COMP 696: Parallel Computing - Jacobian Iterative Scheme

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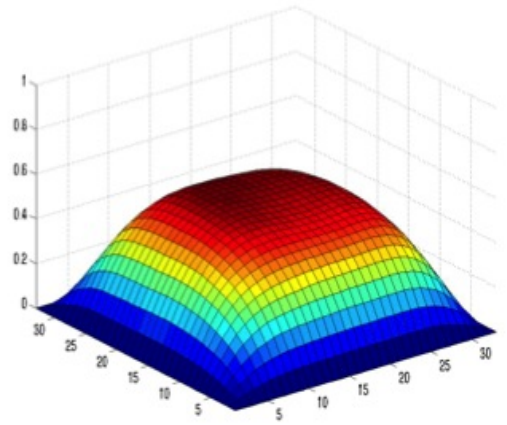


Partial Differential Equations

- Heat/diffusion equation : Heat transfer, particle diffusion, approximation of nuclear transport
- Poisson/Laplace equation : Electromagnetics
- Wave equation : wave propagation, vibration
- Fluid dynamics

PDE Solver methods

- Direct solvers
  - Gauss elimination
  - LU decomposition
- Iterative solvers
  - Basic iterative solvers
    - Jacobi
    - Gauss-Seidel
    - Successive over-relaxation
    - Relaxation methods are iterative methods for solving systems of equations, including nonlinear systems.
    - Relaxation methods were developed for solving large sparse linear systems using finite-difference
  - Krylov subspace methods
    - Generalized minimum residual (GMRES)
    - Conjugate gradient

2D Laplacian - Heat Equation

2D Laplacian:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0,$$

Boundary Conditions:

u(x,0) = $sin(\pi x)$ $\quad 0 <= x <= 1$

u(x,1) = $sin(\pi x)\, e^{-x}$ $\quad 0 \leq x \leq 1$

u(1,y) = 0 $\quad 0 <= y <= 1$

Analytical solution: $sin(\pi x)\, e^{-xy}$ $\quad (0 \leq x \leq 1); (0 \leq y \leq 1)$.

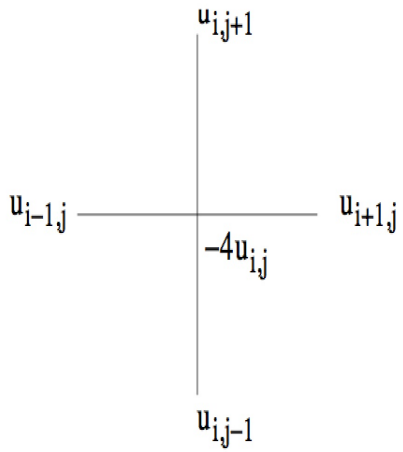
Jacobi Iterative Scheme

Jacobi Iteration - Finite Difference Approximation

Use Taylor Series expansion on uniform grid to yield linear system of equations

$$\nabla^2 u_{i,j} = \frac{1}{h^2}[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}] = 0$$

