Introduction to the mini-app code (Assignment 4)

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Overview

- What is a mini-app?
- An overview of our mini-app
- First look at the code.
- Run the code and visualize output

HPC Mini-Apps

- Full HPC applications have complicated behavior
  - difficult to model or understand performance behavior
- Mini applications (mini-apps) are smaller codes that aim to characterize larger applications
  - typically a few hundred to a few thousand lines of code
- Are simpler to test and understand than full applications
- Used to test different hardware and programming languages
- Good for learning new techniques!

Our Mini-App

- We will be using a mini-app to reinforce the lessons
  - During talks there will be small programming exercises to test out what you learn
  - Then you will get the opportunity to apply the techniques to the mini-app
- We will start with a serial version that has no parallel optimizations
  - By the end of the course we will have several different versions, one for each technique

The Application

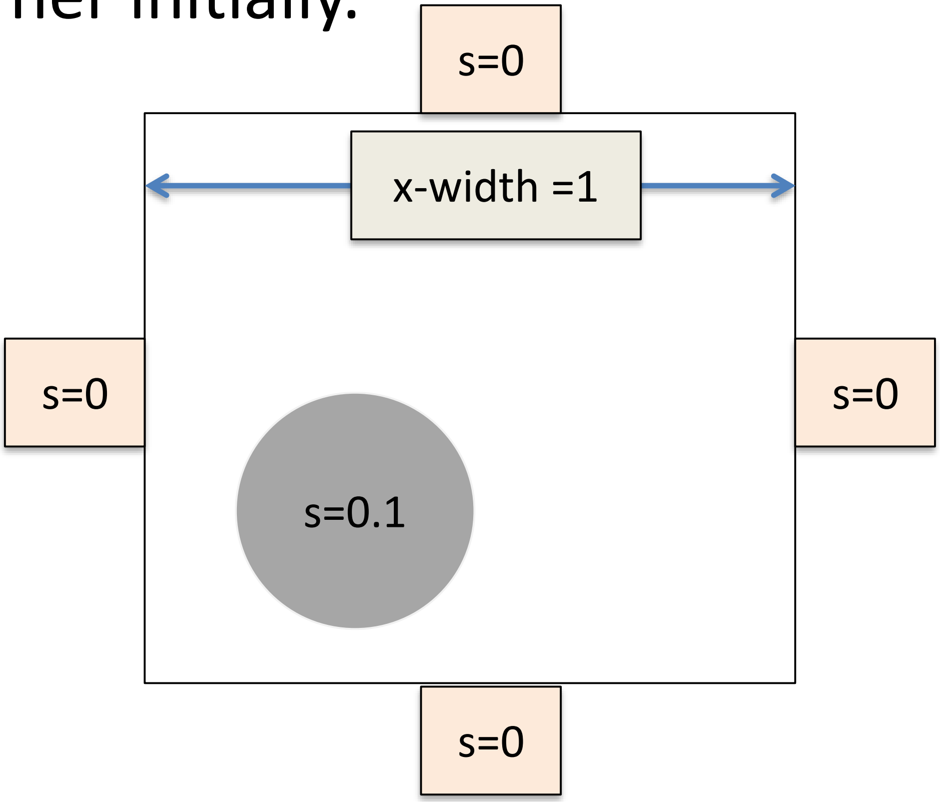
- The code solves a reaction diffusion equation known as Fischer's Equation

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

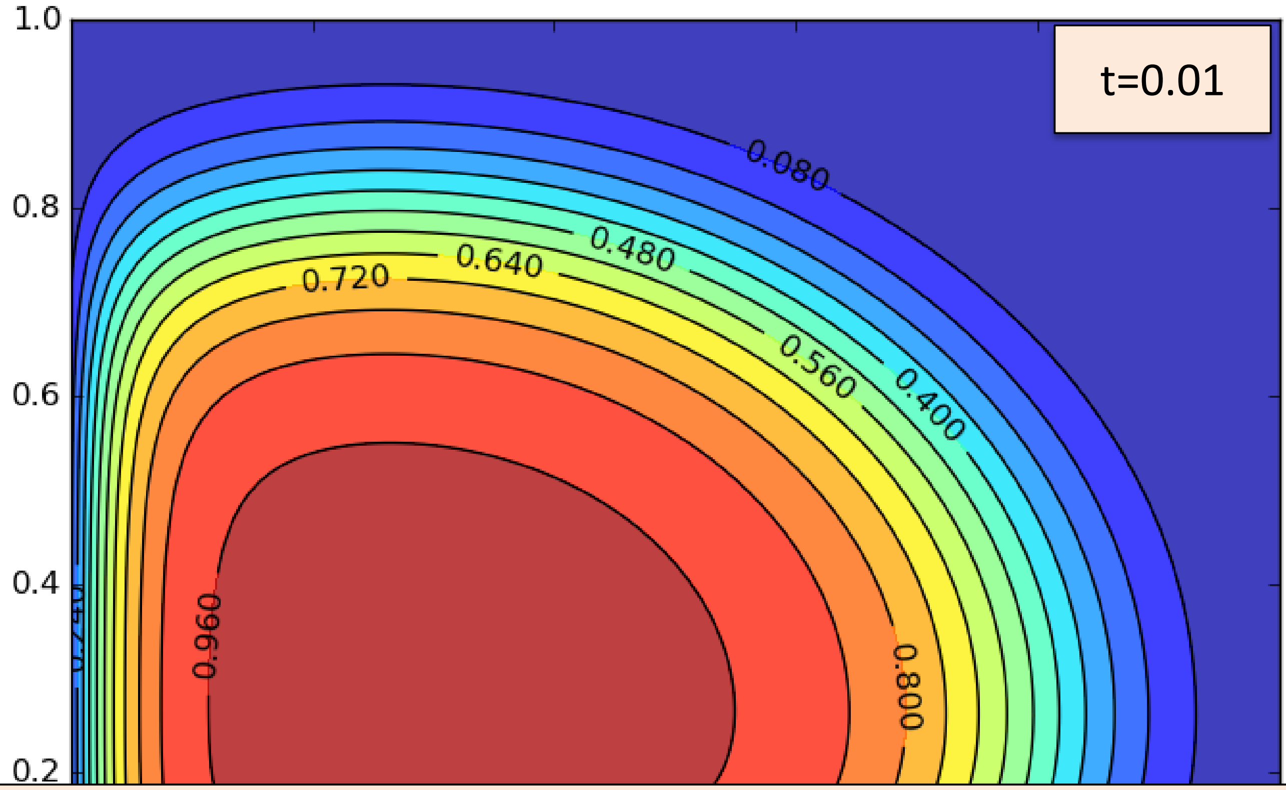
- Used to simulate travelling waves and simple population dynamics
  - The species s diffuses
  - And the population grows to a maximum of s=1

