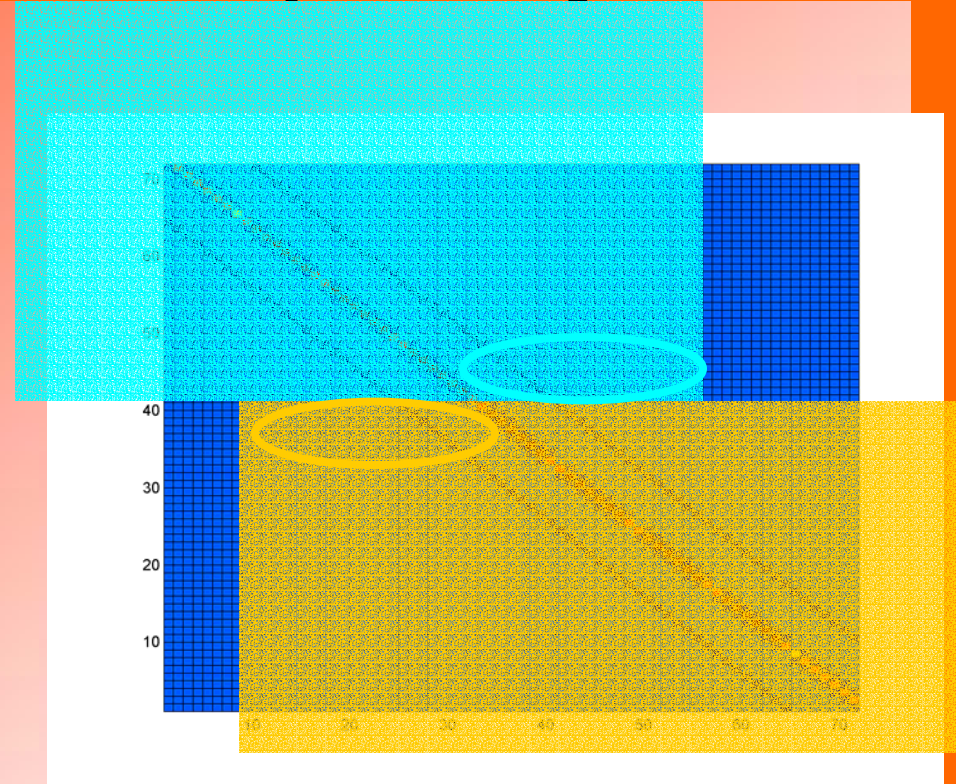
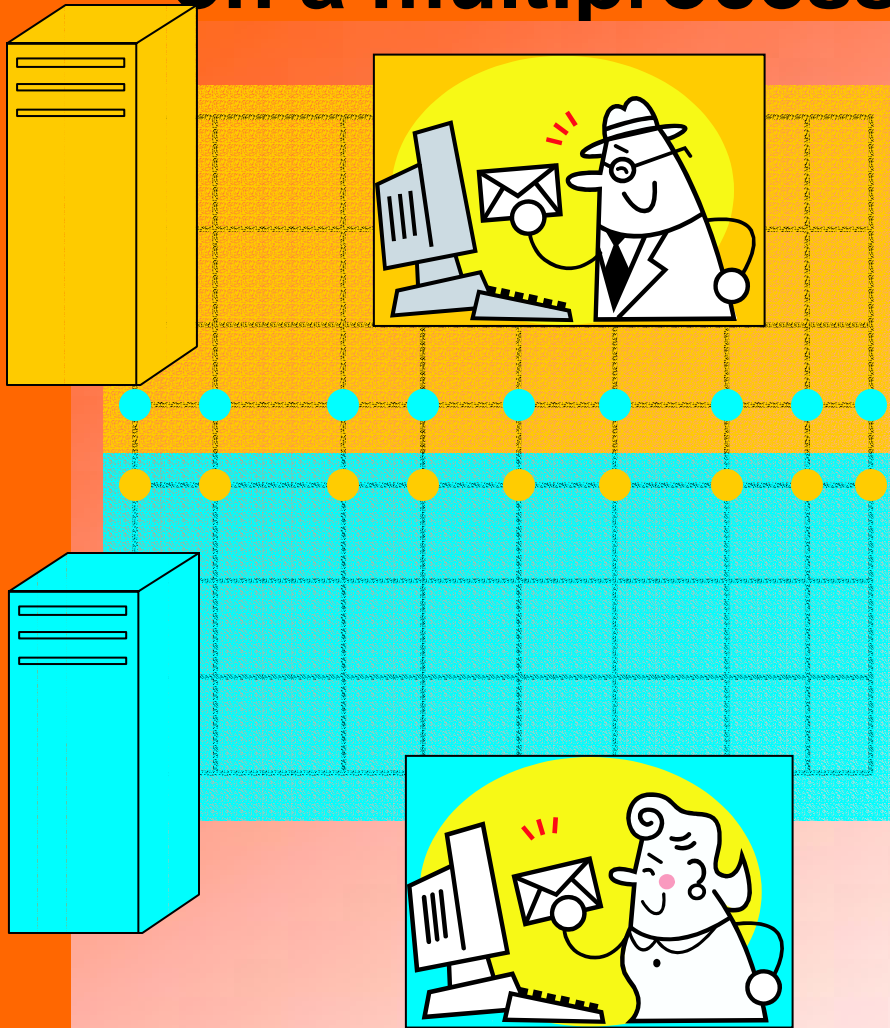
- external iteration
- solve for interface degrees of freedom (external iteration)



