

Today:

- Gauss-Seidel and SOR iterative methods
- Totalview debugging

Next:

- GPUs, Python

Read: Class notes and references

$$(U_{i-1} - 2U_i + U_{i+1}) = -\Delta x^2 f(x_i)$$

Solve for U_i :

$$U_i = \frac{1}{2} (U_{i-1} + U_{i+1} + \Delta x^2 f(x_i)).$$

Note: With no heat source, $f(x) = 0$,
the temperature at each point is average of neighbors.

Suppose $U^{[k]}$ is a approximation to solution. Set

$$U_i^{[k+1]} = \frac{1}{2} (U_{i-1}^{[k]} + U_{i+1}^{[k]} + \Delta x^2 f(x_i)) \quad \text{for } i = 1, 2, \dots, n.$$

Repeat for $k = 0, 1, 2, \dots$ until convergence.

Can be shown to converge (eventually... **very slow!**)

Jacobi iteration in Fortran

```

uold = u  ! starting values before updating
do iter=1,maxiter
  dumax = 0.d0
  do i=1,n
    u(i) = 0.5d0*(uold(i-1) + uold(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold(i)))
  enddo
  ! check for convergence:
  if (dumax .lt. tol) exit
  uold = u  ! for next iteration
enddo

```

Note: we must use old value at $i - 1$ for Jacobi.

Otherwise we get the **Gauss-Seidel** method.

Gauss-Seidel iteration in Fortran

```

do iter=1,maxiter
  dumax = 0.d0
  do i=1,n
    uold = u(i)
    u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold))
  enddo
  ! check for convergence:
  if (dumax .lt. tol) exit
enddo

```

Note: Now $u(i)$ depends on value of $u(i-1)$ that has already been updated for previous i .

Good news: This converges about twice as fast as Jacobi!

But... loop carried dependence! Cannot parallelize so easily.

Red-black ordering

We are free to write equations of linear system in any order...
reordering rows of coefficient matrix, right hand side.

Can also number unknowns of linear system in any order...
reordering elements of solution vector.

Red-black ordering: Iterate through points with odd index first
($i = 1, 3, 5, \dots$) and then even index points ($i = 2, 4, 6, \dots$).

Then all black points can be updated in any order,
all red points can then be updated in any order.

Same asymptotic convergence rate as natural ordering.



Red-Black Gauss-Seidel

```
do iter=1,maxiter
  dumax = 0.d0

  ! UPDATE ODD INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold)
  do i=1,n,2
    uold = u(i)
    u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! UPDATE EVEN INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold)
  do i=2,n,2
    uold = u(i)
    u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! check for convergence:
  if (dumax .lt. tol) exit
enddo
```

Gauss-Seidel method in 2D

If $\Delta x = \Delta y = h$:

$$\frac{1}{h^2} (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j}) = -f(x_i, y_j).$$

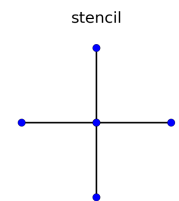
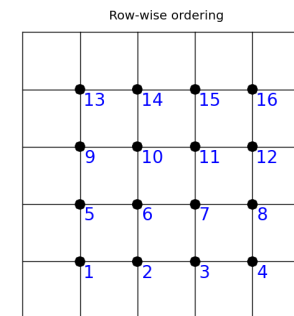
Solve for $U_{i,j}$ and iterate:

$$u_{i,j}^{[k+1]} = \frac{1}{4} (u_{i-1,j}^{[k+1]} + u_{i+1,j}^{[k]} + u_{i,j-1}^{[k+1]} + u_{i,j+1}^{[k]} - h^2 f_{i,j})$$

Again no need for matrix A .

Note: Above indices for old and new values assumes we iterate
in the **natural row-wise order**.

Gauss-Seidel in 2D

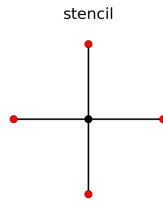
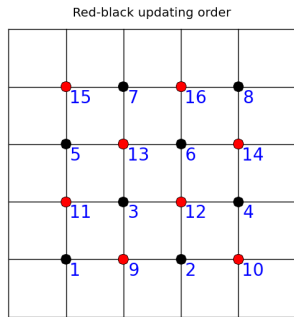


Updating point 7 for example (u_{32}):

Depends on **new values** at points 6 and 3, **old values** at points 7 and 10.

$$U_{32}^{[k+1]} = \frac{1}{4} (U_{22}^{[k+1]} + U_{42}^{[k]} + U_{21}^{[k+1]} + U_{41}^{[k]} + h^2 f_{32})$$

Red-black ordering in 2D



Again all black points can be updated in any order:

New value depends only on red neighbors.

Then all red points can be updated in any order:

New value depends only on black neighbors.

SOR method

Gauss-Seidel move solution in right direction but not far enough in general.

Iterates “relax” towards solution.

Successive Over-Relaxation (SOR):

Compute Gauss-Seidel approximation and then go further:

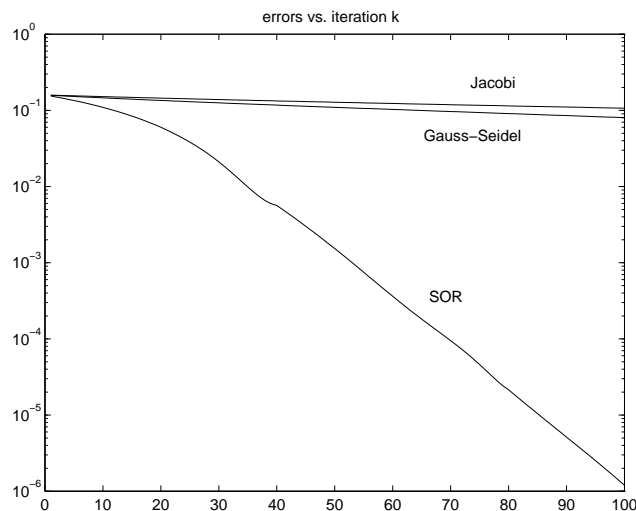
$$U_i^{GS} = \frac{1}{2}(U_{i-1}^{[k+1]} + U_{i+1}^{[k]} + \Delta x^2 f(x_i))$$

$$U_i^{[k+1]} = U_i^{[k]} + \omega(U_i^{GS} - U_i^{[k]})$$

where $1 < \omega < 2$.

Optimal omega (For this problem): $\omega = 2 - 2\pi\Delta x$.

Convergence rates



Red-Black SOR in 1D

```

do iter=1,maxiter
  dumax = 0.d0

  ! UPDATE ODD INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold, ugs)
  do i=1,n,2
    uold = u(i)
    ugs = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    u(i) = uold + omega*(ugs-uold)
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! UPDATE EVEN INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold, ugs)
  do i=2,n,2
    uold = u(i)
    ugs = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    u(i) = uold + omega*(ugs-uold)
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! check for convergence...

```

Note that uold, ugs must be private!

Totalview debugger

`http://www.roguewave.com/products/totalview-family`

Student versions available — see email to class.