Introduction to the mini-app code (Mini-Project 4)

Olaf Schenk

USI Lugano

Università della Svizzera italiana

Institute of Computational Science ICS

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The Application

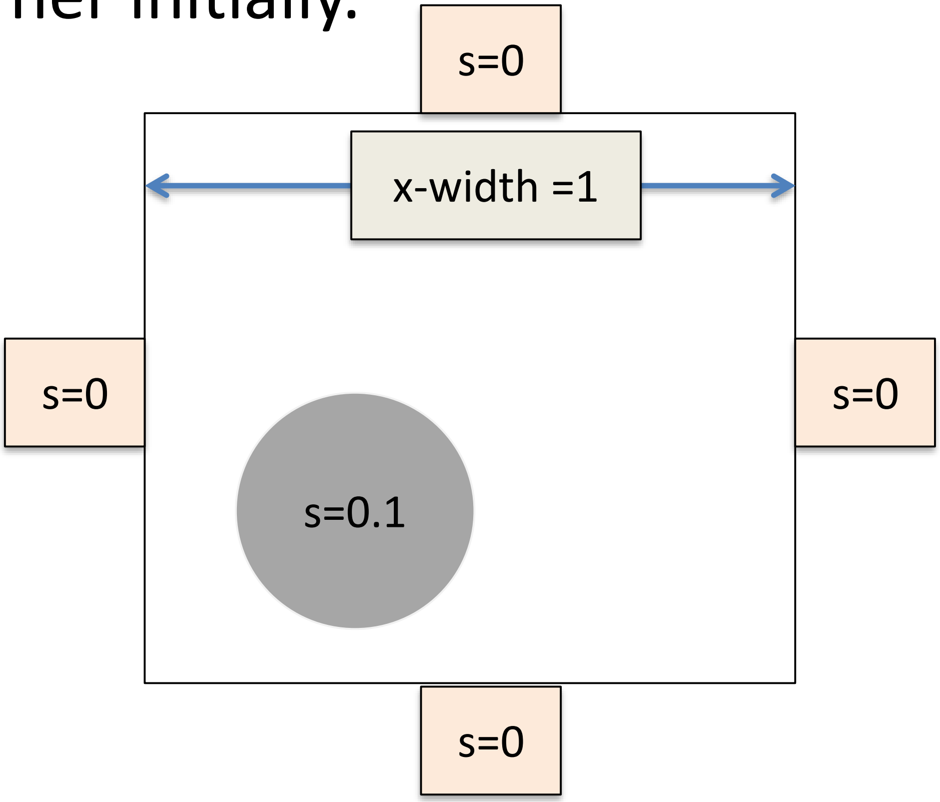
- The code solves a reaction diffusion equation known as Fischer's Equation

$$\frac{\partial s}{\partial t} = D \overbrace{\left(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2} \right)}^{\text{diffusion}} + \overbrace{Rs(1-s)}^{\text{reaction/growth}}$$

- Used to simulate travelling waves and simple population dynamics
  - The species s diffuses
  - And the population grows to a maximum of s=1

