High Performance Computations for Random Network Models of Parental Vaccine Acceptance and Disease Spread using CuPy

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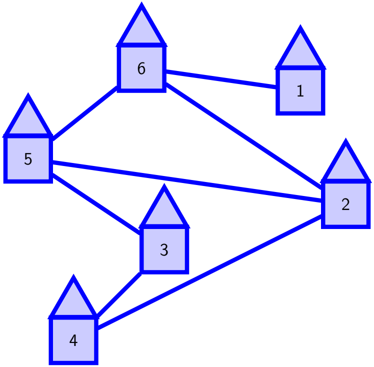
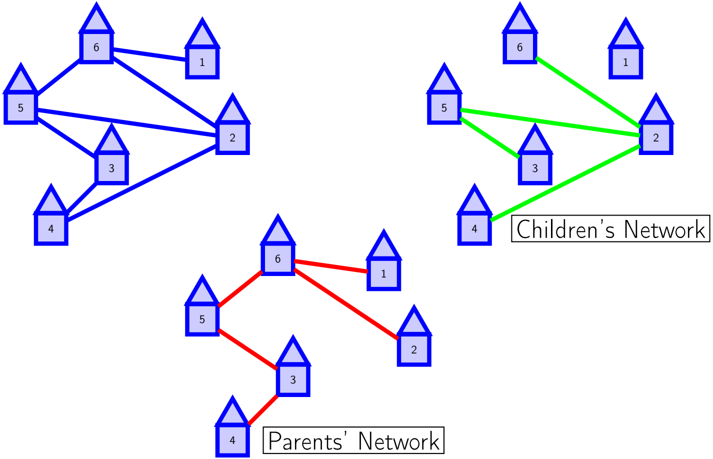
Previous work

- Computational implementation of coupled social and biological networks to examine
  - the influence of imperfect information on the diffusion of vaccination opinion
  - spread of vaccine-preventable pediatric diseases.
- Random network considered: Erdős-Rényi network
- High performance parallel stochastic simulations using Graphical Processing Units (GPUs) (2496 CUDA cores per GPUs).
- CuPy: CUDA and Python combined.

Network of Households (two overlapping networks)



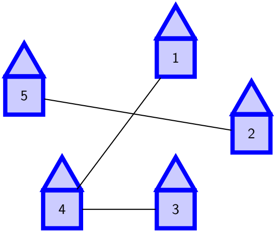
Children Spreading Infection, Parents Spreading Information about Disease and Vaccination



Network Settings (programmed previously)

- N – households
- A maximum number of M_c children placed into each household
- $0 \leq Children(i) \leq M_c$, for $1 \leq i \leq N$ (binomial distribution, $P_c = 0.5$ probability of having a child)
- Initially all these children are susceptible
- I_0 infected children are distributed among households randomly
- Erdős-Rényi model for the children's biological network: household i and j are connected with probability $P_{link}\sqrt{Children(i)Children(j)}$
- Parent's (Social) Network
  - Children's connections are retained with probability P_{ret}
  - New connections are added with probability P_{add}
- Separate epidemic/vaccination/birth processes go through the networks.

Adjacency Matrices (Children and Parents)



- $x_{ij} = 1$ if and only if households i and j are connected.
- Symmetric matrix with zero diagonal

$$\begin{bmatrix} \color{blue}{0} & 0 & 0 & \color{red}{1} & 0 & \dots \\ 0 & \color{blue}{0} & 0 & 0 & \color{red}{1} & \dots \\ 0 & 0 & \color{blue}{0} & \color{red}{1} & 0 & \dots \\ 1 & 0 & 1 & \color{blue}{0} & 0 & \dots \\ 0 & 1 & 0 & 0 & \color{blue}{0} & . \end{bmatrix}$$

