Numerical Algorithms for HPC

Solution of Boundary Value Problems

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Overview of Lecture

- Overview of linear solving methods
- Relaxation methods
  - Jacobi algorithm
  - testing for convergence
  - Gauss Seidel
  - over-relaxation
- Notes
  - parallelisation
  - non-linear equations
- Pollution problem
  - solution using relaxation methods
  - 2D equations including wind

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Many methods for solving $Au = b$

- Direct methods
  - give the solution after a fixed number of operations
    - Gaussian elimination
    - LU factorisation
- Relaxation methods (this lecture)
  - gradually improve solution, starting from an initial guess
  - stop when the answer is sufficiently accurate
  - simple to implement but may be slow to converge on solution
    - or may fail completely!
- Krylov subspace methods (following lectures)
  - iterative (like relaxation methods) but more sophisticated
  - harder to implement but more efficient and reliable

Why not use Direct Methods?

- Direct methods explicitly operate on the matrix A
  - e.g. decompose it into L and U factors
- For PDEs, A is very sparse indeed
  - may contain 99% zeros so clearly we use compressed storage
  - we want to take advantage of this when we solve equations
- Difficult to exploit sparsity for direct methods
  - e.g. L and U may be dense even though A is sparse
  - for large systems of equations, we may run out of memory!
- Relaxation and Krylov methods (see later) exploit sparsity
  - relaxation methods operate on the equations not the matrix
  - Krylov methods comprise mostly matrix-vector multiplications
    - can write efficient routines to do $y = A\,x$ when A is sparse
  - start to show the solution earlier during process of solving

Relaxation vs Matrix Methods

- Operate directly on the difference equations
  - can forget (almost!) all about the matrix representation $Au = b$ for this lecture
  - it turns out that relaxation methods can usefully be understood in terms of matrix-vector operations (not immediately obvious)
    - See lecture on "Matrix Splitting Techniques" later
- For illustrative purposes, look at 1D problem
  - for simplicity with no wind
  - exercise will involve extending this to the 2D problem
    - quite straightforward in practice

Relaxation Methods

- 1D diffusion equations are

$$-u_{i-1} + 2u_i - u_{i+1} = 0 \qquad i = 1,2,\ldots,N$$

- Equivalently: $u_i = {}^1/_2\,(u_{i-1} + u_{i+1})$
  - why not make an initial guess at the solution
  - then loop over each lattice point i and set $u_i = {}^1/_2\,(u_{i-1} + u_{i+1})$
  - i.e. we solve the equation exactly at each point in turn
- Updating u_i spoils the solution we just got for u_{i-1}
  - so simply iterate the whole process again and again ...
  - ... and hope we eventually get the right answer!
- This is called the Jacobi Algorithm
  - the simplest possible relaxation method

Jacobi Algorithm

- Use superscript n to indicate iteration number
  - n counts the number of times we update the *whole* solution
  - equivalent to computer time
- Jacobi algorithm for diffusion equation is:

$$u_i^{(n+1)} = {}^1\!/_2 \left(u_{i-1}^{(n)} + u_{i+1}^{(n)} \right)$$

- Each iteration, calculate $u^{(n+1)}$ in terms of $u^{(n)}$
  - don't need to keep copies of all the previous solutions
  - only need to remember two solutions at any time: u and u_{new}
    - corresponding to iterations n and $n+1$