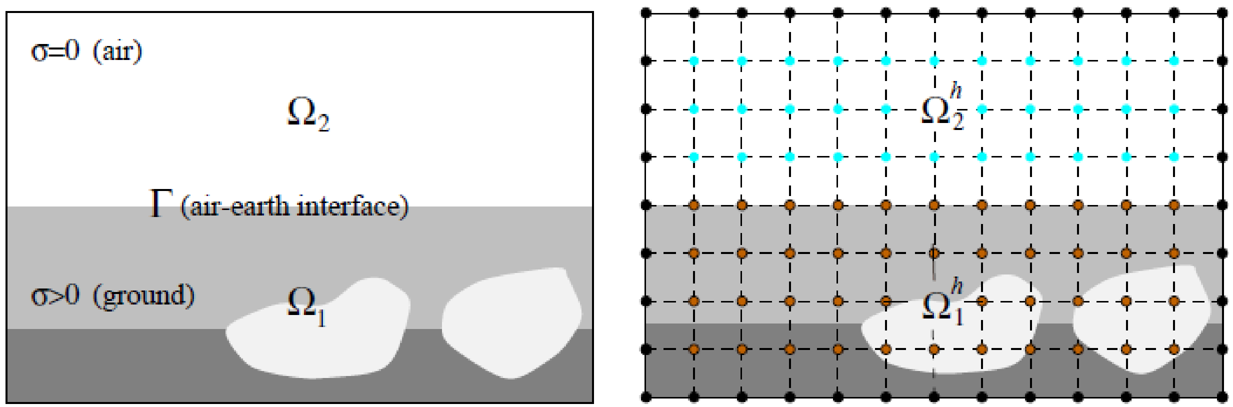
Initial and boundary conditions

- The domain is rectangular, with fixed value of s=0 on each boundary, and a circular region of s=0.1 in the lower left corner initially.



The need to discretize

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



(a) An earthly domain

(b) With a discretization grid

$$\frac{\partial s(x_i,y_i)}{\partial t} \approx \frac{s_{i,j}^{t+1} - s_{i,j}^{t}}{\Delta t} = \frac{s_{i,j} - s_{i,j}^{t}}{\Delta t} \qquad s(x_i, y_i) := s^{t+1}(x_i, y_i) = s_{i,j}^{t+1}$$

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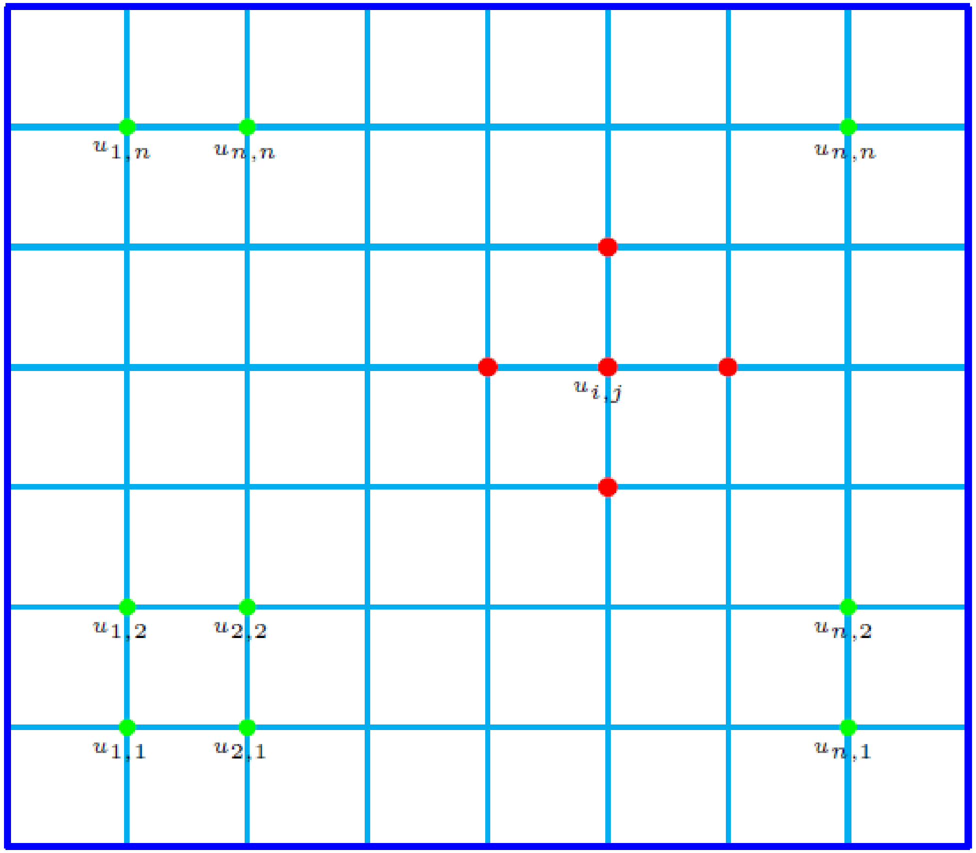