Sparse Symmetric Matrix Storage

- Symmetric sparse matrix with zero diagonal

$$\begin{bmatrix} \color{blue}{0} & 0 & 0 & \color{red}{1} & 0 & \dots \\ 0 & \color{blue}{0} & 0 & 0 & \color{red}{1} & \dots \\ 0 & 0 & \color{blue}{0} & \color{red}{1} & 0 & \dots \\ 1 & 0 & 1 & \color{blue}{0} & 0 & \dots \\ 0 & 1 & 0 & 0 & \color{blue}{0} & . \end{bmatrix} \xRightarrow{\text{indexing}} \begin{bmatrix} . & 1 & 2 & \color{red}{4} & 7 & \dots \\ . & . & 3 & 5 & \color{red}{8} & \dots \\ . & . & . & \color{red}{6} & 9 & \dots \\ . & . & . & . & 10 & \dots \\ . & . & . & . & . & . \end{bmatrix}$$

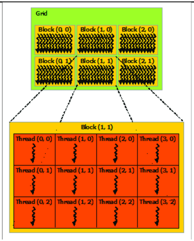
- Only the indices of nonzero elements in the upper part are stored: $k \in \{4, 6, 8, \dots\}$ (Children_mtx_indx, Parents_mtx_indx)
- We switch between indexing formulas as needed:

$$k = i + \frac{(j-2)(j-1)}{2}$$

$$\text{col index } j = \text{floor}\left(\frac{3+\sqrt{8k-7}}{2}\right)$$

$$\text{row index } i = k - \frac{(j-2)(j-1)}{2}$$

Parallel computations using CUDA on Graphical Processing Units

NVIDIA Tesla K40 Computing Accelerator 4.2 TFLOPS 12GB memory	2880 CUDA cores maximum size of a thread block $(1024, 1024, 64)$
	

CUDA/GPGPU

CUDA

- CUDA is a parallel computing platform and programming model developed by NVIDIA for general computing on its own GPUs.
- CUDA enables developers to speed up compute-intensive applications by harnessing the power of GPUs for the parallelizable part of the computation.

GPGPU

- General-purpose GPU computing (GPGPU) is the use of a GPU to do general purpose computing.
- The model for GPU computing is to use a CPU and GPU together in a heterogeneous co-processing computing model.
    - The sequential part of the application runs on the CPU.
    - The computationally-intensive part is accelerated by the GPU.

CUDA with different programming languages

- Originally CUDA is written in C/C++. Problem: matrices and matrix operations
- CUDA Fortran: very convenient handling of matrices; object oriented, but not popular anymore on the job market
- Python: popular in both academia and business, easy to read
- Python with CUDA: CuPy
  - NumPy-compatible matrix library accelerated by CUDA
  - Example: cupy.flatnonzero() - indices of nonzero entries
  - Example: a + b - adding vectors/matrices in parallel
- Current CuPy code is based on previously written CUDA Fortran code
- Typically, every process is done simultaneously (parallel) for each household.
- CUDA C++ kernel functions are still useful.

Disease progression (daily process)

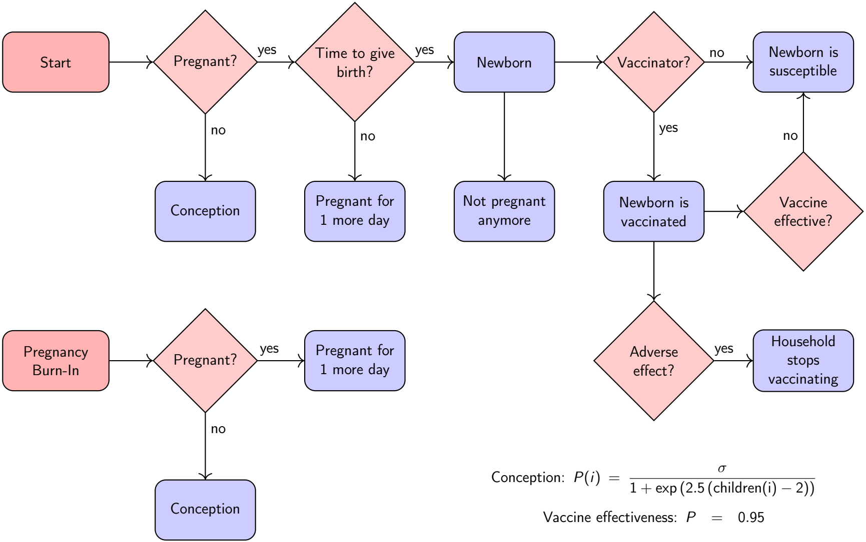
Immunized ← Susceptible → Infected → Recovered