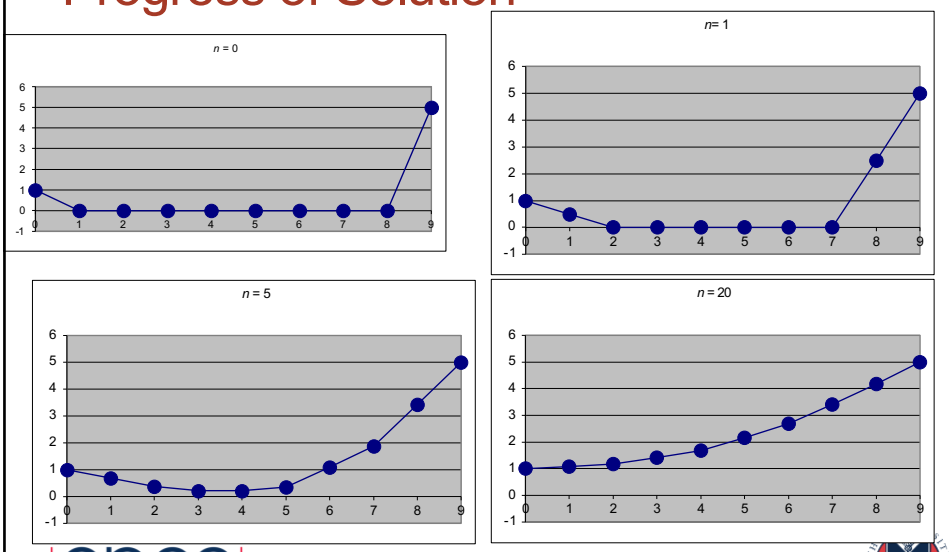
Jacobi Pseudo-Code

```
declare arrays:    u(0, 1, ..., M+1)
                 unew(0, 1, ..., M+1)

initialise: set boundaries: u(0)   = fixed value u0
                            u(M+1) = fixed value uM+1
          initial guess:  u(1, 2, ..., M) = guess value

loop over n = 1, 2, ...

  update:    loop over internal points: i = 1, 2, ... M
               unew(i) = 0.5*( u(i-1) + u(i+1) )
             end loop over i

  copy back: u(1, 2, ..., M) = unew(1, 2, ..., M)

end loop over n
```


Implementation Notes

- Array declarations
  - Fortran: `real, dimension(0:M+1) :: u`
  - Java: `float[] u = new float[M+2];`
  - C: `float u[M+2];`
- Arrays explicitly contain boundaries u_0 and u_{M+1}
  - we set them according to boundary conditions
    - but we NEVER update them!
  - e.g. when we copy u_{new} back to u, only copy internal values
  - in pseudo-code, boundary values for u_{new} are never set
    - complete solution is therefore only ever present in u
    - might be more elegant to set boundaries in u_{new} as well
- What to choose for initial guess $u_i^{(0)}$?
  - for a simple implementation just set interior values to zero

Progress of Solution



When to Stop the Iterative Loop

- The solution *appears* to be getting better
  - must quantify this!
- For dense systems we used the residual
  - we tried to solve $Ax = b$, so $r = b - Ax$ should be a zero vector
  - in practice, there is a numerical error in solution of each equation
  - error in equation i is the value of r_i
    - Norm of residual is computed from the sum of the squares of r_i
  - Can calculate residue as before: $\frac{||r||_2}{||b||_2}$
- Can do the same thing for relaxation methods
  - compute the sum of the squares of the error in each equation
  - do this at the end of each iterative loop over n
    - stop if this is small enough

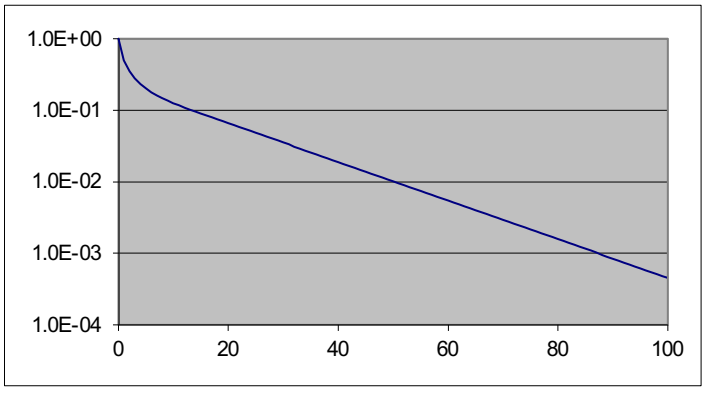
Pseudocode for Residual Calculation

```
loop over n = 1, 2, ...
  update:     ...
  copy back:  ...

  compute residue: rnorm = 0.0
                   loop over i = 1, 2, ..., M
                     rnorm = rnorm + (-u(i-1)+2*u(i)-u(i+1))^2
                   end loop over n
                   rnorm = sqrt(rnorm)

   normalise:      res = rnorm / bnorm

   if (res < tolerance) finish

end loop over n
```