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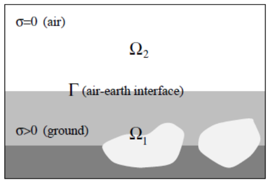

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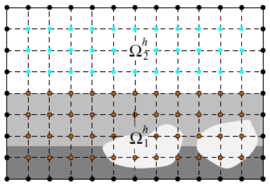
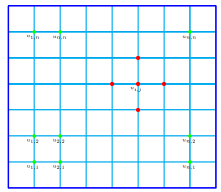


(b) With a discretization grid



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

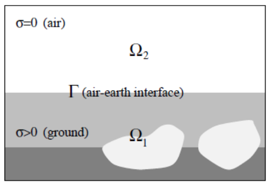
$$\frac{\partial s(x_i,y_i)}{\partial t} \approx \frac{s_{i,j}^{t+1} - s_{i,j}^{t}}{\Delta t} = \frac{s_{i,j} - s_{i,j}^{t}}{\Delta t} \qquad s(x_i,y_i) := s^{t+1}(x_i,y_i) = s_{i,j}^{t+1}$$

$$\frac{s_{ij} - s_{ij}^{t}}{\Delta t} = D\left(\frac{\partial^2 s(x,y)}{\partial^2 x} + \frac{\partial^2 s(x,y)}{\partial^2 y}\right) + Rs(x,y)[1 - s(x,y)]$$

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

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

The need to discretize



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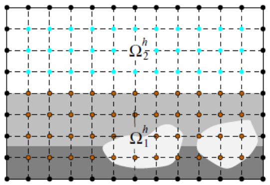
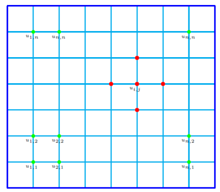

(b) With a discretization grid

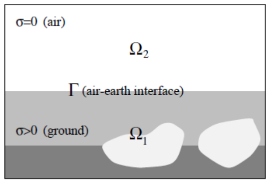


$$\frac{s_{ij}-s_{ij}^t}{\Delta t} = D\left(\frac{\partial^2 s(x,y)}{\partial^2 x} + \frac{\partial^2 s(x,y)}{\partial^2 y}\right) + Rs(x,y)[1 - s(x,y)]$$

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

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

The need to discretize



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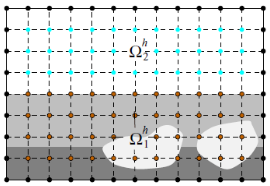

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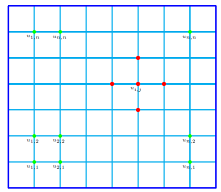

$$\frac{s_{ij}-s_{ij}^t}{\Delta t} = D\frac{1}{\Delta^2}(-4s_{i,j}+s_{i+1,j}+s_{i-1,j}+s_{i,j+1}+s_{i,j-1})+Rs_{i,j}[1-s_{i,j}]$$

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

$$-4s_{i,j}+s_{i+1,j}+s_{i-1,j}+s_{i,j+1}+s_{i,j-1}+\frac{R\Delta^2}{D}s_{i,j}-\frac{R\Delta^2}{D}s_{i,j}^2+\frac{\Delta^2}{D\Delta t}s_{ij}=-\frac{\Delta^2}{D\Delta t}s_{ij}^t$$

$$(-4+\alpha+\beta)s_{i,j}+s_{i+1,j}+s_{i-1,j}+s_{i,j+1}+s_{i,j-1}-\beta s_{i,j}^2=-\frac{\Delta^2}{D\Delta t}s_{ij}^t$$

Nonlinear!

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Solving nonlinear equations

$$
\begin{aligned}
s_1(x_1, x_2, \ldots, x_n) &= 0, \\
s_2(x_1, x_2, \ldots, x_n) &= 0, \\
\vdots &= \vdots \\
s_n(x_1, x_2, \ldots, x_n) &= 0.
\end{aligned}
$$

Or, using vector notation, $\mathbf{s}(\mathbf{x}) = 0$.

