MPI4PY on Compute Canada Clusters

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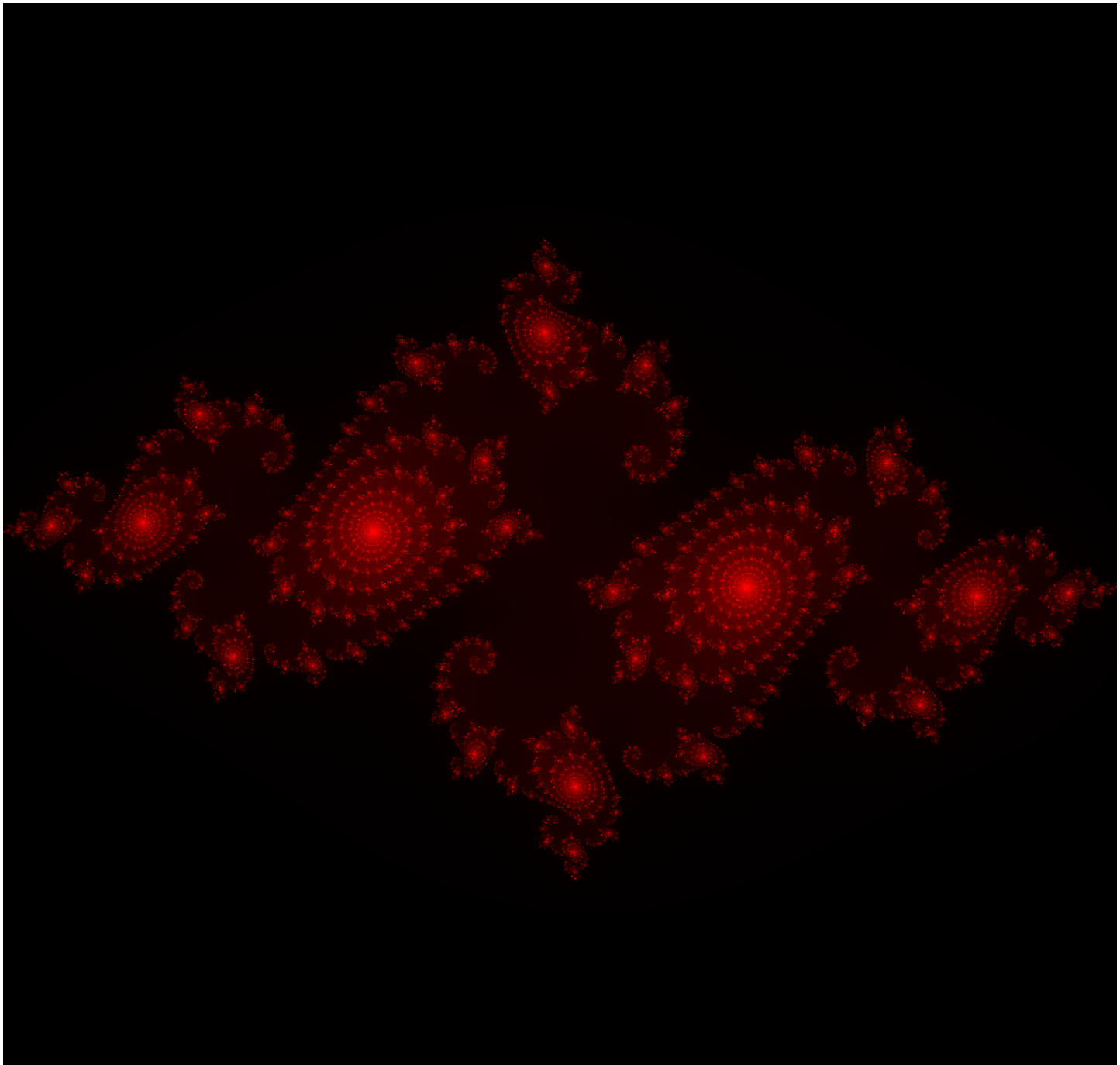
Outline I