Notes on Residual

- For a perfect solution, residue will be zero
  - in practice we will get a finite value
  - usually stop when it is "small", e.g. a tolerance of res $< 10^{-6}$
  - there will be a limit to how small the residual can get
    - can easily hit the limits of single precision
    - use double precision everywhere (or at least perform residual calculation using doubles)
- Normalisation
  - need to divide by the norm of the *b* vector
  - we saw before that *b* corresponds to the boundary values
  - in 1D: `bnorm = sqrt(u(0)*u(0) + u(M+1)*u(M+1))`
    - in 2D, need to sum values of squares of $u_{i,j}$ over all edges

Residual Against Iteration



- Decreases exponentially
  - with a zero initial guess for u, should equal 1.0 at iteration zero

Parallelisation

- Very simple for Jacobi
- Decompose the problem domain regularly across processes/threads
  - for MPI we need halo regions due to $i \pm 1, j \pm 1$ references
  - halos are 1 cell wide for 5-point stencil
  - could be wider for larger stencils
  - swap halos between neighbouring processes every iteration
- Require global sums for, e.g., residue calculation

Relaxation Methods

- About to cover some variations on Jacobi
  - which we hope will be faster!
- How can we tell if a method will work at all?
- Necessary (but not sufficient) condition
  - if the method arrives at the correct solution it must stay there
- Is this true for Jacobi? $u_i^{(n+1)} = {}^1/_2\left(u_{i-1}^{(n)} + u_{i+1}^{(n)}\right)$
  - for solution: $-u_{i-1}^{(n)} + 2u_i^{(n)} - u_{i+1}^{(n)} = 0$, i.e. ${}^1/_2\left(u_{i-1}^{(n)} + u_{i+1}^{(n)}\right) = u_i^{(n)} = u_i^{(n+1)}$
  - so, $u_i^{(n+1)} = u_i^{(n)}$ and we stay at the solution
    - worth checking this for other methods

Gauss Seidel

- Why do we need both u_{new} and u?

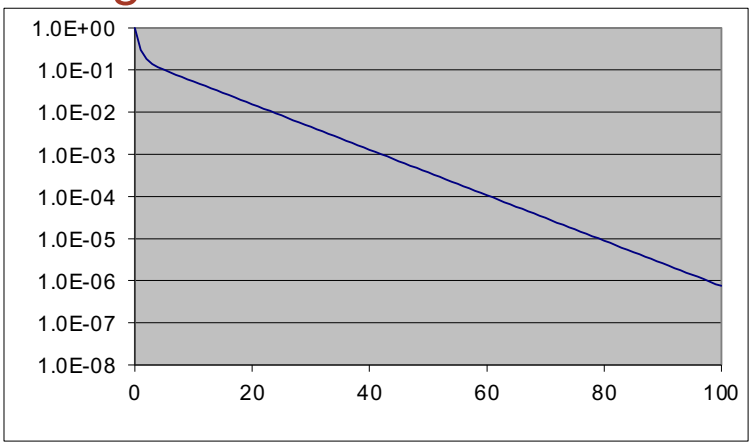
```
update:     loop over internal points: i = 1, 2, ... M
              unew(i) = 0.5*( u(i-1) + u(i+1) )
            end loop over i
copy back: u(1, 2, ..., M) = unew(1, 2, ..., M)
```

- Why not do the update in place?

```
update:     loop over internal points: i = 1, 2, ... M
              u(i) = 0.5*( u(i-1) + u(i+1) )
            end loop over i
```

  - this is called the *Gauss-Seidel* method

Convergence of Gauss-Seidel



- Converges twice as fast as Jacobi
  - for less work and less storage!