Solving nonlinear equations

- Equipped with knowledge on how to **solve nonlinear equations** and **linear systems**, it is time to close the circle and consider systems of nonlinear equation

$$\begin{aligned} s_1(x_1, x_2, \ldots, x_n) &= 0, \\ s_2(x_1, x_2, \ldots, x_n) &= 0, \\ \vdots &= \vdots \\ s_n(x_1, x_2, \ldots, x_n) &= 0. \end{aligned}$$

Or, using vector notation, $\mathbf{s}(\mathbf{x}) = \mathbf{0}$.

Solving nonlinear equations

Suppose we have one function, f:

- one variable: $s(x+p) = s(x) + s'(x)p + \frac{1}{2}s''(x)p^2 + \dots$
- n variables: $s(x+p) = s(x) + g(x)^T p + \frac{1}{2}p^T H(x)p + \dots$

Example: given the function

$$s = x_1^4 - 2x_1^3x_2^2 + 4x_1x_2^3,$$

Gradient:

$$g(x) = \nabla s = \begin{pmatrix} 4x_1^3 - 6x_1^2x_2^2 + 4x_2^3 \\ -4x_1^3x_2 + 12x_1x_2^2 \end{pmatrix};$$

Hessian:

$$H = \nabla^2 s = \begin{pmatrix} 12x_1^2 - 12x_1x_2^2 & -12x_1^2x_2 + 12x_2^2 \\ -12x_1^2x_2 + 12x_2^2 & -4x_1^3 + 24x_1x_2 \end{pmatrix}.$$

We obtain the Taylor expansion using the above formula, for a given $p = \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$.

m functions, n variables

Let $x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$, function $s = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{pmatrix}$, direction $p = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}$.

Assume that s is sufficiently smooth (at least two bounded derivatives). Then the Taylor expansion is

$$s(x+p) = s(x) + J(x)p + \mathcal{O}(\|p\|^2),$$

where $J(x)$ is the **Jacobian** matrix of first derivatives of s at x, given by

$$J(x) = \begin{pmatrix} \frac{\partial s_1}{\partial x_1} & \frac{\partial s_1}{\partial x_2} & \cdots & \frac{\partial s_1}{\partial x_n} \\ \frac{\partial s_2}{\partial x_1} & \frac{\partial s_2}{\partial x_2} & \cdots & \frac{\partial s_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial s_m}{\partial x_1} & \frac{\partial s_m}{\partial x_2} & \cdots & \frac{\partial s_m}{\partial x_n} \end{pmatrix}.$$

Newton's method

By Taylor series,

$$s(\mathbf{x}) = s(\mathbf{x}_k) + J(\mathbf{x}_k)(\mathbf{x} - \mathbf{x}_k) + \mathcal{O}\|(\mathbf{x} - \mathbf{x}_k)\|^2.$$

For $\mathbf{x} = \mathbf{x}^*$, also $s(\mathbf{x}) = 0$.
Neglect nonlinear term and define method by

$$0 = s(\mathbf{x}_k) + J(\mathbf{x}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k).$$

Given an initial guess x_0:

for $k = 0, 1, \ldots,$ until convergence

solve $J(\mathbf{x}_k)p = -s(\mathbf{x}_k)$,
set $\mathbf{x}_{k+1} = \mathbf{x}_k + p$.

end

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Newton's method

By Taylor series,

$$s(\mathbf{x}) = s(\mathbf{x}_k) + J(\mathbf{x}_k)(\mathbf{x} - \mathbf{x}_k) +$$

