

Case Study

Lecture 2

Sunita Chandrasekaran

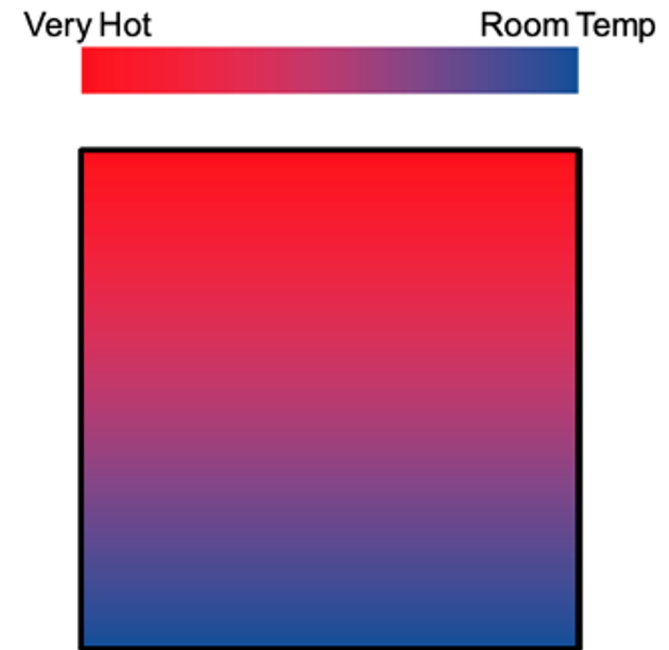
Associate Professor, University of Delaware

PDC Summer School, Aug 2023

Materials also prepared by Dr. Felipe Cabarcas, Postdoctoral Fellow, UDEL

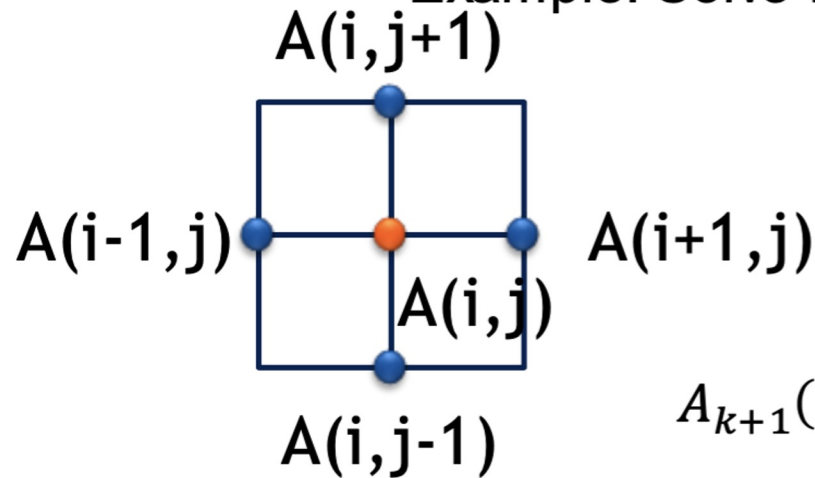
Laplace Heat Transfer

- A simple simulation of heat distributing across a metal plate
- Apply a consistent heat to the top of the plate
- Simulating the heat distribution across the plate



Laplace solver using Jacobi Iteration

- Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.
- Common, useful algorithm
- Example: Solve Laplace equation in 2D: $\nabla^2 f(x, y) = 0$



$$A_{k+1}(i, j) = \frac{A_k(i-1, j) + A_k(i+1, j) + A_k(i, j-1) + A_k(i, j+1)}{4}$$

```
while ( error > tol && iter < iter_max )  
{  
    error = 0.0;
```

Iterate until converged

```
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        Anew[j][i] = 0.25 * ( A[j][i+1] + A[j][i-1] + A[j-1][i] + A[j+1][i]);  
        error = fmax( error, fabs(Anew[j][i] - A[j][i]));  
    }  
}
```

Iterate across matrix elements

Calculate new neighbors

Compute max error for convergence

```
for( int j = 1; j < n-1; j++)  
{  
    for( int i = 1; i < m-1; i++ )  
    {  
        A[j][i] = Anew[j][i];  
    }  
}
```

Swap input/output arrays

Profiling Sequential Code

LLVM

```
$ clang -Ofast -fopenmp -fno-inline -pg -o jacobi-serial  
jacobi.c  
Jacobi relaxation Calculation: 4096 x 4096 mesh  
  0, 0.250000  
 100, 0.002397  
 200, 0.001204  
 300, 0.000804  
 400, 0.000603  
 500, 0.000483  
 600, 0.000403  
 700, 0.000345  
 800, 0.000302  
 900, 0.000269  
total: 25.557923 s
```

NVC

```
$ nvc -O3 -o jacobi-serial jacobi.c  
Jacobi relaxation Calculation: 4096 x 4096 mesh  
  0, 0.250000  
 100, 0.002397  
 200, 0.001204  
 300, 0.000804  
 400, 0.000603  
 500, 0.000483  
 600, 0.000403  
 700, 0.000345  
 800, 0.000302  
 900, 0.000269  
total: 23.364053 s
```

How are we going to parallelize Jacobi?

- OpenMP + Multicore – PDC's Dardel
 - Clang, AMD OpenMP
- OpenMP offloading to GPU – PDC's Dardel
 - Clang, AMD OpenMP
- OpenACC + Multicore – demo on LBNL's Perlmutter
 - NVIDIA HPC SDK
- OpenACC on GPU -- demo on LBNL's Perlmutter
 - NVIDIA HPC SDK