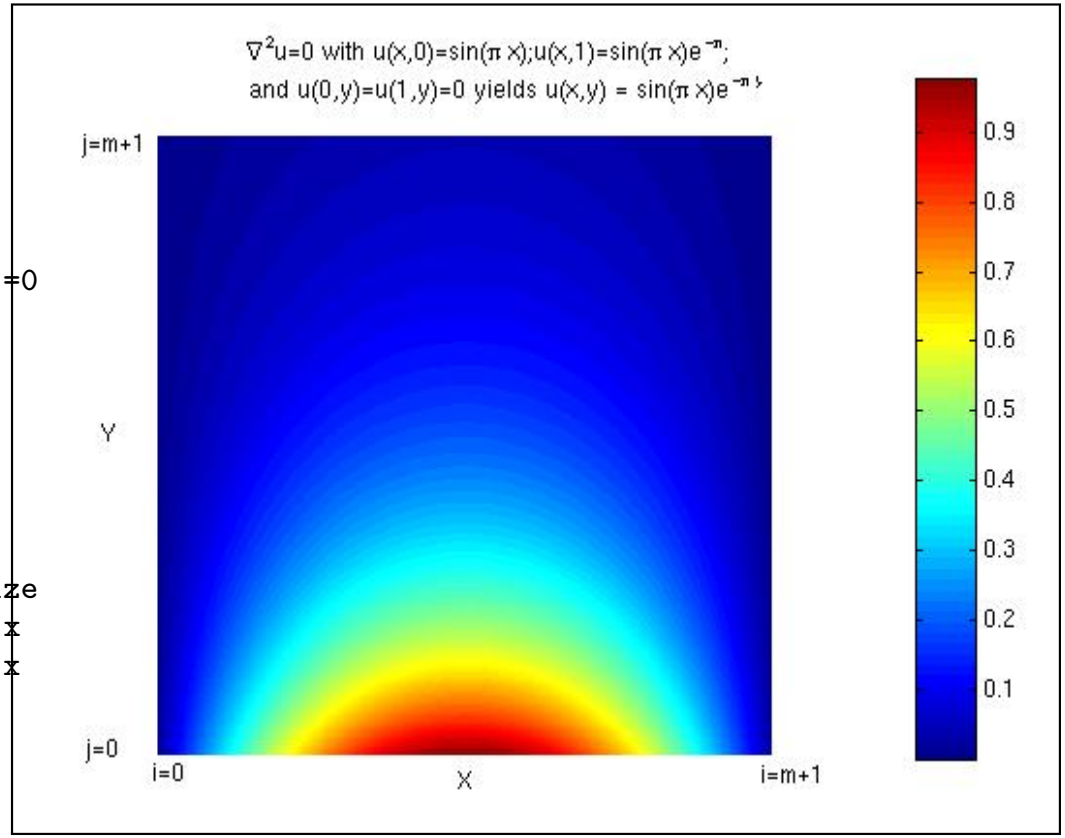
```
c => u(1:m  ,1:m  )    ! i  ,j  Current/Central
                                ! for 1<=i<=m; 1<=j<=m
n => u(1:m  ,2:m+1) ! i  ,j+1  North (of Current)
e => u(2:m+1,1:m )  ! i+1,j    East  (of Current)
w => u(0:m-1,1:m  ) ! i-1,j    West  (of Current)
s => u(1:m  ,0:m-1)  ! i  ,j-1  South (of Current)
```



Source: http://www.eng.utah.edu/~cs3200/notes/cs3200-Finite-Differences.pdf

Serial Jacobi Iterative Scheme - Boundary Conditions

```
  SUBROUTINE bc(u, m)
! PDE: Laplacian u = 0;       0<=x<=1;  0<=y<=1
! B.C.: u(x,0)=sin(pi*x);
!        u(x,1)=sin(pi*x)*exp(-pi); u(0,y)=u(1,y)=0
! SOLUTION: u(x,y)=sin(pi*x)*exp(-pi*y)
    IMPLICIT NONE
    INTEGER m, j
    REAL(real8), DIMENSION(0:m+1,0:m+1) :: u
    REAL(real8), DIMENSION(:,:), POINTER :: c
    REAL(real8), DIMENSION(0:m+1) :: y0
    y0 = sin(3.141593*(/(j,j=0,m+1)/)/(m+1))
    u = 0.0d0      ! at x=0,1; all y plus initialize
    u(:,  0) = y0                  ! at y = 0; all x
    u(:,m+1) = y0*exp(-3.141593) ! at y = 1; all x
    RETURN
  END SUBROUTINE bc
```