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end

```
// main timeloop
for (int timestep = 1; timestep <= nt; timestep++) {
  // set x_new and x_old to be the solution
  ss_copy(x_old, x_new, N);
  for (it=0; it<50; it++) {
    // compute residual : requires both x_new and x_old
    diffusion(x_new, b);
    residual = ss_norm2(b, N);
    // check for convergence
    if (residual < tolerance) { converged = true; break; }
   // solve linear system to get –deltax
   ss_cg(deltax, b, 200, tolerance, cg_converged);
   // check that the CG solver converged
   if (!cg_converged) break;
   // update solution
   ss_axpy(x_new, -1.0, deltax, N);
 }
 iters_newton += it+1;
}
```

Newton's method

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solve $J(\mathbf{x}_k)p = -s(\mathbf{x}_k)$,

set $\mathbf{x}_{k+1} = \mathbf{x}_k + p$.

end

```
// the interior grid points
#pragma omp parallel for
  for (int j=1; j < jend; j++) {
    for (int i=1; i < iend; i++) {
      S(i,j) = -(4. + alpha) * U(i,j)// central point
               + U(i-1,j) + U(i+1,j)  // east and west
               + U(i,j-1) + U(i,j+1)  // north and south
               + alpha * x_old(i,j)
               + dxs * U(i,j) * (1.0 - U(i,j));
  }
}
```

The CG method

Algorithm: Conjugate Gradient.
Given an initial guess $\mathbf{x}_0$ and a tolerance `tol`, set at first $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$, $\delta_0 = \langle \mathbf{r}_0, \mathbf{r}_0 \rangle$, $b_\delta = \langle \mathbf{b}, \mathbf{b} \rangle$, $k = 0$ and $\mathbf{p}_0 = \mathbf{r}_0$. Then:

while $\delta_k > \mathtt{tol}^2\, b_\delta$

$$\mathbf{s}_k = A\mathbf{p}_k$$

$$\alpha_k = \frac{\delta_k}{\langle \mathbf{p}_k, \mathbf{s}_k \rangle}$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k$$

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{s}_k$$

$$\delta_{k+1} = \langle \mathbf{r}_{k+1}, \mathbf{r}_{k+1} \rangle$$

$$\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \frac{\delta_{k+1}}{\delta_k}\mathbf{p}_k$$

