CSCS
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Introduction to GPUs in HPC

CSCS Summer School 2024

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Intro to the Diffusion MiniApp

Overview

In this session we will cover:

1. What is a miniapp?
2. The summer school miniapp overview.
3. First look at the code.
4. Compile, run and visualize the miniapp.

What is a HPC miniapp?

- Full HPC applications are complicated.
  - Difficult to model/understand performance behavior.
- A miniapp is a smaller code that aim to characterize performance of larger applications.
  - simpler to understand and benchmark than full applications
  - can be used to test different hardware, languages and libraries
  - good for learning new techniques!

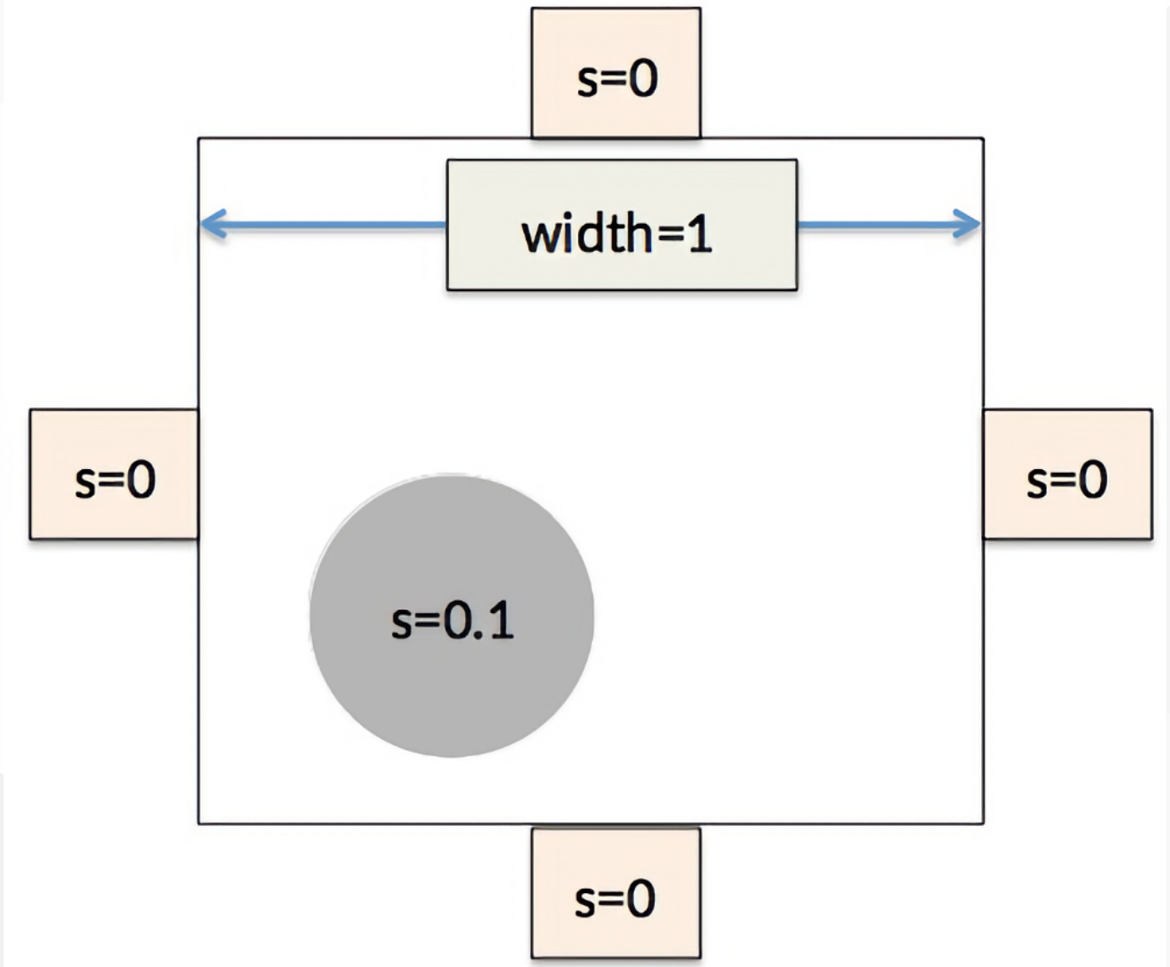
The Application

- The code solves **Fisher's equation**, a **reaction diffusion** model:

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

- Used to simulate travelling waves and simple population dynamics.
  - The species s diffuses
  - The species reproduces to a maximum of $s = 1$

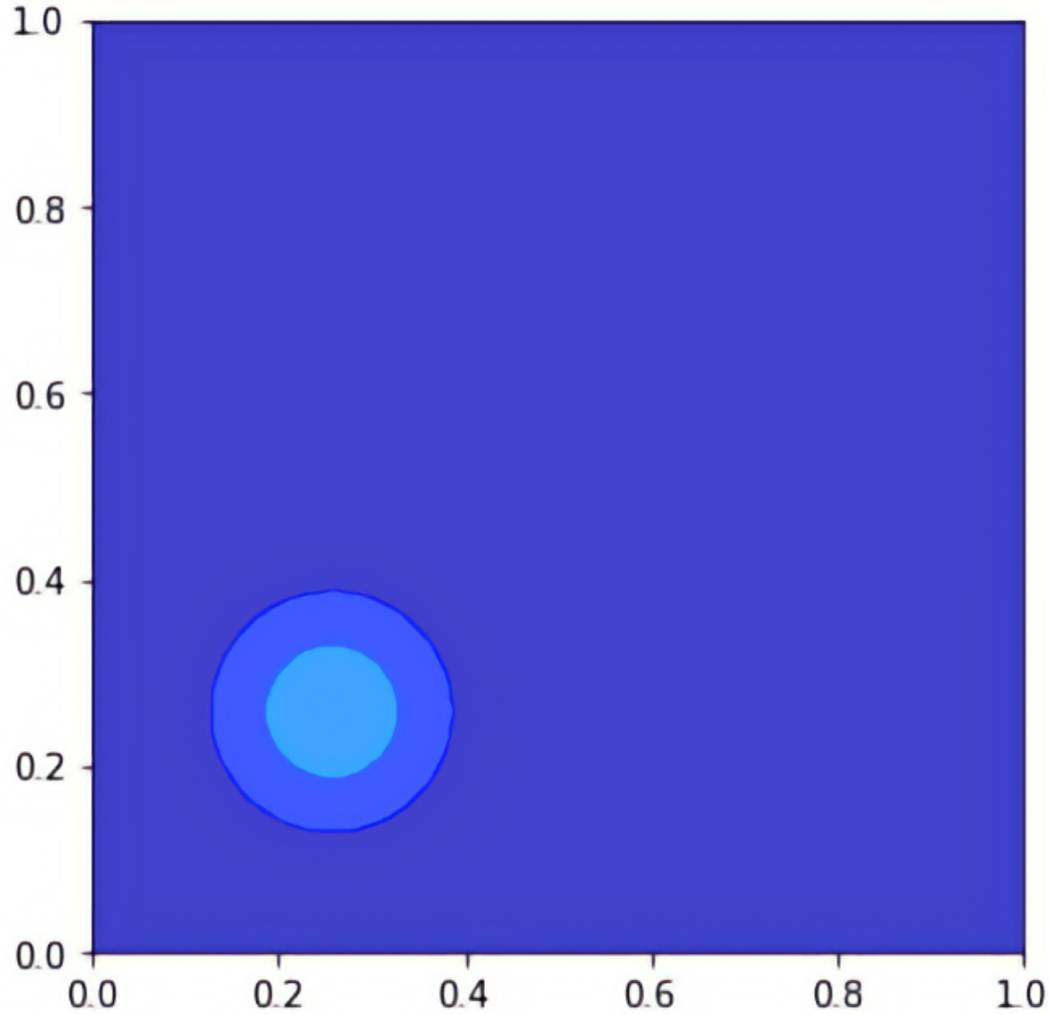
Initial and Boundary Conditions



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.