Source: Kaden Notes: `http://scv.bu.edu/~kadin/alliance/apply/solvers/`

Serial Jacobi Iterative Scheme - Boundary Conditions

```
PROGRAM Jacobi
USE serial_jacobi_module
REAL(real8), DIMENSION(:,:), POINTER :: c, n, e, w, s

write(*,*)'Enter matrix size, m:'
read(*,*)m
! start timer, measured in seconds
CALL cpu_time(start_time)
 ! mem for unew, u
ALLOCATE ( unew(m,m), u(0:m+1,0:m+1) )

c => u(1:m  ,1:m  )    ! i  ,j  Current/Central
                                ! for 1<=i<=m; 1<=j<=m
n => u(1:m  ,2:m+1) ! i  ,j+1  North (of Current)
e => u(2:m+1,1:m )  ! i+1,j    East  (of Current)
w => u(0:m-1,1:m  ) ! i-1,j    West  (of Current)
s => u(1:m  ,0:m-1)  ! i  ,j-1  South (of Current)

CALL bc(u, m)          ! set up boundary values

 ! iterate until error below threshold
DO WHILE (gdel > tol)
  ! increment iteration counter
  iter = iter + 1
  IF(iter > 5000) THEN
    WRITE(*,*)'Iteration terminated (exceeds 5000)'
    STOP                        ! nonconvergent solution
  ENDIF
  unew = ( n + e + w + s )*0.25 ! new solution, Eq. 3
  gdel = MAXVAL(DABS(unew-c))    ! find local max error
  IF(MOD(iter,10)==0) WRITE(*,"('iter,gdel:',i6,e12.4)")i
  c = unew                      ! update interior u
ENDDO

CALL CPU_TIME(end_time)       ! stop timer
PRINT *,'Total cpu time =',end_time - start_time,' x 1'
PRINT *,'Stopped at iteration =',iter
PRINT *,'The maximum error =',gdel

write(40,"(3i5)")m,m,1
write(41,"(6e13.4)")u
DEALLOCATE (unew, u)

END PROGRAM Jacobi
```