- New Infections in a household i
  - $\beta = 0.01$ – transmission probability <u>between</u> households
  - $\beta_h = h\beta = 2\beta$ – transmission probability <u>within</u> households

$$P_{\text{infection}}(i) = 1 - (1-\beta)^{\frac{\textbf{infected connections}(i)}{\textbf{Children}(i)}} (1-\beta_h)^{\text{Infected(i)}}$$

  - Infected connections are based on the children's network
- Recovery period: based on discretized gamma distribution. Mean: 22 days; Maximum: 28 days (Measles)
  - An infectious recovers on day $0 \leq j \leq 28$ with probability $P(j)$
  - $P(28) = 1$

Pregnancy and Newborns (daily process)

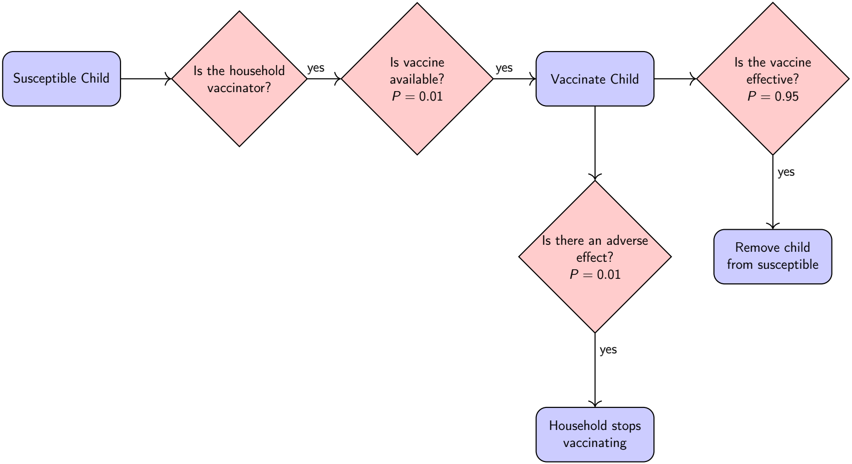


$$\text{Conception: } P(i) = \frac{\sigma}{1 + \exp\left(2.5\left(\text{children(i)} - 2\right)\right)}$$

$$\text{Vaccine effectiveness: } P = 0.95$$

$$\text{Vaccine adverse effect: } P = 0.01$$

Vaccination (daily process)



Probability of household i to vaccinate (daily process)

- Probability to vaccinate against the disease without any social influence, based on only the pay-off between the dangers of infection and the dangers of adverse effects:

$$p_0 = \frac{1}{1 + \exp\left(\gamma(\text{total adverse events}) - \alpha(\text{total infected})\right)}$$

- Probability to vaccinate:

$$P_V(i) = \frac{p_0 \cdot q^{n_V(i)} \cdot (1-q)^{n_N(i)}}{p_0 \cdot q^{n_V(i)} \cdot (1-q)^{n_N(i)} + (1-p_0) \cdot (1-q)^{n_V(i)} \cdot q^{n_N(i)}}$$

- q – probability that parents give the correct/honest signal on their stance/attitude toward vaccination
- $n_V(i)$ – number of socially connected vaccinating households
- $n_N(i)$ – number of socially connected non-vaccinating households

Description of CuPy Code: library imports

```
import numpy as np # numerical library
import cupy as cp # CUDA accelerated library
import os  # for reading random seed from OS
import sys # for stopping code if needed
import math # for ceiling functions
from scipy import stats
import matplotlib.pyplot as plt
from kernel_functions import * # our kernel functions
    (CUDA c++)