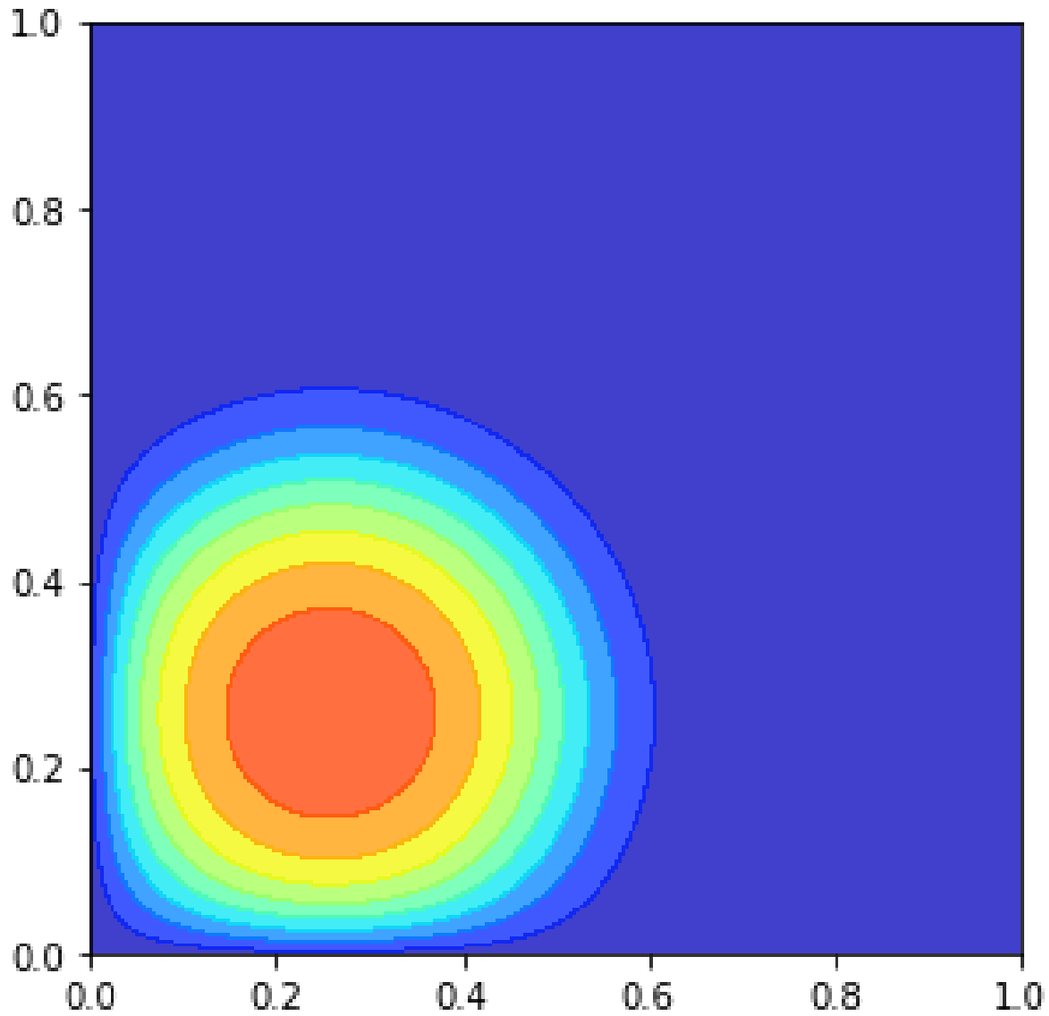
Time Evolution of the Solution

$$t = 0.001$$



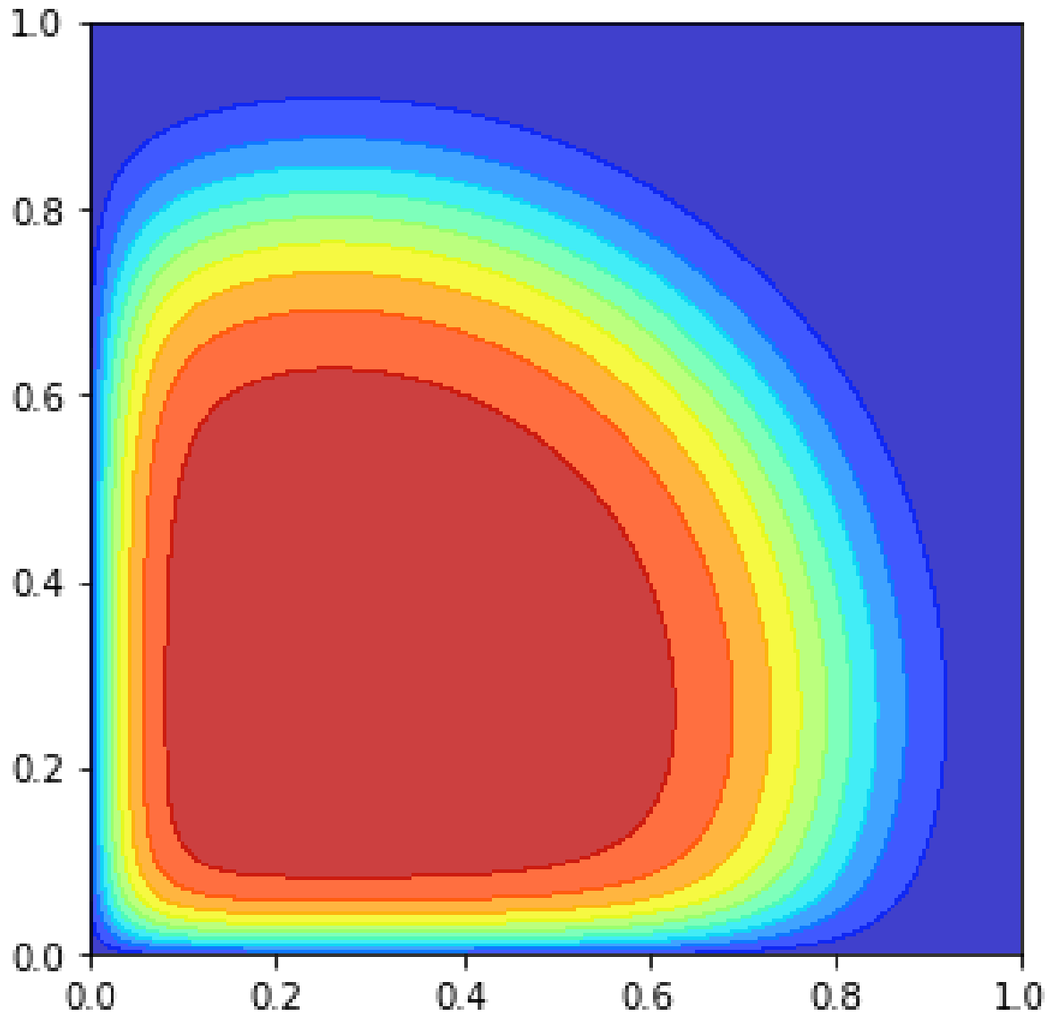
Time Evolution of the Solution

$$t = 0.005$$



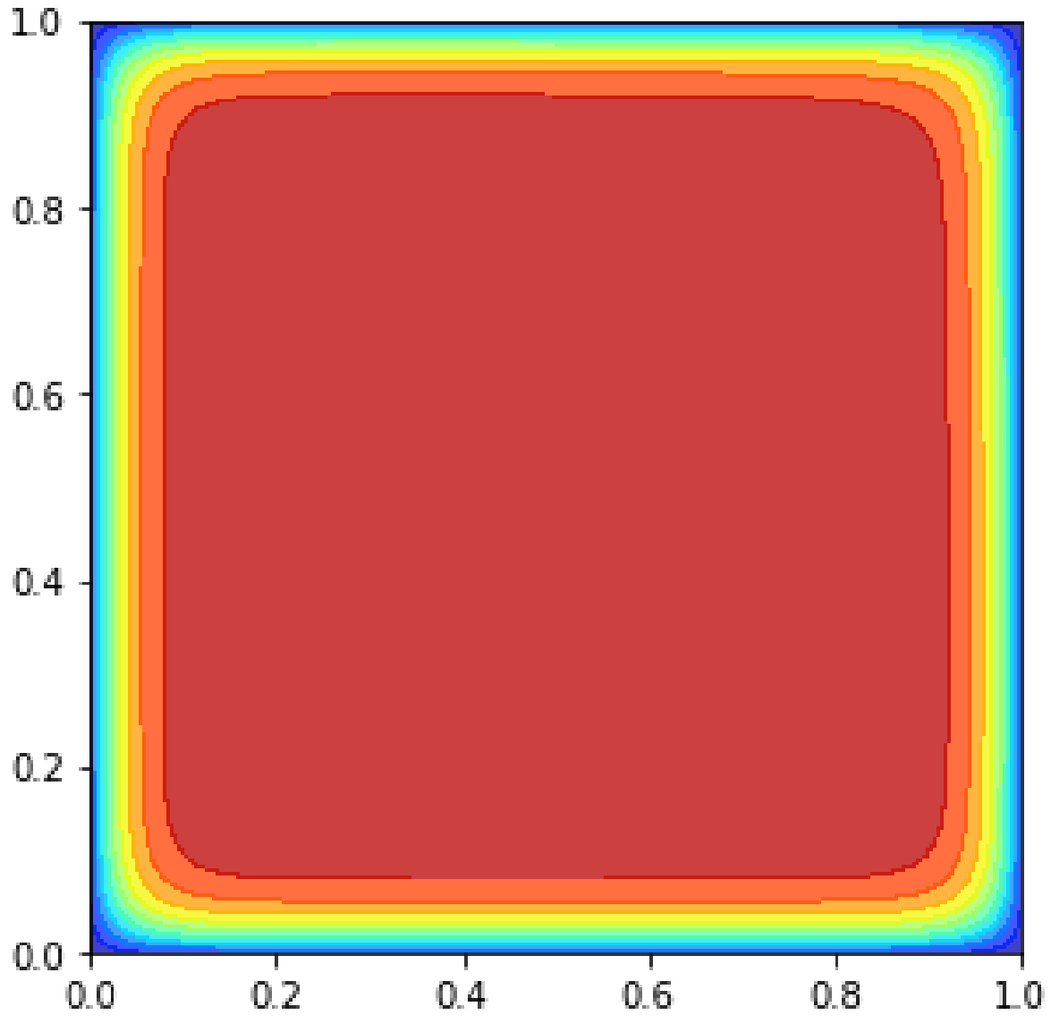
Time Evolution of the Solution

$$t = 0.01$$



Time Evolution of the Solution

$$t = 0.02$$



Numerical Solution

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

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

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

Numerical Solution

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

- Don’t worry if you don’t understand everything.
- 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 miniapp 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. . .

The Code

- The application is written in **C++**
- It could be faster. . .
  - We avoid aggressive optimization to make the code easier to understand
  - It is not a fine example of design

Code Walkthrough

There are three main files of interest:

1. `main.cpp` : Initialization and time stepping code
2. `linalg.cu` : BLAS level-1 vector-vector operations and conjugrate gradient solver
3. `operators.cu` : The stencil kernel

