CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

Introduction to the Summer School MiniApp

Sebastian Keller, Prashanth Kanduri and Ben Cumming, CSCS

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!

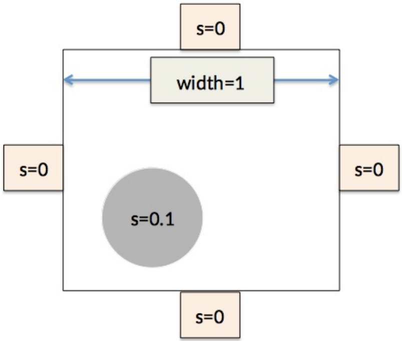
The Summer School Miniapp

- Throughout the summer school we will be using a miniapp 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 miniapp.
- We will start with a serial version that has no parallel optimizations.
- By the end of the course we will have different versions, one for each technique.

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 $s = 1$.

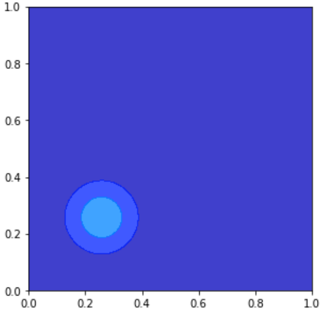
Initial and Boundary Conditions



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.

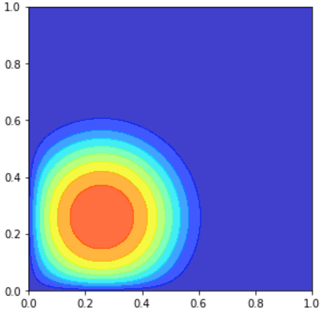
Time Evolution of the Solution

$t = 0.001$



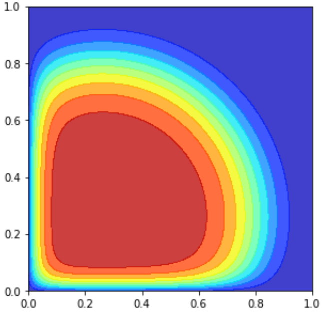
Time Evolution of the Solution

$$t = 0.005$$



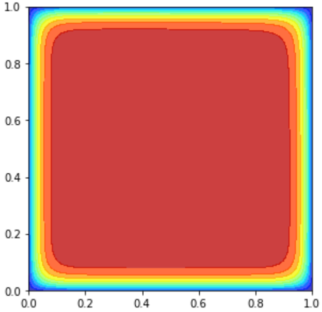
Time Evolution of the Solution

$$t = 0.01$$



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

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

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

Numeric 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.cpp`: BLAS level-1 vector-vector operations and conjugrate gradient solver.
3. `operators.cpp` The stencil kernel.

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

Linear Algebra: linalg.cpp

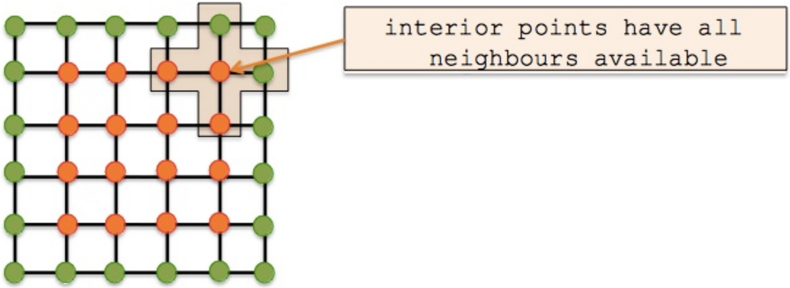
- This file defines simple kernels for operatiing on vectors, e.g.:
  - dot product $x^T y$ or $x \cdot y$: `ss_dot`.
  - linear combination $z = \alpha x + \beta y$: `ss_lcomb`.
- The kernels of interest are named `ss_xxxx`.
- Each will have to be parallelized using CUDA, MPI and OpenACC.
- The `ss_cg`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

Stencil operator: operators.cpp

This file has the function that applies the stencil operator:

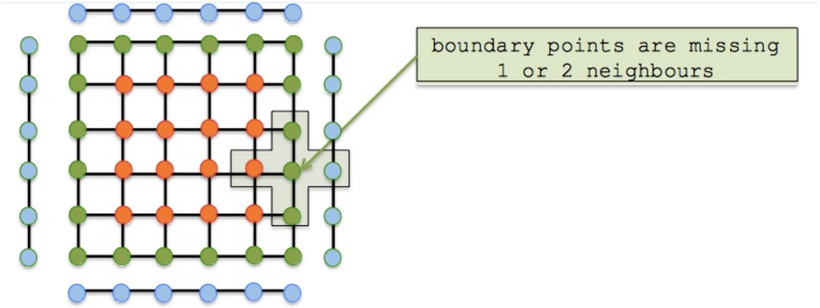
```
for i=2:nx-1
    for j=2:ny-1
        S(i,j) = -(4. + alpha) * U(i,j)
                                + U(i-1,j) + U(i+1,j)
                                + U(i,j-1) + U(i,j+1)
                                + alpha * x_old(i,j)
                                + dxs * U(i,j) * (1.0 - U(i,j));
    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/SummerUniversity2022
    .git
> cd SummerUniversity2022/miniapp/openmp
> module load daint-gpu
> module swap PrgEnv-cray PrgEnv-gnu
> make
```

Run the miniapp

```
> srun -Cgpu --reservation=course ./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 MPI 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?