Who Am I

- BSc in Computer Science from Wilfirid Laurier University
  - Majors in Computer Electronics Applied Mathematics
  - Minor in Biochemistry
- MSc in Biology from University of Waterloo
  - Petabase-scale Data Mining Identifies Novel Clostridial Species and Neurotoxins Associated with Ancient Human DNA
- Experience programming in several languages
  - Python, Bash, C/C++, Java/Groovey, PIC Assembly, MATLAB/R
- Over ten years of experience using various HPC systems
  - Carbon Compute Cluster : Argonne National Labs
  - Sharcnet : University of Waterloo, University of Toronto
  - Compute Canada (now the Digital Research Alliance of Canada) : BC, Ontario, Quebec
- Thousands of compute hours running
  - Black white boxes
- custom scripts / pipelines / visualizations
- Run Linux as my daily OS
- Used Python with MPI4PY for my CP431 projects with Julia sets for my final project

Julia Sets



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All this can make developing new code “easier” and faster.

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You should use the right tool for the job. Sometimes that's Python and sometimes that's C/C++ or even Assembly.

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See Dr. Pawel Pomorski Slides Numpy, Cython, Multiprocessing and Numba.

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What you lose in performance, you gain in shorter development time, and potentially fewer lost neurons.

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  - MPI_Init() is called when you import the module
  - MPI_Finalize() is called before the Python process ends

Hello to the World

```
#!/usr/bin/env python3
"""
Parallel Hello World
"""
from mpi4py import MPI

size = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()
name = MPI.Get_processor_name()

print('Greetings. I am process {} of {} on {}'.format
    ↪ (rank, size, name ) )
```

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See Texas tutorials for more options

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- MPI4Py handles the packing and unpacking for user defined data types
- Two types of communication: Blocking and non - Blocking

Collective Communications

Used to send messages to multiple processes at once. Eg. Broadcast, Scatter, Gather, Reduction

See Texas tutorials for examples and specifics

Transferring Python Data

```
#!/usr/bin/env python3
"""
Send Python Data
"""

from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0 :
    data = { 'a': 7 , 'b' : 3.14 }
    comm.send( data , dest=1, tag=11)
    print( 'Message set, data is : ', data )
elif rank == 1 :
    data = comm.recv( source=0, tag=11)
    print( 'Message Received, data is : ', data )
```

Transferring Numpy Data I

```
#!/usr/bin/env python3
"""
Send Numpy Data
"""

from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

# pass explicit MPI data types
if rank == 0 :
    data = numpy.random.randint(0,100, size=(2, 4),
        ↪ dtype='i')
    comm.Send( [ data, MPI.INT ] , dest=1, tag=77)
```

Transferring Numpy Data II

```
elif rank == 1 :
    data = numpy.empty ( (2,4), dtype='i' )
    comm.Recv( [ data, MPI.INT ], source=0 , tag=77)
    print(data)

# automatic MPI data type discovery
if rank == 0 :
    data = numpy.random.randint(0,100, size=(2, 3, 4)
        ↪ , dtype='i')
    comm.Send( data, dest=1, tag=13)
elif rank == 1 :
    data = numpy.empty( (2,3,4), dtype='i' )
    comm.Recv( data, source=0, tag=13)
    print(data)
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- Use comm.Iprobe(source=target, tag=11) to check for incoming if you wanted to use irecv

Compute Canada Clusters

- Documentation at
  `https://docs.computecanada.ca/wiki/Graham`
- Python documentation at
  `https://docs.computecanada.ca/wiki/Python`
- MPI documentation at
  `https://docs.computecanada.ca/wiki/MPI`

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```
#!/bin/bash
#SBATCH --account=def-some-user
#SBATCH --nodes=2
#SBATCH --ntasks=8 # number of MPI processes
#SBATCH --mem-per-cpu=512M # memory; default unit is
    ↪ megabytes
#SBATCH --time=0-00:15 # time (DD-HH:MM)

module load StdEnv/2020 intel/2020.1.217 openmpi
    ↪ /4.0.3 scipy-stack/2022a mpi4py/3.1.2 python
    ↪ /3.9
#export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK #Use
    ↪ this with multi-threaded code
echo 'Hello World Example'
srun ./hello_world.py # mpirun or mpiexec also work
echo 'Send Python Data Example'
srun ./send_python_data.py
echo 'Send Numpy Data Example'
srun ./send_numpy_data.py
```