```

Reading network data of children and parents

```
data=np.load("erndata.npz")

N=np.asscalar(data['N'])
NC=np.asscalar(data['NC'])
NP=np.asscalar(data['NP'])
Plink=np.asscalar(data['Plink'])
Pret=np.asscalar(data['Pret'])
Padd=np.asscalar(data['Padd'])
I0=np.asscalar(data['I0'])
Children_mtx_indx=cp.asarray(data['Children_mtx_indx'
    ],dtype=cp.int64)
Parents_mtx_indx=cp.asarray(data['Parents_mtx_indx'],
    dtype=cp.int64)
AllInfected=cp.asarray(data['Infected'],dtype=cp.int32
    )
Susceptible=cp.asarray(data['Susceptible'],dtype=cp.
    int32)

Children=cp.add(AllInfected,Susceptible)
```

Setting the parameters

```
q=0.5     # Probability of signal matching opinion
rho=0.01 # Probability of vaccination access
Padv=0.01  # Probability of adverse effect
aalpha=10**(-4) # Household view of infection
ggamma=0.1  # Household view of adverse effect
bbeta=0.01  # Transmission rate between households
bbetah=2*bbeta  # Transmission rate within households
NV0=0.05 # Proportion of all-time never-vaccinator
    households
Peff=0.45  # Probability of vaccine effectiveness
ssigma=0.005 # Birth rate
gestation=280
MaxDays=1000
ip=28    # Days it takes to recover

Infected=cp.zeros((N,ip),dtype=cp.int32)
```

Recovery process follows gamma distribution

```
shape = 22; disc=np.arange(ip+1) # ip=28; Measles
#shape = 11.5;  ip=16; disc=np.arange(ip+1); Flu
cumprob=stats.gamma.cdf(disc, shape, scale=1)
Pincubtrans=cp.asarray((cumprob[1:ip+1]-cumprob[0:ip])
    /(cumprob[ip]-cumprob[0:ip]), dtype=cp.float32)
```

Arrays

```
Pregnancy=cp.zeros(N, dtype=cp.int32)
Vaccinator_yesnonever=cp.zeros(N, dtype=cp.int32)
Nbrvacc_yes=cp.zeros(N, dtype=cp.int32)
Nbrvacc_no=cp.zeros(N, dtype=cp.int32)
Adverse=cp.zeros(N, dtype=cp.int32)
Vaccinated_new=cp.zeros(N, dtype=cp.int32)
Vaccinated=cp.zeros(N, dtype=cp.int32)
Recovered=cp.zeros(N, dtype=cp.int32)
InfNeighb=cp.zeros(N, dtype=cp.int32)
Infected_Total=cp.zeros(MaxDays, dtype=cp.int32)
Daily_Incidence=cp.zeros(MaxDays, dtype=cp.int32)
Daily_Vaccinations=cp.zeros(MaxDays, dtype=cp.int32)
Daily_Suscep=cp.zeros(MaxDays, dtype=cp.int32)
Daily_Vaccinators=cp.zeros(MaxDays, dtype=cp.int32)
Daily_NonVaccinators=cp.zeros(MaxDays, dtype=cp.int32)
Daily_Recovered=cp.zeros(MaxDays, dtype=cp.int32)
Daily_P0=cp.zeros(MaxDays, dtype=cp.float32)
Daily_Children=cp.zeros(MaxDays, dtype=cp.int32)
PV_info=cp.zeros(N, dtype=cp.float32)
P_infection=cp.zeros(N, dtype=cp.float32)
Infected[:,1]= AllInfected
```

Pregnancy Burn-In

```
blocksize_x = 1024 # maximum size of 1d block is 1024 threads
blocks=(blocksize_x,1,1) # number of blocks in the grid to cover all indices see 'grids' later
grids=(math.ceil(N/blocksize_x),1,1) # set grid size N

seed=int.from_bytes(os.urandom(4),'big') # Random seed from OS
# Uses the number of existing children and birth rate (ssigma) to create pregnancies at different stages in each household.
# Pregnancy[i] = 0 - no pregnancy
# Pregnancy[i] = j, 0 < j < gestation - jth day of pregnancy
pregnancy_burn_in(grids, blocks, (N, cp.float32(ssigma), seed, Children, Pregnancy, gestation))
```