Source: Kaden Notes: http://scv.bu.edu/~kadin/alliance/apply/solvers/

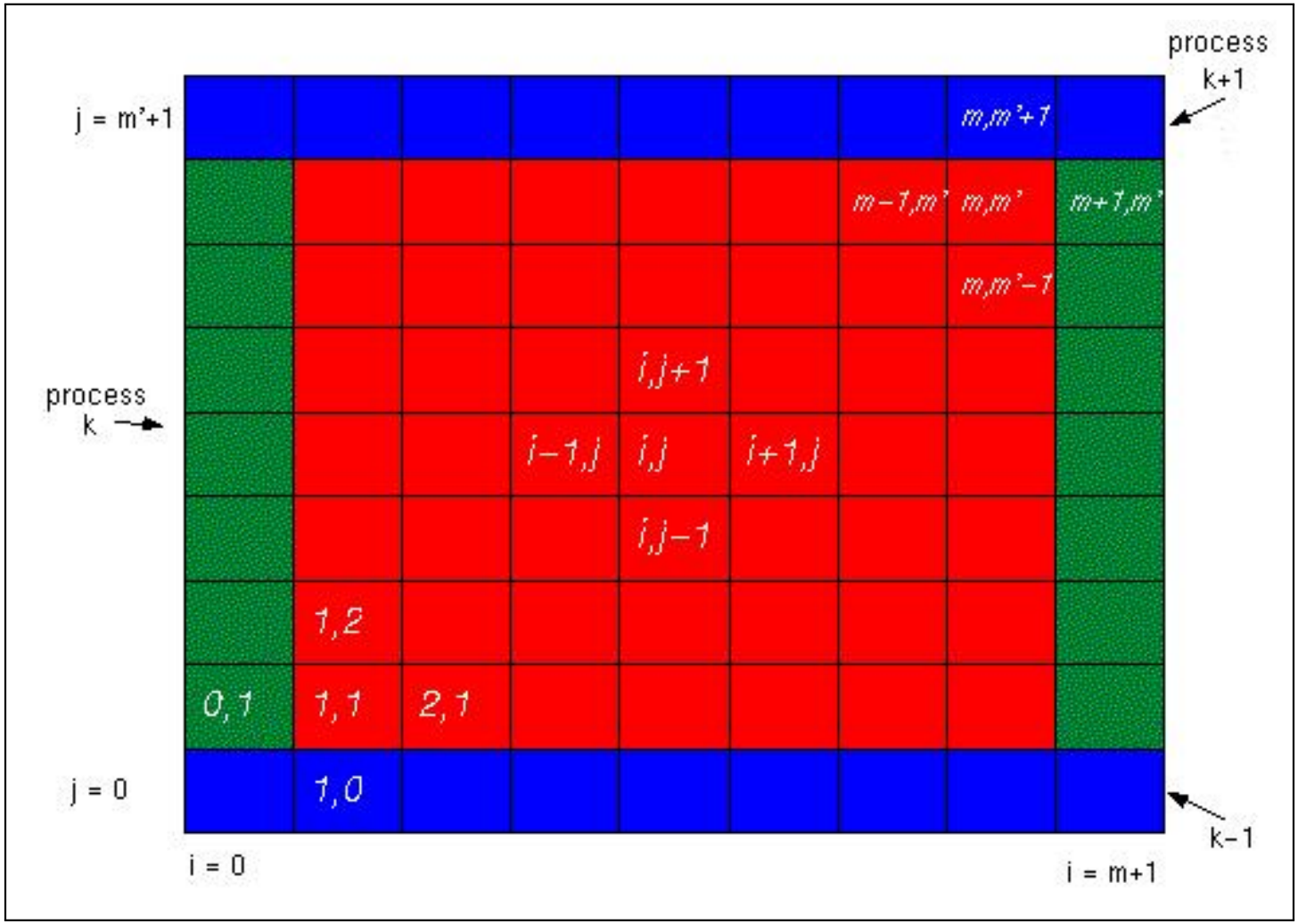
Parallel Jacobi Approach

- Divide work evenly among processors (mxm/p),
- Divide work into P (number of PEs) horizontal strips
- Rewrite FD equation for solving u on PE k:

$$u_{i,j}^{n+1,k} = \frac{u_{i+1,j}^{n,k} + u_{i-1,j}^{n,k} + u_{i,j+1}^{n,k} + u_{i,j-1}^{n,k}}{4}$$

- n is the iteration number
- **Red** cells hold solution at iteration $(n+1)$
- **Blue** cells on top/bottom are the neighbor cells –¿ need to get them from other processor
- Green cells hold boundary conditions

Ghost Cell Layout



Source: Kaden Notes: `http://scv.bu.edu/~kadin/alliance/apply/solvers/`

Parallel Jacobi Code

```
PROGRAM Jacobi
USE types_module;   USE jacobi_module;
USE mpi_module
REAL, DIMENSION(:,:), POINTER :: c, n, e, w, s
CALL MPI_Init(ierr)  ! starts MPI
! get current process id
CALL MPI_Comm_rank(MPI_COMM_WORLD, k, ierr)
! get # procs from env
CALL MPI_Comm_size(MPI_COMM_WORLD, p, ierr)
if( k == 0) then
  write(*,*)'Enter matrix size, m:'   ;
  read(*,*)m
endif
CALL MPI_Bcast(m, 1, MPI_INTEGER, 0, &
              MPI_COMM_WORLD, ierr)
 ! start timer, measured in seconds
CALL cpu_time(start_time)
mp = m/p     ! columns for each proc
! mem for vnew, v
ALLOCATE ( vnew(m,mp), v(0:m+1,0:mp+1) )
c => v(1:m  ,1:mp  )      ! i  ,j
   ! for 1<=i<=m; 1<=j<=mp
n => v(1:m  ,2:mp+1)   ! i  ,j+1
e => v(2:m+1,1:mp  )   ! i+1,j
w => v(1:m  ,0:mp-1)   ! i-1,j
s => v(0:m-1,1:mp  )    ! i  ,j-1
```

```
CALL bc(v, m, mp, k, p)        ! set up boundary values
! determines domain border flags
CALL neighbors(k, below, above, p)
! iterate until error below threshold
DO WHILE (gdel > tol)
  iter = iter + 1     ! increment iteration counter
  IF(iter > 5000) THEN
    WRITE(*,*)'Iteration terminated (exceeds 5000)'
    STOP       ! nonconvergent solution
  ENDIF
  vnew = ( n + e + w + s )*0.25  ! new solution
  ! find local max error
  del = MAXVAL(DABS(vnew-c))
  IF(MOD(iter,10)==0)   &
       WRITE(*,"('k,iter,del:',i4,i6,e12.4)")k,iter,del
  IF(m==4 .and. MOD(iter,10) == 0)   &
     CALL print_mesh(v,m,mp,k,iter)
  c = vnew                        ! update interior v
  CALL MPI_Allreduce( del, gdel, 1,   &
        MPI_DOUBLE_PRECISION, MPI_MAX,   &
        MPI_COMM_WORLD, ierr )  ! find global max error

  CALL update_bc_2( v, m, mp, k, below, above)
! CALL update_bc_1( v, m, mp, k, below, above)
ENDDO
```

