Introduction to Project 3
Nonlinear PDE

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Overview

- Overview of Project 3
- Short review of the code
- Running the code and visualizing the output

The HPC PDE Application

The code solves a reaction diffusion equation known as Fischer's Equation

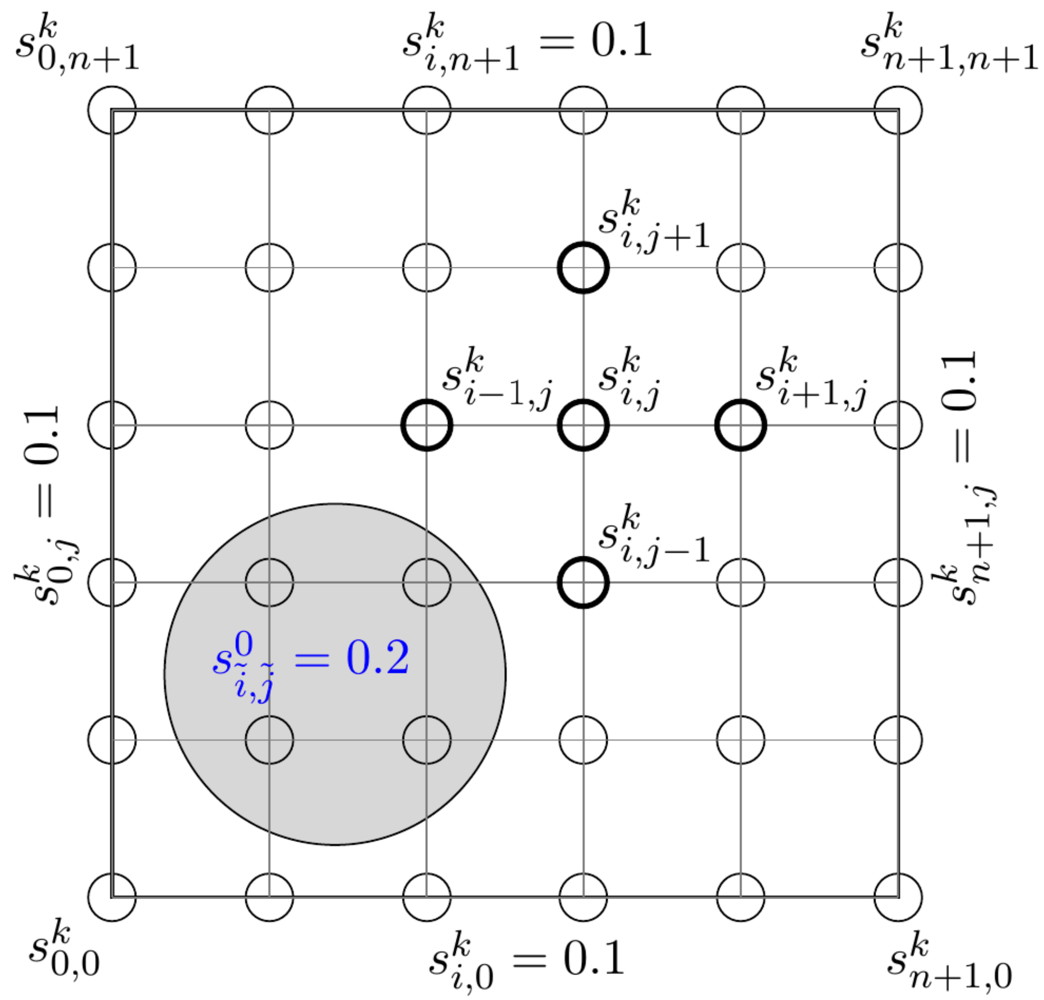
$$\frac{\partial s}{\partial t} = D(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2}) + Rs(1-s)$$

Used to simulate travelling waves and simple population dynamics

- **The species s diffuses**
- **And the population grows to a maximum of s=1**

Initial and boundary conditions

- set the domain to be the unit square, i.e. $\Omega = (0,1)^2$
- fixed boundary values with $s(x) = 0.1 \; for \; x \in \partial\Omega$
- Initial values s^{init} are set to 0.1 except for a circular region with initial values of 0.2 in the lower left corner



Numerical Solution

The rectangular domain is discretized with a grid of dimension (n+2)x(n+2) points

- **A second order finite difference discretization gives the following approximation for the spatial derivatives**

$$(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2})_{i,j} \approx \frac{1}{\Delta x^2}(-4s_{i,j} + s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1})$$

- **A first order finite difference discretization is used for the approximation of the temporal derivative**

$$(\frac{\partial s}{\partial t})^k_{i,j} \approx \frac{1}{\Delta t}(s^k_{i,j} - s^{k-1}_{i,j}),$$

