Supplementary Material

S1 Fig. Scalability performance. The optimization routine concluded 500 generations of 20 particles in ~36 hours of runtime running on 128 compute cores of a physical server. To account for first-order uncertainty, we replicated the solution obtained using each parameter set 500 times and calibrated against the average fitness. The scalability of the calibration routine is tested against various numbers of processes for a smaller problem (one generation with two population members). An initial increase in the number of cores showed almost linear scaling while there is a diminishing return of the number of cores assigned (Fig S1). This is due to the nature of I/O operations simulation runs and biopsy routines need.
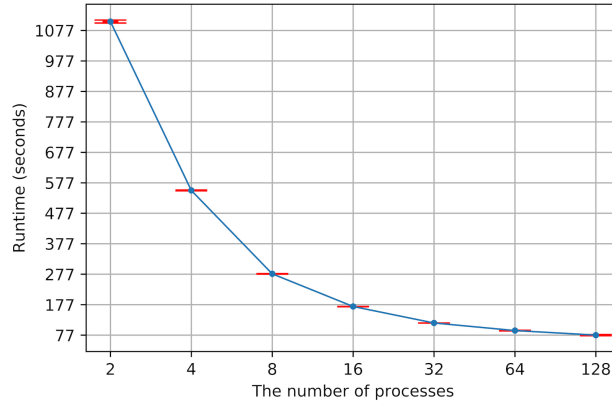

Fig 1. Scaling of the calibration routine with the number of processes (cores) leveraged.

S2 Fig. Evolution of optimization algorithm. Figs S2 A and B show the improvement of the fitness function and the average fitness of particles over time, respectively. The calibration routine is re-initialized with a random particle population

in every 100 generations that fluctuates the average fitness in Fig S2 A. Fig S2 C illustrates the points in the solution space that were visited over 500 generations. Blue lines in Fig S2 D represent the trajectory of best solutions and the red dot is the final best solution that optimization algorithm landed on.
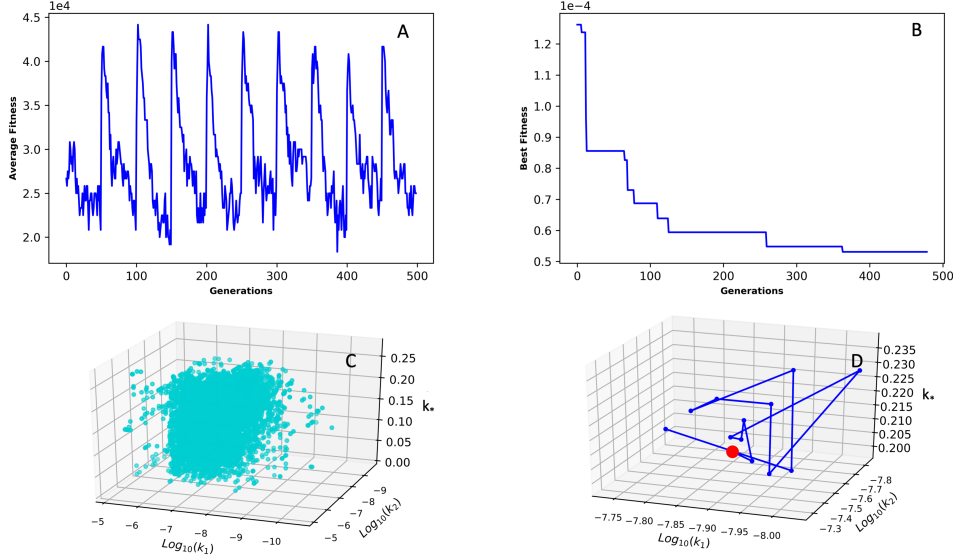

Fig 2. Outputs of simulation algorithm and parameter exploration.
Average fitness and best fitness over generations (A and B respectively), and visualization of the explored state-space of the model toward optimal parameters and the best parameters over time (C and D respectively).

S3 Code repository. The calibration and simulation code-base are in `https://code.ornl.gov/ozi/cisnet.git`. To gain access please go to `xcams.ornl.gov` and create an account, and let **ozmeno@ornl.gov** or **nutarojj@ornl.gov** know of your xcams username to acquire access.