Pregnancy Burn-In kernel function

```
import cupy as cp

pregnancy_burn_in = cp.RawKernel(r'''
    #include <curand_kernel.h>
    extern "C" __global__
    void pregnancy_burn_in(const int N, const float ssigma,
    int seed, const int* Children,
                    int* Pregnancy, const int gestation){
        int i = blockDim.x * blockIdx.x + threadIdx.x;
        int j, seq, offset;
        seq = 0;
        offset = 0;
        curandState h;
        if(i<N){
        curand_init(seed+i,seq,offset,&h);
          for(j=1; j < gestation; j++){
              if(Pregnancy[i]>0) { ++Pregnancy[i]; }
              else if( curand_uniform(&h) < ssigma/(1.0+exp
    (2.5*(Children[i]-2)))) { Pregnancy[i]=1; }
          }
        }
    }
    ''', 'pregnancy_burn_in', backend='nvcc')
```

Vaccinators_Init

```
seed=int.from_bytes(os.urandom(4),'big')
# Initial set up of vaccinators and non-vaccinators, based
    on the initial infected (I0)
# Vaccinator_yesnonever[i] = 0/1, family i doesn't vaccinate
    /does vaccinate. Can change, see Vaccinator_update
Vaccinators_Init(grids, blocks, (N, cp.float32(1.0/(1.0+np.
    exp(-aalpha*I0))),seed,Vaccinator_yesnonever))
```

Vaccinators_Init kernel function

```
Vaccinators_Init = cp.RawKernel(r'''
    #include <curand_kernel.h>
    extern "C" __global__
    void Vaccinators_Init(const int N, const float VProb,
   int seed, int* Vaccinator_yesnonever){
        int i = blockDim.x * blockIdx.x + threadIdx.x;
        int seq, offset;
        seq = 0;
        offset = 0;
        curandState h;
        if(i<N){
            curand_init(seed+i,seq,offset,&h);
            if(curand_uniform(&h)<VProb) {
   Vaccinator_yesnonever[i] = 1; }
            else { Vaccinator_yesnonever[i] = 0; }
        }
    }
    ''', 'Vaccinators_Init', backend='nvcc')
```

```
# Vaccinator_yesnonever[i] = -1
# NV0 proportion of non-vaccinators

# Number of vaccinators
Nvacc=np.asscalar(cp.count_nonzero(Vaccinator_yesnonever).
    get())

 # Calculates the number of never-vaccinators
 N_nevervacc=int(round(NV0*(N-Nvacc)))

 # Indices of non-vaccinators, min value of
    Vaccinator_yesnonever is 0
idx_Nonvacc=cp.argmin(Vaccinator_yesnonever)

# From the number of non-vaccinators (N-Nvacc), choose
    randomly N_nevervacc indices (never vaccinators)
idx_Nevervacc=cp.random.choice(N-Nvacc, size=N_nevervacc,
    replace=False, p=None)

# Place never-vaccinators (-1) into Vaccinator_yesnonever
cp.put(Vaccinator_yesnonever, idx_Nevervacc, -(cp.ones(
    N_nevervacc,dtype=cp.int16)))
```

```
while (Infected_Total[day].get() > 0):
    day = day + 1
    # Marks households NbrNbrvacc_yes=0/1 & Nbrvacc_no=0/1
    grids=(math.ceil(N/blocksize_x),1,1) # set grid size N
    Vaccinators_Separate(grids, blocks, (N,
    Vaccinator_yesnonever, Nbrvacc_yes, Nbrvacc_no))

    # Counts vaccinating/non-vaccinating neighbors
    grids=(math.ceil(NP/blocksize_x),1,1) # set grid size NP
    Pressure_Update(grids, blocks, (NP, Parents_mtx_indx,
    Vaccinator_yesnonever, Nbrvacc_yes, Nbrvacc_no))

    # p0 - probability to vaccinate without social influence
    p0=1.0/(1.0+np.exp(ggamma*np.asscalar(cp.sum(Adverse).
    get())-aalpha*np.asscalar(cp.sum(Infected_Total).get()))
    )

    grids=(math.ceil(N/blocksize_x),1,1) # set grid size N
    # PV_info - probability to vaccinate with social
    influence
    pv_info_update(grids, blocks, (N, PV_info, cp.float32(p0
    ), cp.float32(q), Nbrvacc_yes, Nbrvacc_no,
    Vaccinator_yesnonever))
```