- form the Schur complement (eliminate interface unknowns)

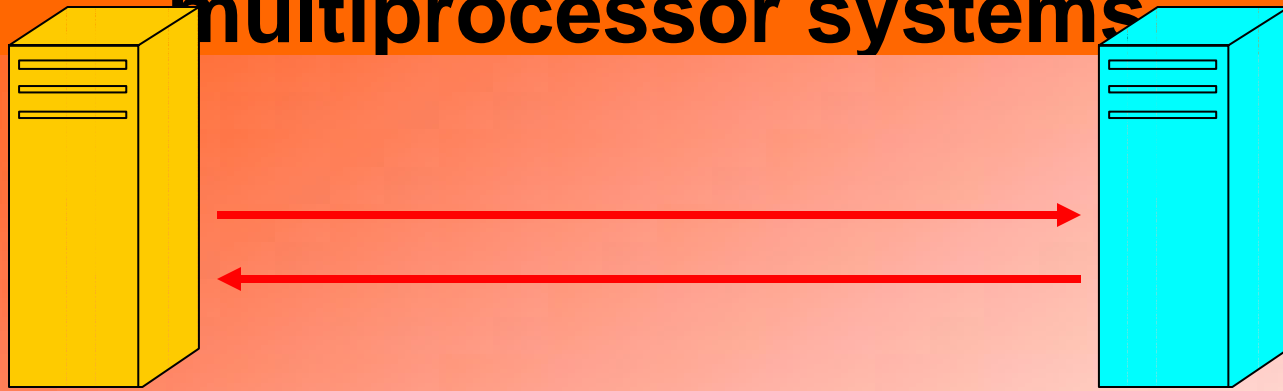


Solve system $AU = b$ on a multiprocessor computer system



- Need to communicate data between processors
 - distributed memory or shared memory ?

Parallel solution: distributed memory multiprocessor systems



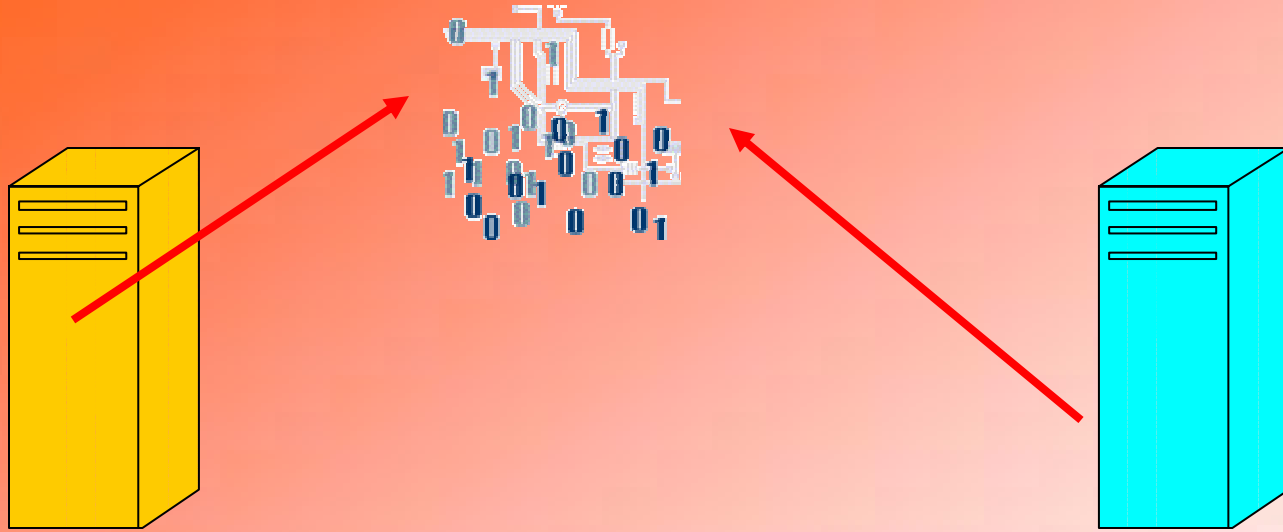
- Issues: computation time versus communication time