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

Linear Algebra: `linalg.cu`

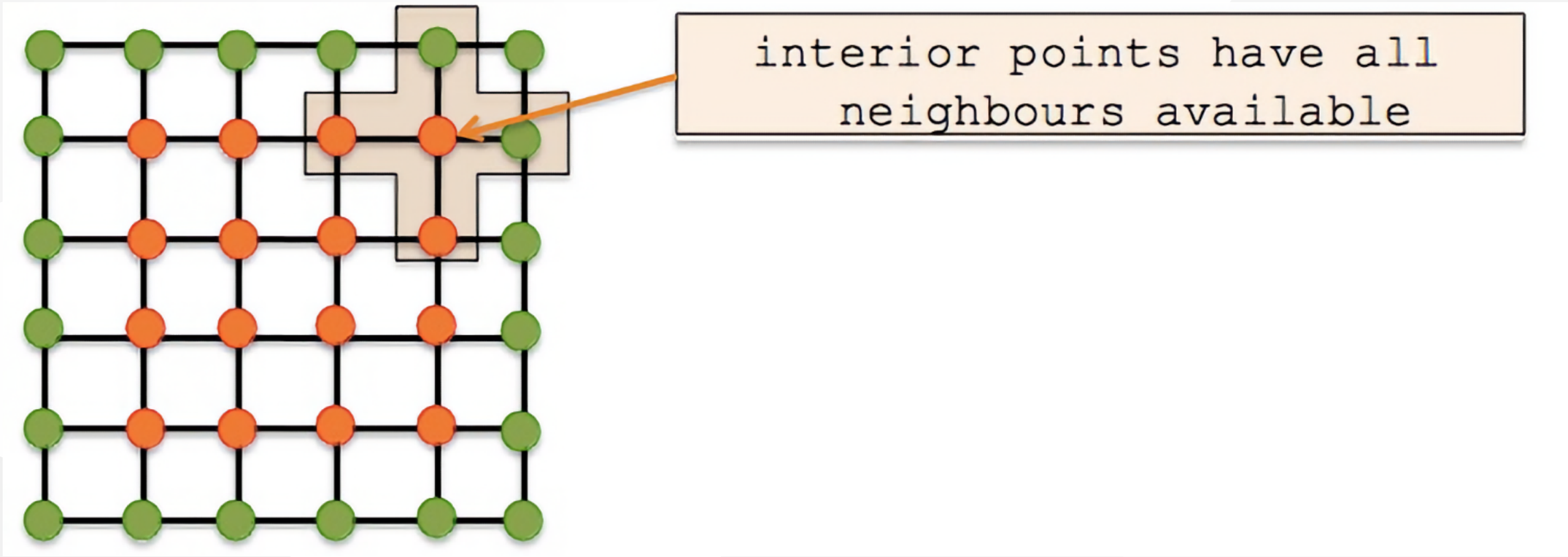
- This file defines simple kernels for operatiing on vectors, e.g.:
  - dot product $x^T y$ or $x \cdot y$: `ss_dot`
  - linear combination $z = \alpha x + \beta y$: `ss_lcomb`
- The kernels of interest are named `ss_xxxx`
- Each will have to be parallelized using CUDA
- The `ss_cg` function implements conjugate gradient using the vector and stencil operations

Stencil Operator: `operators.cu`

This file has the function that applies the stencil operator:

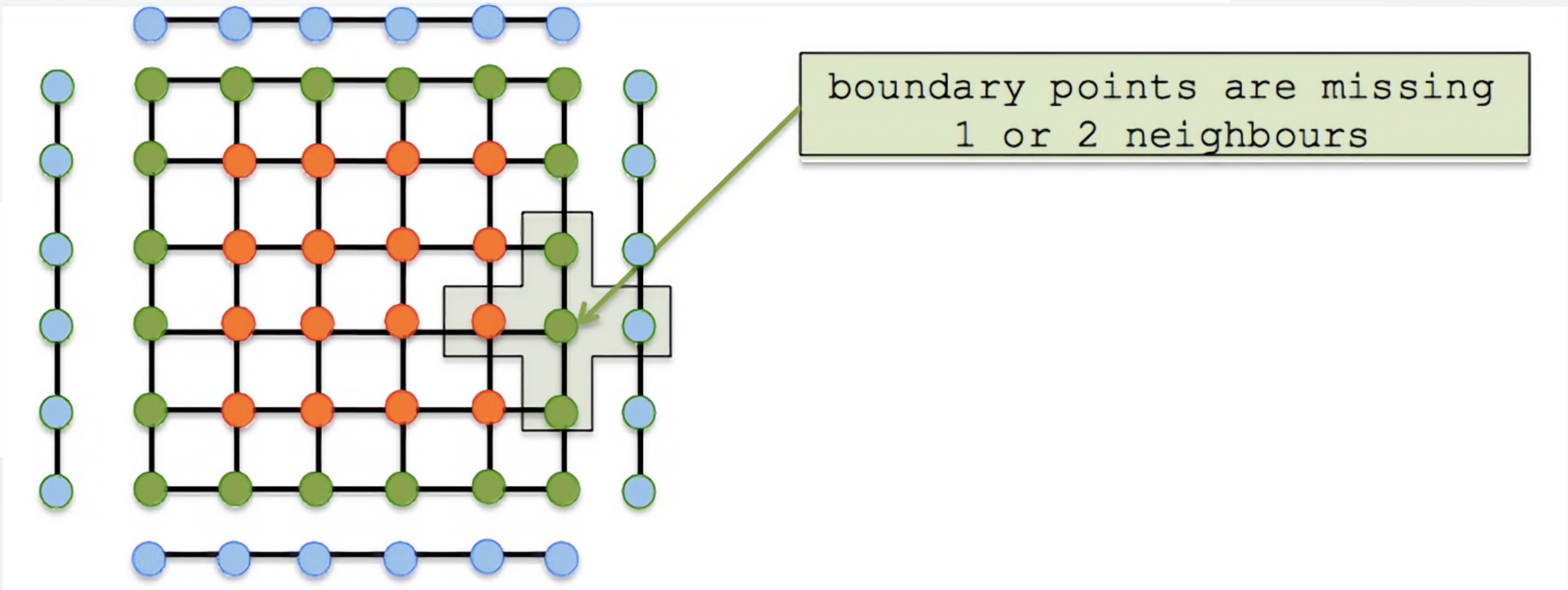
```
for i=2:nx-1
    for j=2:ny-1
        S(i,j) = -(4. + alpha) * U(i,j)
                                + U(i-1,j) + U(i+1,j)
                                + U(i,j-1) + U(i,j+1)
                                + alpha * x_old(i,j)
                                + dxs * U(i,j) * (1.0 - U(i,j));
    end
end
```

Stencil Operator: Interior Grid Points




```
S(i,j) = -(4+alpha)*U(i,j)
           + U(i-1,j) + U(i+1,j) + U(i,j-1) + U(i,j+1) + ...
```

Stencil Operator: Boundary Grid Points



Points on the boundary need to use one or two external boundary points.

```
S(i,j) = -(4+alpha)*U(i,j)
           + U(i-1,j) + bndE[j] + U(i,j-1) + U(i,j+1) + ...
```

Testing the Code

Get the code and compile miniapp

```
> git clone https://github.com/eth-cscs/SummerUniversity2024.git
> cd SummerUniversity2024/cuda/miniapp
> module load daint-gpu cudatoolkit
> module swap PrgEnv-cray PrgEnv-gnu
> make
```

Testing the Code

Run the miniapp

```
> srun -A class05 -Cgpu --reservation=su2024 ./main 128 128 100 0.01
==================================================
Welcome to mini-stencil!
version   :: C++ serial
mesh      :: 128 * 128 dx = 0.00787402
time      :: 128 time steps from 0 .. 0.01
iteration :: CG 200, Newton 50, tolerance 1e-06
==================================================
--------------------------------------------------
simulation took 1.07502 seconds
7439 conjugate gradient iterations, at rate of 6919.88 iters/second
959 newton iterations
--------------------------------------------------
```

Exercise: Run the MiniApp

- Run with 4 different resolutions
  - `128 128 100 0.01`
  - `256 256 200 0.01`
  - `512 512 200 0.01`
  - `1024 1024 400 0.01`
- For each case record:
  1. the number of CG iterations.
  2. the number of CG iterations per second.
- We will refer to these results when testing the OpenMP and GPU versions of the code

Exercise: Visualize the Results

- The application generates two data files with the final solution: `output.bin` and `output.bov`
- There is a Python script that will show a contour plot of the solution
- Now is a good time to test if X-windows is working

```
> module load daint-gpu
> module load jupyterlab
> python3 ./plotting.py -s  # -s to get image in pop up
```

Questions?