Daily Process (continued)

```python
    # Update vaccinators based on PV_info. Never-vaccinators will not change
    seed=int.from_bytes(os.urandom(4),'big')
    Vaccinator_update(grids, blocks, (N, PV_info, seed, Vaccinator_yesnonever))

    # Vaccinates susceptibles if the household is a vaccinator and the vaccine is available
    # The vaccine is effective with probability Peff and causes adverse effects with probability Padv
    seed=int.from_bytes(os.urandom(4),'big')
    Vaccinated_new.fill(0) # Resets newly vaccinated
    Vaccinate_Susceptibles(grids, blocks, (N, Vaccinated_new, Vaccinated, Vaccinator_yesnonever, Susceptible, seed, cp.float32(rho),cp.float32(Padv), Adverse, cp.float32(Peff)))

    seed=int.from_bytes(os.urandom(4),'big')
    Pregnancy_Newborns(grids, blocks, (N, Vaccinated_new, Vaccinated, Vaccinator_yesnonever, Susceptible, seed, cp.float32(Padv), Adverse, cp.float32(Peff), Pregnancy, gestation, Children, cp.float32(ssigma)))
```

Pregnancy_Newborns kernel function

```
if(i<N){     // in parallel for each household i simultaneously
    curand_init(seed+i,seq,offset,&h); // initialize random seed for each thread
    if (Pregnancy[i]==0){  // no pregnancy, might get pregnant
        if(curand_uniform(&h) < ssigma/(1.0+exp(2.5*(Children[i]-2.0)))) { Pregnancy[i]= 1; }
    }
    // else, the household is pregnant for another day
    else if(Pregnancy[i]<gestation){ Pregnancy[i]=Pregnancy[i]+1; }
    else if(Pregnancy[i] == gestation) { // else, newborn
        Children[i]=Children[i]+1;
        Pregnancy[i]=0;
        if (Vaccinator_yesnonever[i]==1) {  // household vaccinates
            Vaccinated_new[i]=Vaccinated_new[i]+1;
            Vaccinated[i]=Vaccinated[i]+1;
            // the vaccine is NOT effective
            if(curand_uniform(&h)>Peff) { Susceptible[i]= Susceptible[i]+1; }
            // adverse effect of the vaccine
            if (curand_uniform(&h)<Padv){
                Adverse[i]=Adverse[i]+1;
                Vaccinator_yesnonever[i] = -1;
            }
        }
        // otherwise, if the household does not vaccinate
        else { Susceptible[i]= Susceptible[i]+1; }
    }
}
```

Daily Process (continued)

```
    seed=int.from_bytes(os.urandom(4),'big')
    Recover_Infected(grids, blocks, (N, Infected, Recovered, seed, Pincubtrans, AllInfected, ip))

    grids=(math.ceil(NC/blocksize_x),1,1) # set grid size NC
    InfNeighb.fill(0)
    Infected_Neighbors(grids, blocks, (NC, Children_mtx_indx, AllInfected, InfNeighb))

    grids=(math.ceil(N/blocksize_x),1,1) # set grid size N
    Pinfection_update(grids, blocks, (N, P_infection, InfNeighb, Children, AllInfected, cp.float32(bbeta), cp.float32(bbetah)))

    seed=int.from_bytes(os.urandom(4),'big')
    New_Infected(grids, blocks, (N, P_infection, Infected, Susceptible, seed, AllInfected, ip))
```