- Implementation: MPI (Message Passing Interface)



Parallel solution: shared memory



- Processors communicate with one global (shared) memory: bus contention and latency
- Expensive not always scalable solutions

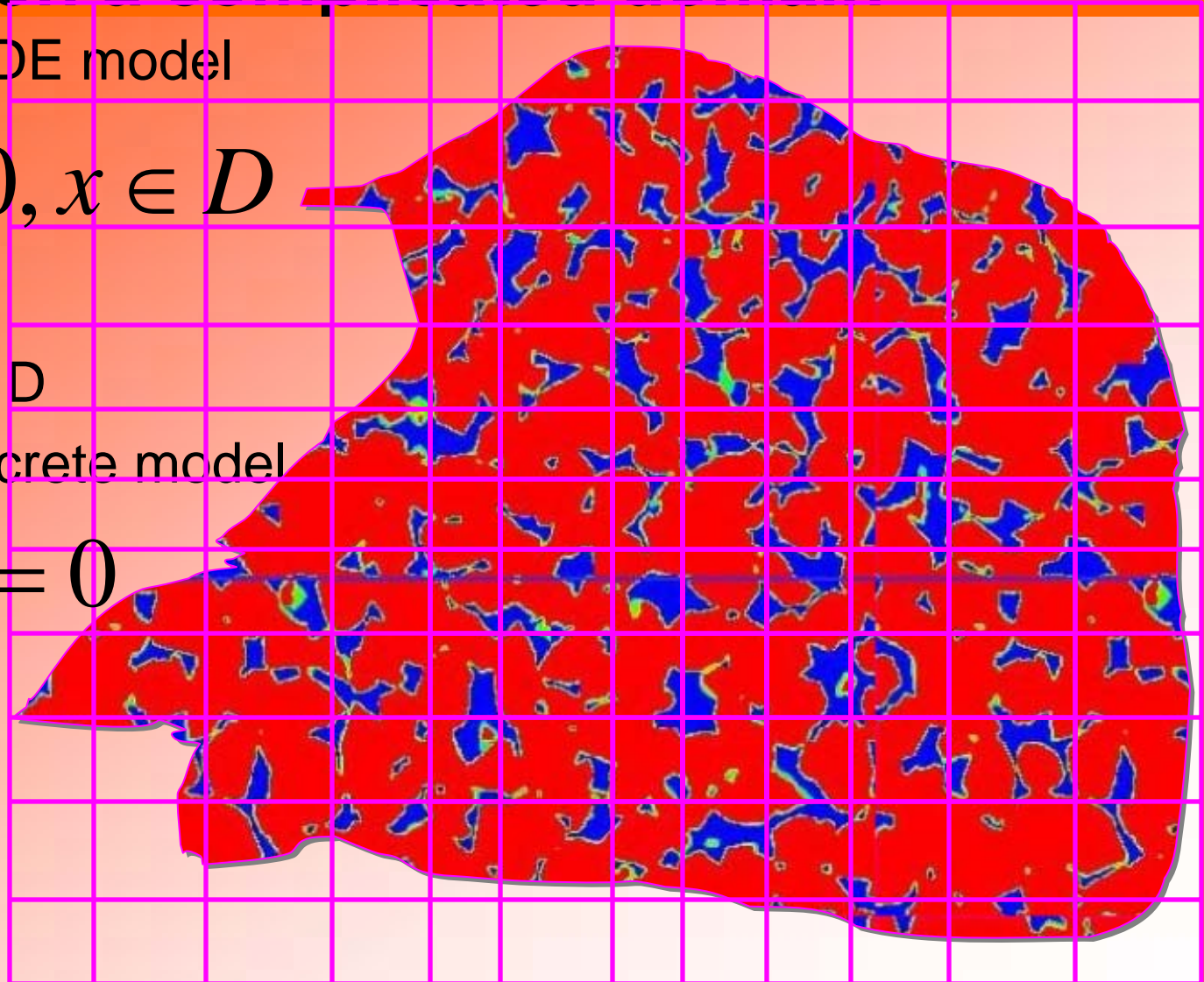
Example: nonlinear PDE on a complicated domain