Parallelisation Gauss Seidel

- Order of the update loop is now significant
  - we used normal (*lexicographic*) order: other orderings possible
- Parallelisation of Jacobi was easy
  - Just divide grid and each processor sends its boundary data to neighbouring processor ("halo-swapping")
- Parallelisation of Gauss Seidel is harder
  - e.g. in 1D $u_i = {}^1/_2\,(u_{i-1} + u_{i+1})$

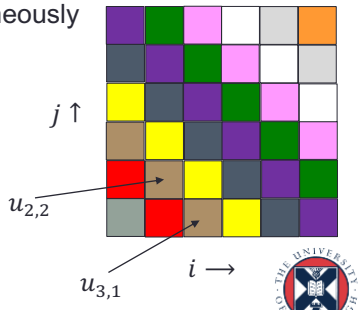
"new" was just updated

"old" just about to be updated

  - Updating of every point depends on the one before, which in turns depends on the one before that…

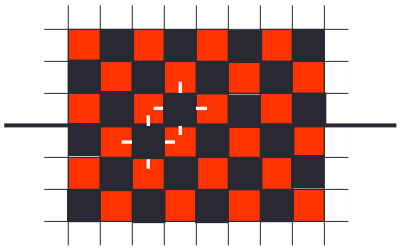
Parallel Gauss Seidel (wavefront)

- Consider dependencies (in 2D)
  - $u_{i,j}$ depends on recently updated values $u_{i-1,j}$ and $u_{i,j-1}$
- In pattern below have inter-colour dependencies,
  - E.g. updates to brown elements depend on red elements
  - …but brown elements don't depend on each other
  - E.g. $u_{2,2}$ does not depend on $u_{3,1}$ or vice versa
  - Brown squares can all be calculated simultaneously
    - i.e. can do the brown (or any colour) in parallel!
- Also works in 3D (more parallelism!)



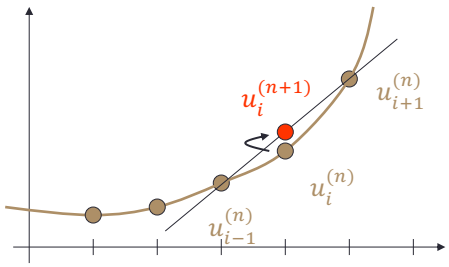
Parallel Gauss Seidel (red-black)

- Red-black order divides grid into chequerboard
  - 2 loops: update all the red squares (in parallel) first then all the black ones (in parallel)
  - new ordering removes some dependence on already updated elements
  - enables Gauss Seidel method to be parallelised
  - ordering can affect convergence (different underlying matrix)



Over Relaxation

- Recall how Jacobi solution progressed



  - we have increased the value of u_i by a small amount
    - but we know the real solution is even higher
  - why not increase by more than suggested
    - i.e. multiply the change by some factor $\omega > 1$

Over-Relaxed Gauss Seidel

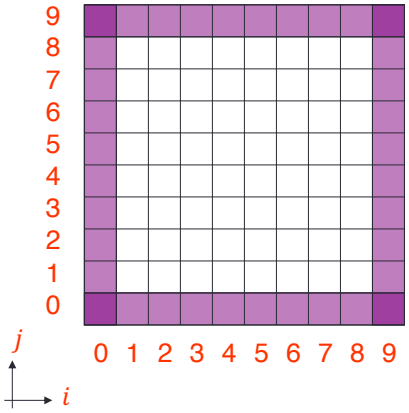
- Gauss-Seidel method: $u_i = {}^1/_2\,(u_{i-1} + u_{i+1})$
  - i.e. $u_i = u_i + {}^1/_2\,[(u_{i-1} - 2u_i + u_{i+1})]$
- Multiply change (in square brackets) by ω
  - over-relaxed update: $u_i = u_i + {}^1/_2\,\omega[(u_{i-1} - 2u_i + u_{i+1})]$
  - or $u_i = (1-\omega)u_i + {}^1/_2\,\omega(u_{i-1} + u_{i+1})$
- Notes
  - original method corresponds to $\omega = 1$
  - if we get to a solution we stay there for any value of ω
  - Theorem by Kahan: ω has to be in range $(0,2)$
  - Sometimes ω known in advance, sometimes trial and error or adaptive