Live Demo

What every could go wrong :)

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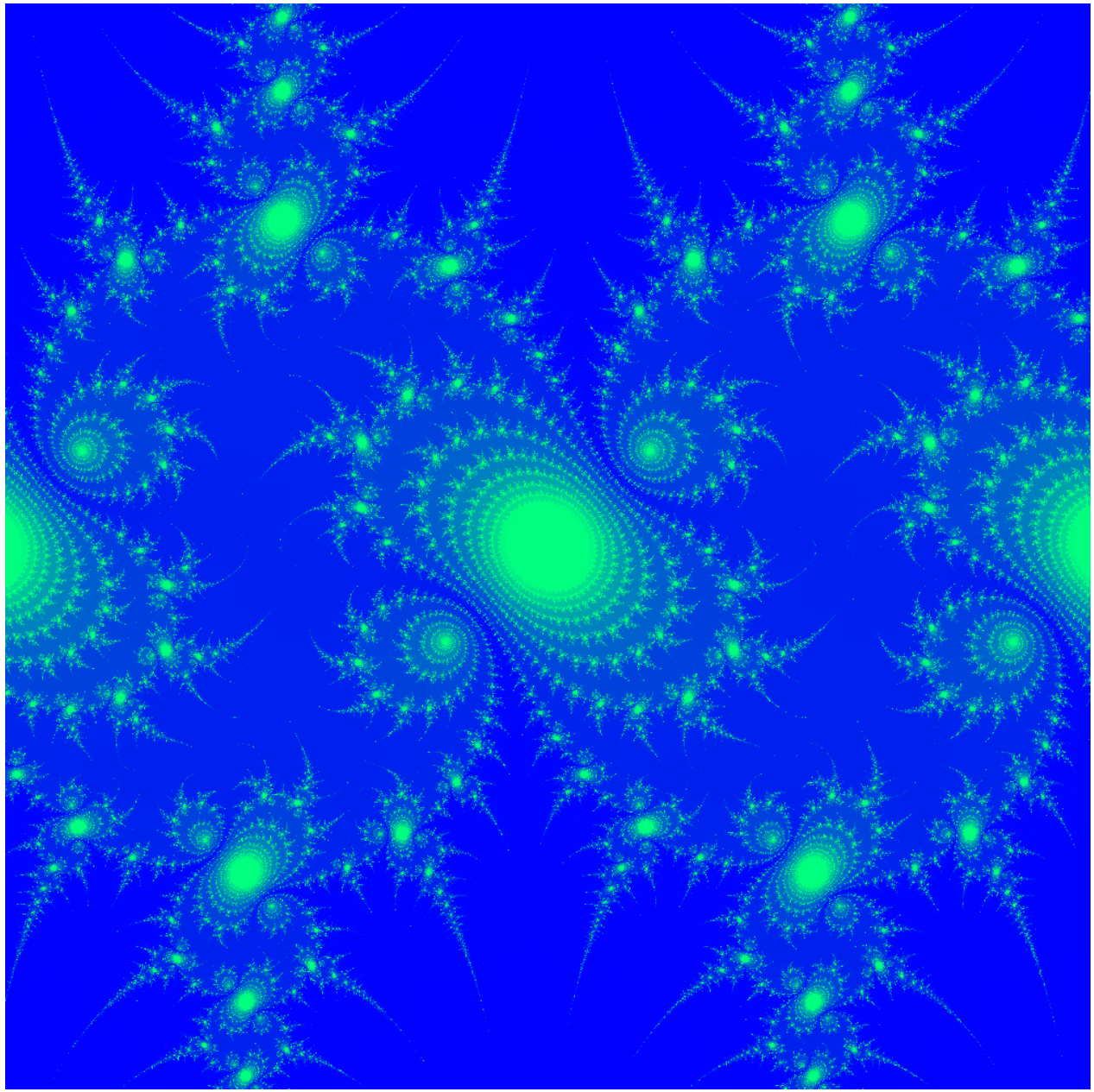
- sbatch run_job.sh or salloc

Questions



References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https://mcgoodwin.net/julia/juliajewels.html