- given a PDE model

$$F(U) = 0, x \in D$$

- discretize D
- define discrete model

$$F_h(U_h) = 0$$



Example of $F(U) = 0$: multi-phase / multi-component flow

Phase: m , component: M

mass conservation

volume constraints

def.: mass
concentration

def.: mass flux

def.: phase velocity

def.: capillary
pressure relation

constitutive eqs.

$$\frac{\partial(\phi N_M)}{\partial t} + \nabla \cdot U_M = q_M$$

$$\sum_m S_m = 1 \quad \sum_M n_{mM} = 1$$

$$N_M = \frac{1}{\rho_{m^*}} \sum_m S_m \rho_m n_{mM}$$

$$U_M = \frac{1}{\rho_{m^*}} \sum_m \rho_m n_{mM} V_m$$

$$V_m = -K \frac{k_m}{\mu_m} (\nabla P_m - \rho_m G \nabla D)$$

$$P_{m_1} - P_{m_2} = P^c_{m_1, m_2}(S_{m_1}, \dots)$$

$$\rho_m = \rho_m(P_m, n_{mM})$$

Specific model

Example: simulate oil and gas recovery

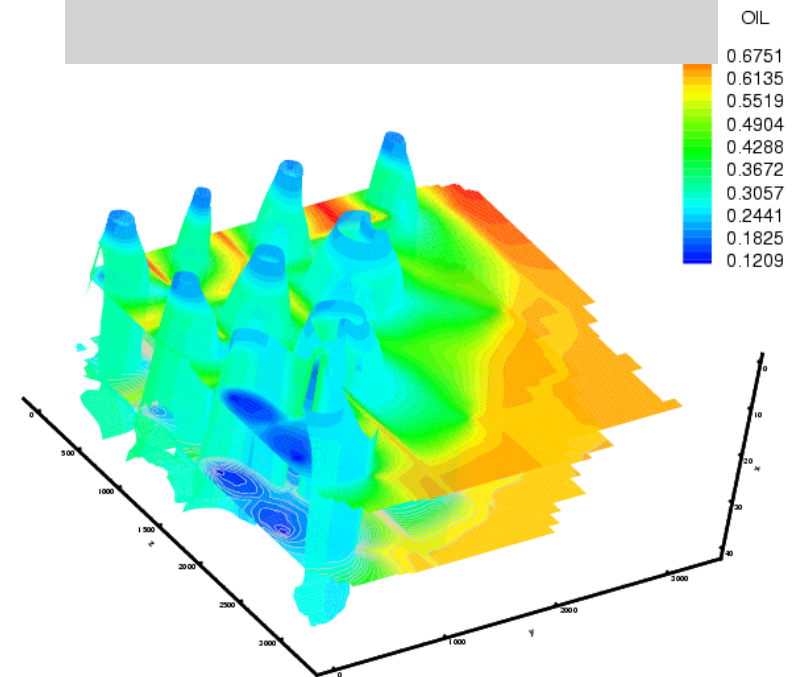
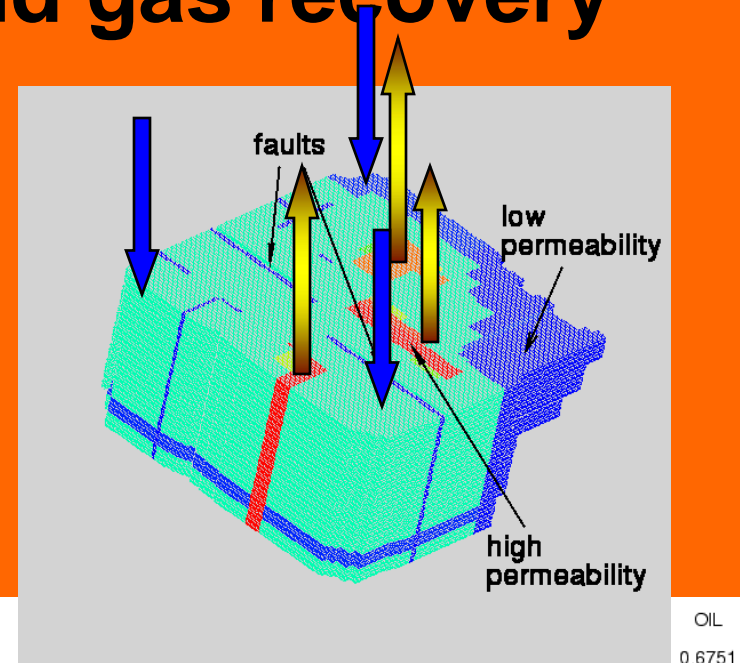
- oil and gas displaced by water contained in D : region in which there is oil and gas and water (brine)