$$k = k + 1$$

end

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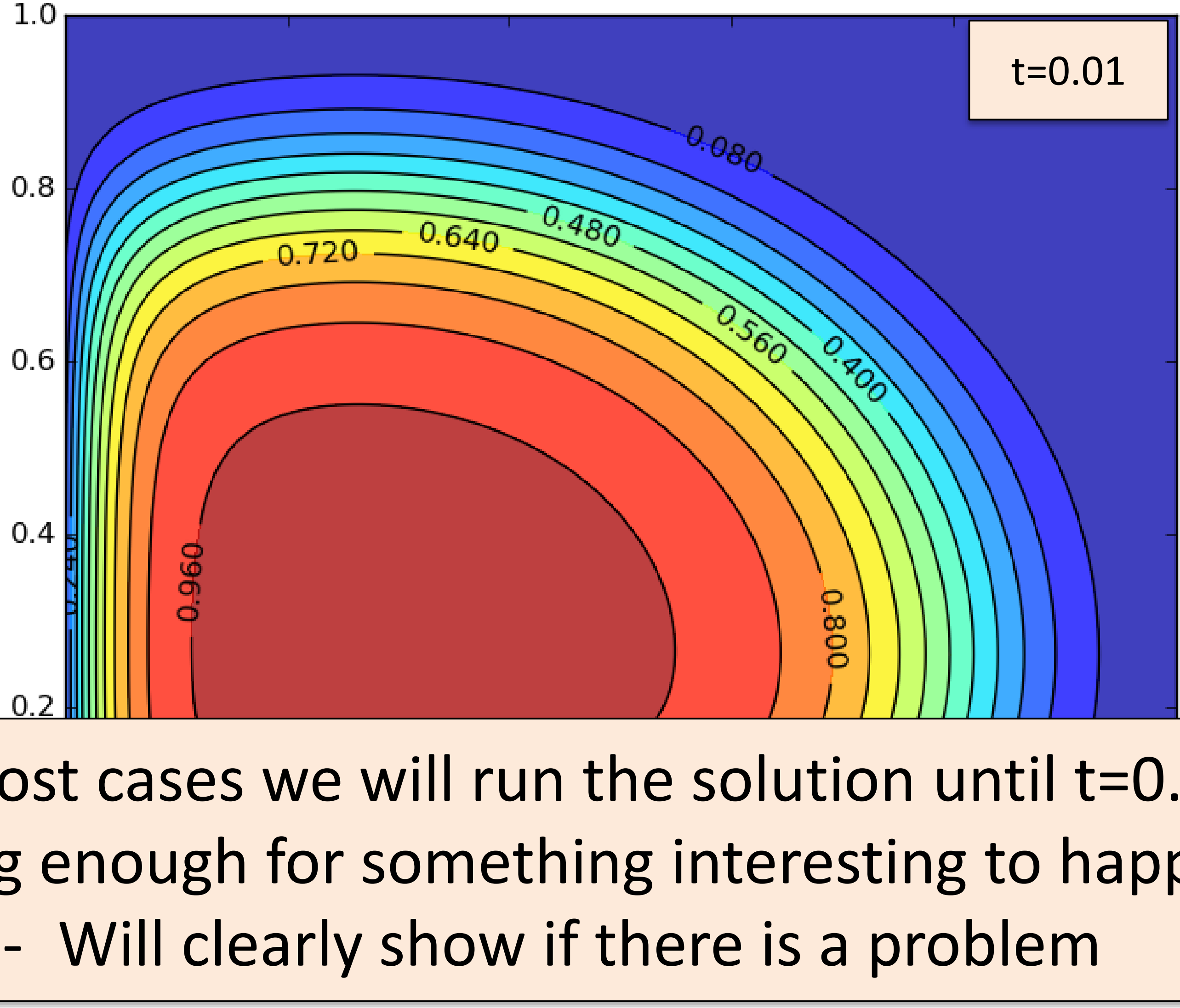
                    + alpha * x_old(i,j)
                    + dxs * U(i,j) * (1.0 - U(i,j));
   }
}
```

Time Evolution of Solution



For most cases we will run the solution until t=0.01.
- Long enough for something interesting to happen
  - Will clearly show if there is a problem

Numerical Solution

- The rectangular domain is discretized with a grid of dimension nx*ny points
- A finite volume discretization and method of lines gives the follow ordinary differential equation for each grid point

$$\frac{\mathrm{d}s_{ij}}{\mathrm{d}t} = \frac{D}{\Delta x^2}\left[-4s_{ij} + s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}\right] + Rs_{ij}\left(1 - s_{ij}\right)$$

- Which we can express as the following nonlinear problem...

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

Numerical Solution

- One nonlinear equation for each grid point
  - together they form a system of N=nx*ny equations
  - Solve with Newton's method
- Each iteration of Newton's method has to solve a linear system
  - Solve with matrix-free Conjugate Gradient solver
- Solve the nonlinear system at each time step
  - This requires in the order of between 5-10 conjugate gradient iterations

- Don’t worry if you don't understand it all!
- We don’t need a deep understanding of the mathematics or domain problem to optimize the code
  - I often work on codes with little domain knowledge
- The mini-app has a handful of kernels that can be parallelized
  - And care was taken when designing it to make parallelization as easy as possible
- So let’s look a little closer at each part of the code

Code Walkthrough

- There are three modules of interest
  - main.f90/main.cpp : initialization and main time stepping loop
  - linalg.f90/linalg.cpp : the BLAS level 1 (vector-vector) kernels and conjugate gradient solver
  - operators.f90/operators.cpp : the stencil operator for the finite volume discretization

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

Linear algebra: linalg.f90/cpp