Numerical Solution

- **Putting these together one obtains**

$$\frac{1}{\Delta t}(s_{i,j}^k - s_{i,j}^{k-1}) = \frac{D}{\Delta x^2}(-4s_{i,j}^k + s_{i-1,j}^k + s_{i+1,j}^k + s_{i,j-1}^k + s_{i,j+1}^k) + Rs_{i,j}^k(1 - s_{i,j}^k)$$

- **Reformulate problem as**

$$f_{i,j}^k := [-(4+\alpha)s_{i,j} + s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1} + \beta s_{i,j}(1 - s_{i,j})]^k + \alpha s_{i,j}^{k-1} = 0$$

$$\alpha := \Delta x^2/(D\Delta t)$$

$$\beta := R\Delta x^2/D$$

Numerical Solution

- **One nonlinear equation for each grid point**

together they form a system of N=n*n equations

Solve with Newton's method

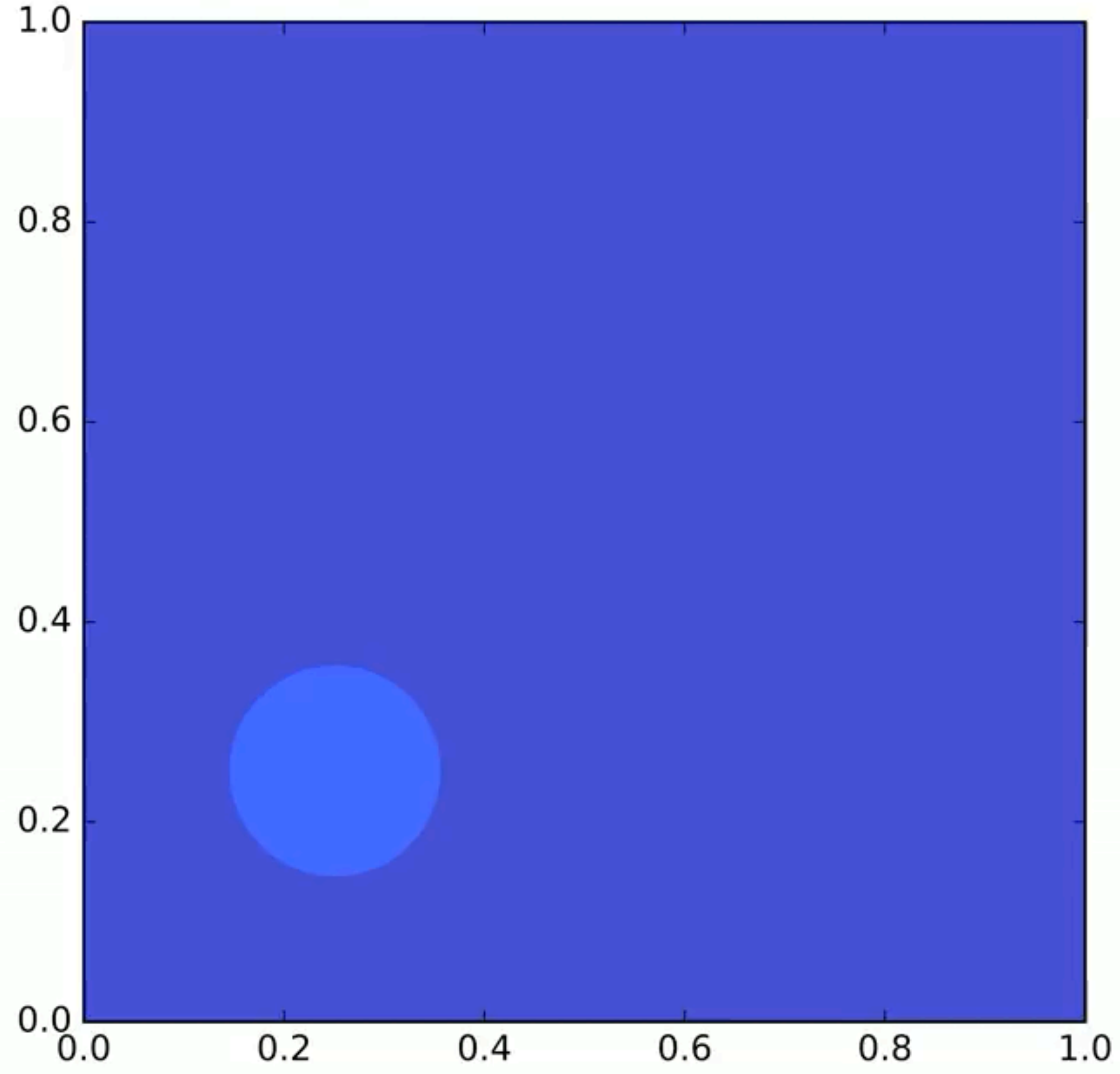
$$y^{l+1} = y^l - [J_f(y^l)]^{-1} f(y^l),$$
$$y^0 := s^{k-1}$$