Non-Linear Equations

- Relaxation methods deal directly with equations
  - doesn't matter that we cannot express them as $Au = b$
  - equally valid for non-linear equations (e.g. fluid dynamics)
- Non-linear equations can be very unstable
  - may need to under-relax to get convergence, i.e. $\omega < 1$

Extending to 2 Dimensions

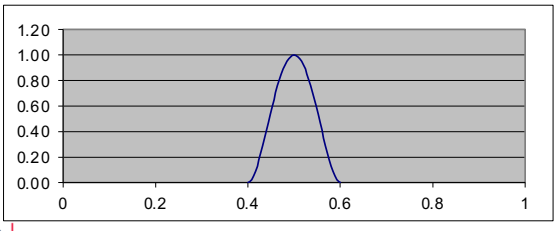
- Initialise
  - set boundary values (purple)
    - zero on top, bottom and left
    - hump function on right
  - zero interior (white)
- Loop over interior
  - $i = 1, 2, \ldots, M$
  - $j = 1, 2, \ldots, M$
  - update $u_{i,j}$ as appropriate
- Repeat until converged
- Write results
  - include boundaries so that the solution looks nice!



2D example with $M = 8$

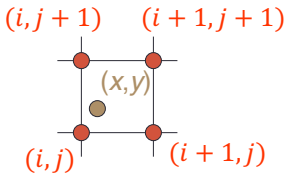
Notes (1)

- How do we convert from (i, j) to (x, y) coordinates?
  - for a domain of size 1×1:
    - $x = ih$ and $y = jh$
- What is the hump function?
  - $u(1.0, y) = k(y_2 - y)^2(y - y_1)^2$
  - a peak, centred at $(y_2 + y_1)/2$, dropping to zero for $y < y_1$ and $y > y_2$
  - for this example, take $y_1 = 0.4$ and $y_2 = 0.6$



Notes (2)

- How do we convert from (x, y) to (i, j) coordinates?
  - e.g. what lattice point do we look at to find $u(0.20,0.33)$?
  - $(0.20,0.33)$ is unlikely to fall exactly on a lattice point
  - the four nearest neighbours are:
    - i = int(x/h)
    - j = int(y/h)



  - do weighted average of these four values (see exercise notes)

Convection-Diffusion Equations

- 1D Gauss-Seidel update

$$u_i = \left(\frac{1}{2+ah}\right)(u_{i-1} + (1+ah)u_{i+1})$$

- 1D Over-Relaxed update

$$u_i = (1-\omega)u_i + \omega\left(\frac{1}{2+ah}\right)(u_{i-1} + (1+ah)u_{i+1})$$

- 2D Discrete Equations

$$u_{i,j} = \frac{1}{(4+(a_x+a_y)h)}\left(u_{i,j-1} + u_{i-1,j} + (1+a_x h)u_{i+1,j} + (1+a_y h)u_{i,j+1}\right)$$

(a_x, a_y) = wind strength from x (East) and y (North) respectively

Notes

- Have multiplied all the equations by h^2
  - equations now explicitly depend on h for a non-zero wind a
  - straightforward to derive update equations for 2D case
- A different convention for Krylov methods (later)
  - maintain the $1/h^2$ factor in matrix A
    - therefore need to multiply RHS by same factor
    - happens to be more convenient
- Finite wind
  - matrix A is now non-symmetric
  - in 1D, lower-diagonal elements are $(1 + ah)$, upper elements are 1
  - gives some minor technical issues when normalising the residue
    - see practical notes
    - if correctly normalised, residue at zero iterations will *always* be 1.0 if the initial guess is a zero solution

Summary

- Relaxation methods
  - guess at an initial solution
  - update many times and stop when residue is small enough
- Update rule is very straightforward
  - solve exactly for each individual u_i
    - obtain formula by rearranging difference equations so u_i is on the LHS
- Interior points updated according to the PDE
  - boundary points set by the boundary conditions
- Jacobi is the simplest method
  - Gauss Seidel acts “in-place” and requires roughly half the iterations
  - appropriate over-relaxation can accelerate this even more
    - finding the best value of ω requires some experimentation!