- This file defines simple kernels for operating on 1D vectors, including
  - dot product : **x•y** : ss_dot
  - linear combination : **z**=*alpha****x** + *beta****y** : ss_lcomb
- The kernels of interest start with ss_xxxxx
  - ss == summer school
- For each parallelization approach that we will see (OpenMP, MPI, CUDA, ... etc), each of these kernels will have to be considered.

Stencil operator: operator.f90/cpp

- This file has a function/subroutine that defines the stencil operator

interior points

for j=2:ydim-1

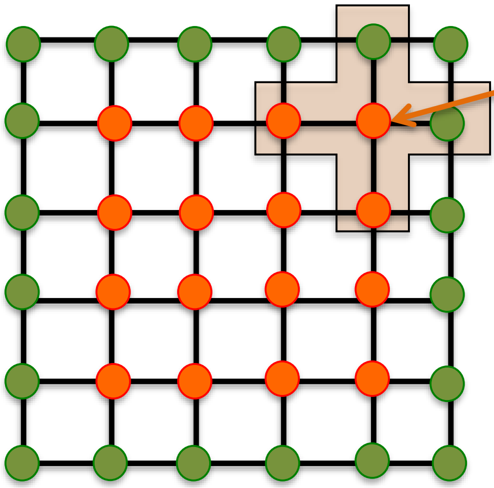
for i=2:xdim-1

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

end

end

Stencil: Interior Grid Points



interior points have all neighbours available

interior points

for j=2:ydim-1

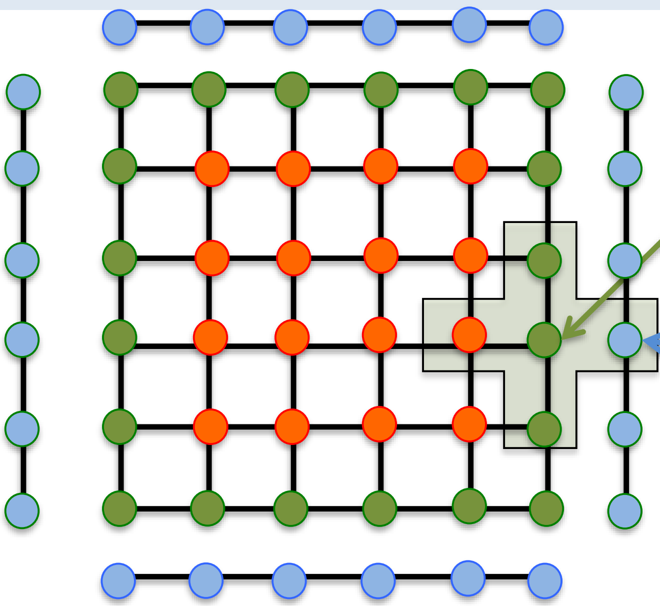
for i=2:xdim-1

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

end

end

Stencil: Boundary Grid Points



boundary points are missing 1 or 2 nieghbours

create 4 halo buffers, that hold "ghost" buffers
bndN, bndE, bndS, bndW

east boundary

i=xdim

for j=2:ydim-1

$$f_{ij} = \left[-\left(4+\alpha\right) s_{ij} + s_{i-1,j} + \boxed{\text{bndE}_i} + s_{i,j-1} + s_{i,j+1} + \beta s_{ij}\left(1 - s_{ij}\right)\right]^{k+1} + \alpha s_{ij}^{k} = 0$$

end

Testing the code

- Get the code, by checking it out from github

```
> git clone https://github.com/rjanalik/HPC_2019.git
> cd HPC_2019/Mini-project4/miniapp_openmp
```

I choose the C++ version here

- Compile and run

```
> make
> srun –n1 ./main 128 128 100 0.01
```

Testing continued...

- Compile

```
> make
```

- Run interactively (use salloc beforehand)

```
> srun ./main 128 128 100 0.01
```

- the grid is 128 x 128 grid points
- take 100 time steps
- run simulation for t=0.01

- Or run batch job

```
> sbatch job.daint
... when job is finished ...
> cat job.out
```

It is possible to choose parameters that will make the simulation fail to converge! The code should tell you gracefully that it was unable to converge.

increasing the spatial resolution may require increasing the number of time steps