$$F(U) = 0$$

- must discretize D (decide which scheme to use)

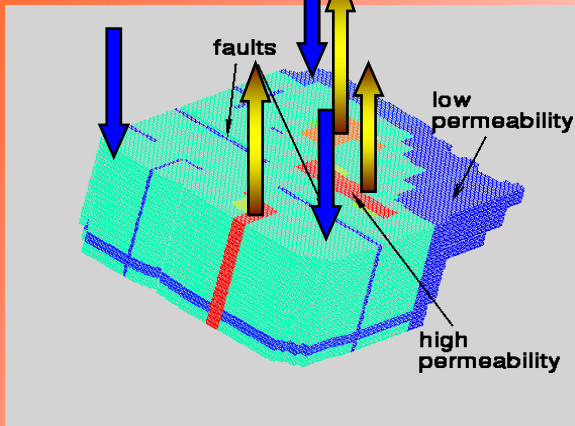
$$F_h(U_h) = 0$$

- must solve the system for U_h
- must post-process the results
 - assess accuracy
 - visualize what is going on



My example: oil and gas recovery

- original domain



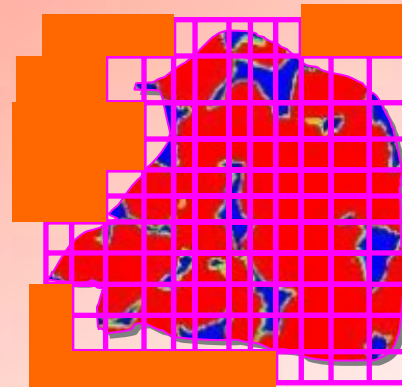
- decomposition into 20 processors

- results

- how accurate is this solution ?
 - that is another story
 - MTH 65* next year ?

Summary of choices: algorithm/implementation

- computing platform
 - serial / workstation
 - parallel / distributed memory: MPI
 - parallel / shared memory
 - parallel supercomputer (PetaFLOPS): a hybrid ?
- discretization method
 - finite differences
 - finite elements
- nonlinear solver
 - Newton-based:
 - » local convergence
 - » global convergence
- linear solver
 - full or sparse matrix ?
 - direct
 - iterative



$$\mathbf{F}(\mathbf{U}) = \mathbf{0}$$

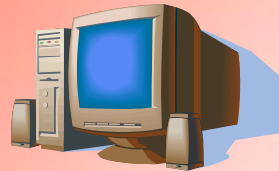
$$\mathbf{A}\mathbf{U} = \mathbf{b}$$

Choices: programming environment



Interpretative environment

- ex: MATLAB
- quick development
- workstation
- graphics available
- may not scale
- not efficient
- not parallel
- portable
 - Windows, Unix, MAC ?
 - but not to supercomputing platforms



Compiled environment

- ex.: FORTRAN, C, C++
- requires post-processing (graphics output to files)
- can reuse “dusty shelves” (legacy code)
- can use highly optimized libraries
- computational kernels as efficient as computer-ly possible
- parallel (MPI)
- can be made portable between supercomputing platforms



In this class we will do both types of implementation

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