- **Each iteration of Newton's method has to solve a linear system**

Solve with matrix-free Conjugate Gradient solver

$$[J_f(y^l)]\delta y^{l+1} = f(y^l)$$
$$y^{l+1} = y^l - \delta y^{l+1}$$

Time Evolution of the Solution



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Numerical Solution

- Most of the code is already implemented
- The focus is on the parallelisation of the code using OpenMP
- So let’s look a little closer at each part of the code

Code Walkthrough

There are three modules of interest

- main.cpp: initialization and main time stepping loop
- linalg.cpp : the BLAS level 1 (vector-vector) kernels and conjugate gradient solver
- operators.cpp : the stencil operator for the finite difference discretization

the vector-vector kernels and diffusion operator are the only kernels that have to be parallelized

Linear algebra: linalg.cpp

This file defines simple kernels for operating on 1D vectors, including

- dot product : $x \cdot y$: hpc_dot()

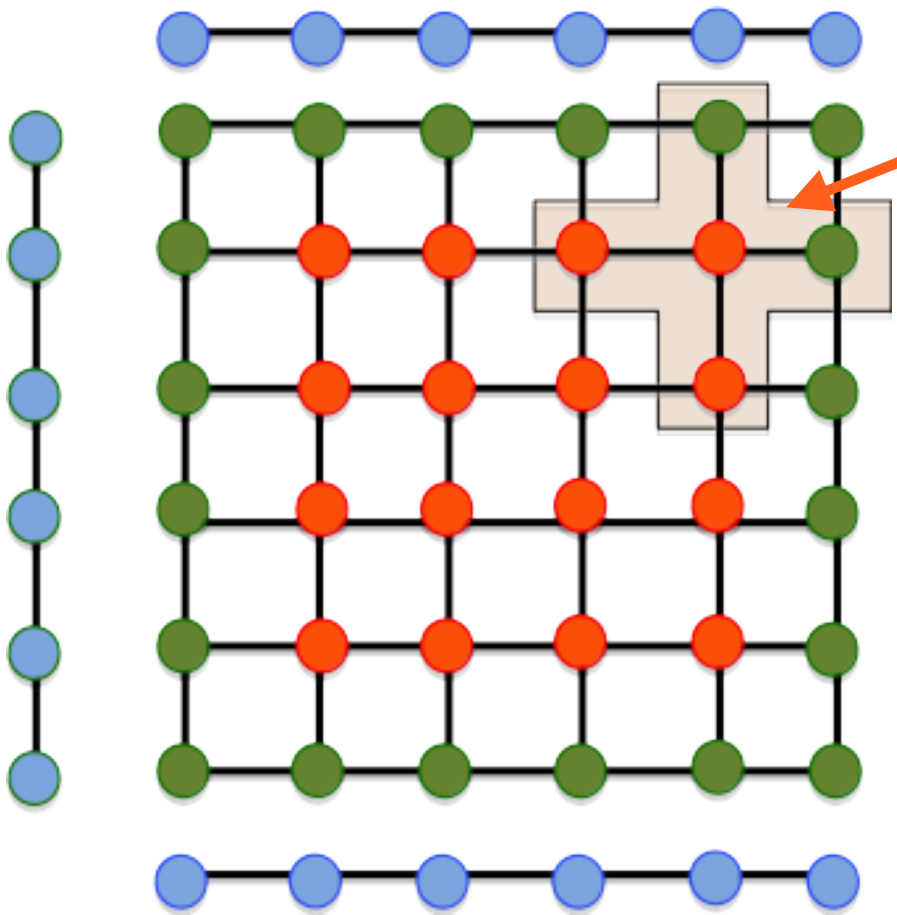
linear combination : $z = \alpha x + \beta y$ where $\alpha, \beta \in \mathbb{R}$: hpc_lcomb()

- The kernels of interest start with hpc_xxxxx()

hpc $==$ HPC Lab for CSE

For each parallelization approach that we will see (OpenMP, and later on MPI), each of these kernels will have to be considered.