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.



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

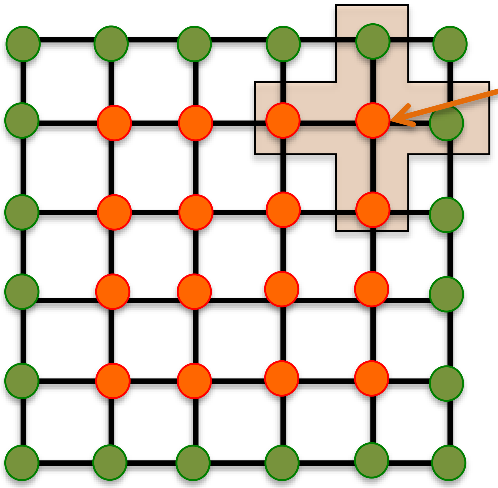
for i=2:xdim-1

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

end

end

Stencil: Interior Grid Points



interior points have all neighbours available

interior points

```
for j=2:ydim-1
 for i=2:xdim-1
```

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

```
 end
end
```

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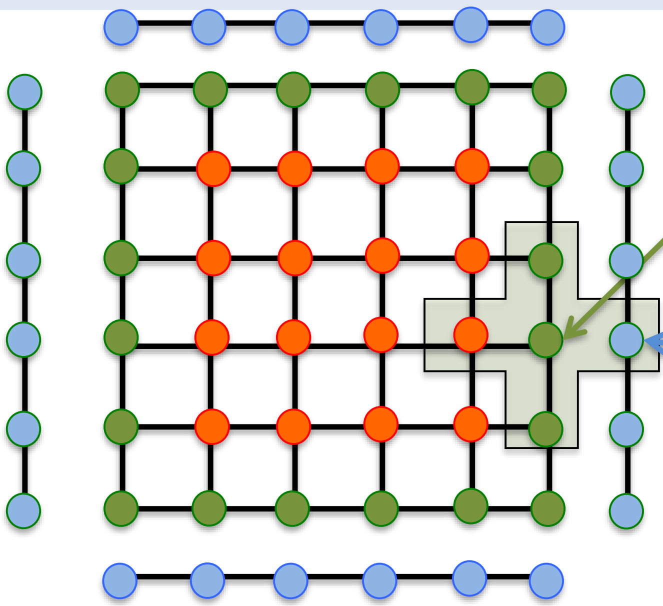
Stencil: Boundary Grid Points



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

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

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

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

- Or run batch job

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

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Exercise

- Compile using the cray programming environment.
  - get time to solution for, note time to solution and total conjugate iterations in each case
    - 128 128 100 0.01
    - 256 256 200 0.01
    - 1024 1024 ??? 0.01
- Recompile using the GNU programming environment
  - this will require make clean to remove previous build:

```
> make clean
> make
```

  - rerun tests above and compare time to solution and the number of conjugate iterations for each case

Output

The number of conjugate gradient iterations, which should always be constant for a given mesh size and time parameters. Can be used to check that changes to the code are still getting the correct result. There will be small variations due to the imprecise nature of floating point operations.

```
==========
W
version :: C++
mesh    :: 128
time    :: 100 t
================================================================
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
8127 conjugate gradient iterations, at rate of 5130.43 iters/second
920 newton iterations
-------------------------------------------------------------
Goodbye!
```

time to solution

best way to compare different implementations

Visualize the answer

- 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

```
> ls output.*
output.bin output.bov
> module load python
> python plotting.py
> display output.png
```

requires X-windowing
make sure you connect with "ssh -X"

Exercise

- Visualize the output from the previous exercise
  - now is a good time to see if X-windows is working!
- If that worked properly, try visualizing output from different final times
  - srun –n1 ./main 128 128 100 0.0025
  - srun –n1 ./main 128 128 100 0.005
  - srun –n1 ./main 128 128 100 0.01