Daily Process Data Collection for Output

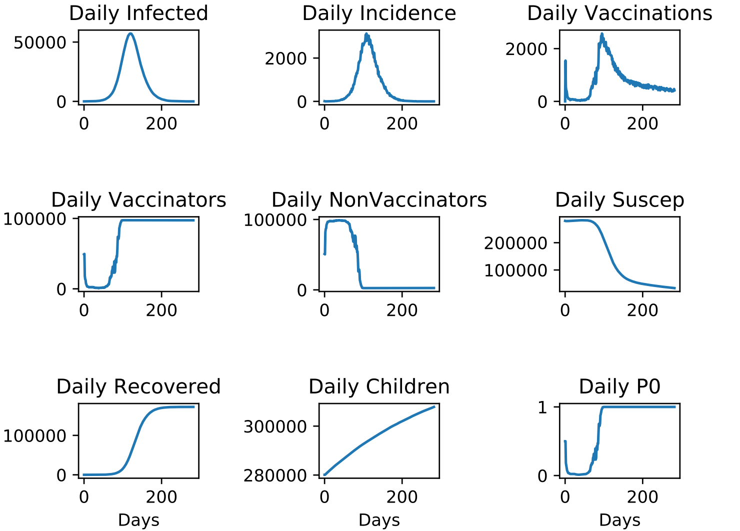
cupy.sum - summation is done in parallel on the GPU

```
    Infected_Total[day] = cp.sum(AllInfected)
    Daily_Incidence[day] = cp.sum(Infected[:,1])
    Daily_Vaccinations[day] = cp.sum(Vaccinated_new)
    Daily_Vaccinators[day] = cp.sum(Vaccinator_yesnonever > 0)
    Daily_NonVaccinators[day] = cp.sum(Vaccinator_yesnonever <= 0)
    Daily_Suscep[day] = cp.sum(Susceptible)
    Daily_Recovered[day] = cp.sum(Recovered)
    Daily_Children[day] = cp.sum(Children)
    Daily_P0[day] = p0
```

Plotting Results

```
Days=np.arange(day+1)
fig = plt.figure()
fig.subplots_adjust(hspace=1.5, wspace=1)

ax=fig.add_subplot(3,3,1)
ax.plot(Days,Infected_Total[0:day+1].get())
ax.set_title("Daily Infected")

ax=fig.add_subplot(3,3,2)
ax.plot(Days,Daily_Incidence[0:day+1].get())
ax.set_title("Daily Incidence")

...

ax=fig.add_subplot(3,3,9)
ax.plot(Days,Daily_P0[0:day+1].get())
ax.set_title("Daily P0")
ax.set_xlabel("Days")

plt.show()
fig.savefig("fig.pdf")
```

Sample Results



Timing Results

- For the epidemic process the speed of the CuPy code is comparable to the speed of the previous CUDA Fortran code, despite Python being an interpreted language.

N	Cuda Fortran	CuPy
$100,000$	$1.4s$	$4.7s$
$500,000$	$14.7s$	$16.5s$
$1,000,000$	$31.9s$	$37.4s$

- For the network generation the CuPy code is significantly faster than previous CUDA Fortran code. This is very important, as the stochastic computations require the calculation repeated thousands of time.

N	Cuda Fortran	CuPy	Speed up
$100,000$	$26s$ $(7.8GB)$	$18s$ $(9.1GB)$	44%
$500,000$	$626s$ $(8,7GB)$	$420s$ $(9.7GB)$	49%
$1,000,000$	$2500s$, $(8.7GB)$	$1700s$ $(10GB)$	47%

- The CuPy code is half as long as the CUDA Fortran code due to many of the NumPy-like library functions available in CuPy.

Summary

- We used the CuPy (CUDA + Python) open-source Python library with accelerated matrix and vector operations on NVIDIA GPUs for the stochastic simulation of an agent-based random network model.
- Two overlapping networks are considered, where the nodes represent households with parents and children in them.
- One network represents the children's physical connections through which disease spread.
- The other network represents the parents' social network though which information is exchanged about the disease and the vaccine.
- Initial results show a realistic disease process.

Future Plans

- Modify the code to run on multiple GPUs for population sizes larger than a million.
- Write code to calculate reproduction number R_0.
- Parameter analysis.
- Modify the code to run thousands of times for statistical purposes.
- Examine different diseases (measles, flu).
- Rewrite some of the kernel functions into CuPy code.

References

[1] R. Okuta, Y. Unno, D. Nishino, S. Hido, and C. Loomis.
Cupy: A numpy-compatible library for nvidia gpu calculations.
In *Proceedings of Workshop on Machine Learning Systems (LearningSys) in The Thirty-first Annual Conference on Neural Information Processing Systems (NIPS)*, 2017.