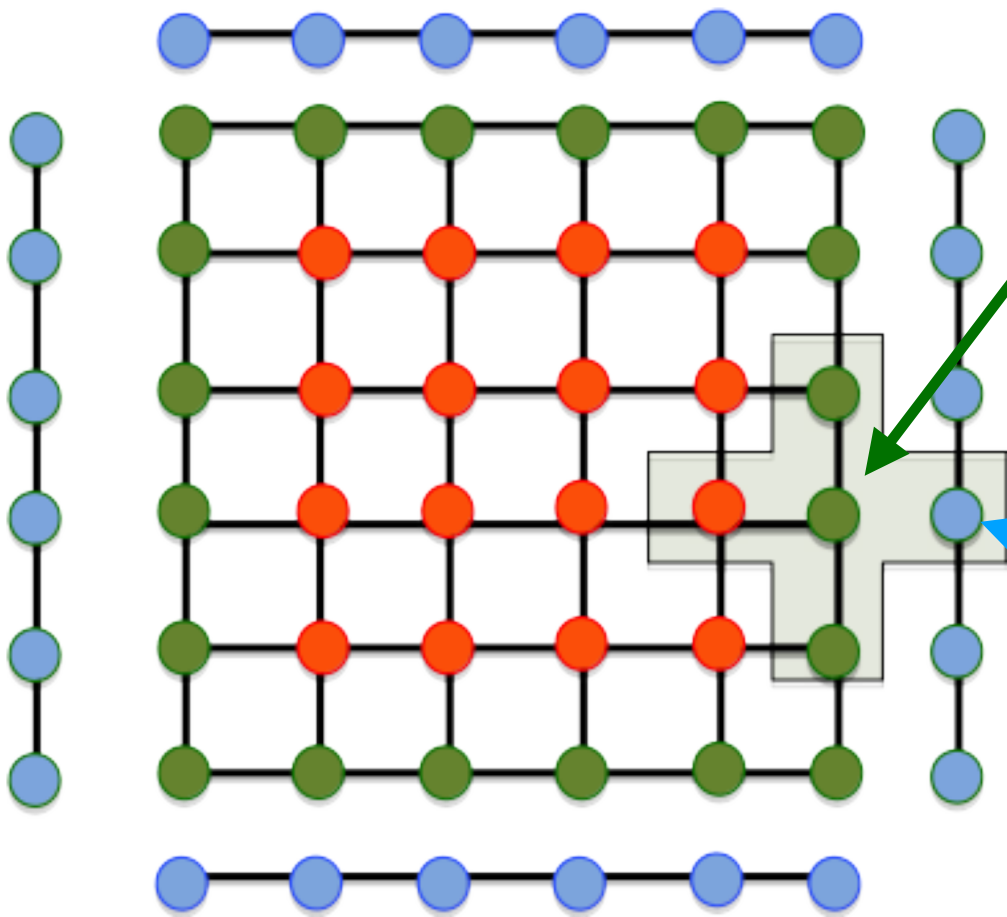
Boundary-free stencil
(interior stencil)



Interior Stencils have all points on interior grid

$$
\begin{aligned}
&for\ j = 1 : n \\
&\qquad for\ \ i = 1 : n \\
&\qquad\quad f_{i,j}^{k} = [-(4+\alpha)s_{i,j} + s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1} + \beta s_{i,j}(1-s_{i,j})]^{k} + \alpha s_{i,j}^{k-1} \\
&\qquad end \\
&end
\end{aligned}
$$

Boundary stencil



Boundary stencils include 1 or 2 grid points on the boundary

Store boundary information in separate arrays bndS, bndW, bndN, bndE

$$
\begin{aligned}
&\mathit{for}\ j = 1:n \\
&\quad \mathit{for}\ i = n+1 \\
&\qquad f^k_{i,j} = [-(4+\alpha)s_{i,j} + s_{i-1,j} + \mathbf{bndE}_i + s_{i,j-1} + s_{i,j+1} + \beta s_{i,j}(1-s_{i,j})]^k + \alpha s^{k-1}_{i,j} \\
&\quad \mathit{end} \\
&\mathit{end}
\end{aligned}
$$

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Testing the code

- **Get the code from Moodle or Github**
- **Compile and run**

```
[user@eu-login]$ make
[user@eu-login]$ export OMP_NUM_THREADS=1
[user@eu-login]$ bsub -n 1 -W 00:10 -R "span[ptile=1]"
./main 128 100 0.005
```

Output

```
=========================================================================
                      Welcome to mini-stencil!
version :: C++ serial
mesh    :: 128 * 128 dx = 0.00787402
time    :: 100 time steps from 0 .. 0.005
=========================================================================
step 1 required 4 iterations for residual 7.21951e-07
step 2 required 4 iterations for residual 7.9975e-07
...
step 99 required 12 iterations for residual 9.36586e-07
step 100 required 12 iterations for residual 9.44772e-07
--------------------------------------------------------------------------------
simulation took 1.58408 seconds
2853 conjugate gradient iterations, at rate 6341.35 iters/second
492 newton iterations
--------------------------------------------------------------------------------
Goodbye!
```

Thank you for your attention and have fun with the Project!