Parallel Jacobi - Update Routines

```
  SUBROUTINE update_bc_1(v, m, mp, k, below, above)
    IMPLICIT NONE
    INCLUDE 'mpif.h'
    INTEGER :: m, mp, k, ierr, below, above
    REAL(real8), DIMENSION(0:m+1,0:mp+1) :: v
    INTEGER status(MPI_STATUS_SIZE)
! Select 2nd index for domain decomposition to have stride 1
! Use odd/even scheme to reduce contention in message passing
    IF(mod(k,2) == 0) THEN     ! even numbered processes
      CALL MPI_Send( v(1,mp  ), m, MPI_DOUBLE_PRECISION, above, 0,  &
                     MPI_COMM_WORLD, ierr)
      CALL MPI_Recv( v(1,0   ), m, MPI_DOUBLE_PRECISION, below, 0,  &
                     MPI_COMM_WORLD, status, ierr)
      CALL MPI_Send( v(1,1   ), m, MPI_DOUBLE_PRECISION, below, 1,  &
                     MPI_COMM_WORLD, ierr)
      CALL MPI_Recv( v(1,mp+1), m, MPI_DOUBLE_PRECISION, above, 1,  &
                     MPI_COMM_WORLD, status, ierr)
    ELSE                           ! odd numbered processes
      CALL MPI_Recv( v(1,0   ), m, MPI_DOUBLE_PRECISION, below, 0,  &
                     MPI_COMM_WORLD, status, ierr)
      CALL MPI_Send( v(1,mp  ), m, MPI_DOUBLE_PRECISION, above, 0,  &
                     MPI_COMM_WORLD, ierr)
      CALL MPI_Recv( v(1,mp+1), m, MPI_DOUBLE_PRECISION, above, 1,  &
                     MPI_COMM_WORLD, status, ierr)
      CALL MPI_Send( v(1,1   ), m, MPI_DOUBLE_PRECISION, below, 1,  &
                     MPI_COMM_WORLD, ierr)
    ENDIF
    RETURN
  END SUBROUTINE update_bc_1
```

Parallel Jacobi - Update Routines

```
SUBROUTINE update_bc_2( v, m, mp, k, below, above )
  INCLUDE "mpif.h"
  INTEGER :: m, mp, k, below, above, ierr
  REAL(real8), dimension(0:m+1,0:mp+1) :: v
  INTEGER status(MPI_STATUS_SIZE)

  CALL MPI_SENDRECV(                                          &
            v(1,mp  ), m, MPI_DOUBLE_PRECISION, above, 0,  &
            v(1,   0), m, MPI_DOUBLE_PRECISION, below, 0,  &
            MPI_COMM_WORLD, status, ierr )
  CALL MPI_SENDRECV(                                          &
            v(1,   1), m, MPI_DOUBLE_PRECISION, below, 1,  &
            v(1,mp+1), m, MPI_DOUBLE_PRECISION, above, 1,  &
            MPI_COMM_WORLD, status, ierr )
  RETURN
END SUBROUTINE update_bc_2
```