README for fitting thermoplate data on MATLAB to generate model parameters

Files:

* FUNCTION: heating\_eval\_fixedrate.m
  + simulates thermoplate behavior (starting from steady state, all wells at ambient temperature) over an input duration using input model parameters given a desired pattern of heated wells.
  + Inputs
    - Parameters
      * 8x1 vector of values representing the parameters that govern model behavior, must be in the following order:
        + Hp, passive movement of heat between non heated wells
        + Ht, diffusion up from a heated well
        + Hb, diffusion down from a heated well
        + Hl, diffusion left from a heated well
        + Hr, diffusion right from a heated well
        + He, diffusion out from edge of plate
        + Loss, loss from every well
        + heat\_rate, fixed rate of heating in heated wells that are below their setpoint
    - Timestep
      * Time in seconds between each frame of the simulation
    - On\_Wells
      * 8 x 12 x t matrix of values that guide the simulation
      * Each 8x12 frame represents the 96 wells of the plate at each timepoint, t
      * values of the matrix represent the set temperature of each well at each timepoint. 0 for unheated wells, and the desired degree C above ambient temperature for set wells
  + outputs
    - timecourse
      * An 8 x 12 x t matrix giving the temperature of each well at each frame of the simulation
* FUNCTION: temp\_fit\_heating\_fixedrate.m
  + fits input data to model using the MATLAB function fminsearch to minimize difference between input data and evaluations of the model (heating\_eval\_fixedrate.m)
  + Inputs
    - Data
      * 8 x 12 x t matrix of values output from thermoplate experimental readings. Values should be temperature above ambient in degrees C
        + We normalized to ambient by subtracting the first reading from each well from every subsequent reading
    - Timestep
      * Time in seconds between each frame of the data
    - On wells
      * 8 x 12 x t matrix of values that describe the heating pattern used in the experimental data
      * Each 8x12 frame represents the 96 wells of the plate at each timepoint, t
      * values of the matrix represent the set temperature of each well at each timepoint. 0 for unheated wells, and the setpoint in degrees C above ambient for the heated wells
    - Initial conditions
      * Initial guesses for model parameters to guide minimization function. We used
        + initial\_conditions(1) = 0.007; %passive movement of heat between non heated wells
        + initial\_conditions(2) = 0.01; %diffusion up from a heated well
        + initial\_conditions(3) = 0.006; %diffusion down from a heated well
        + initial\_conditions(4) = 0.008; %diffusion left from a heated well
        + initial\_conditions(5) = 0.003; %diffusion right from a heated well
        + initial\_conditions(6) = 0.0018; %diffusion out from edge of plate
        + initial\_conditions(7) = 0.0005; %loss from every well
        + initial\_conditions(8) = 0.22; %fixed rate of heating
  + outputs
    - parameters
      * 8x1 vector of parameter values that minimize error to provided data
    - W\_error
      * Error between data and simulation (sum of square differences)
* SCRIPT: Testing\_all\_datasets\_fixed\_rate.m
  + File that fits loads and fits all 8 of our datasets, then simulates all other datasets with each parameter set, as well as average parameters, as well as ‘blinded’ parameters.
  + Also saves table and tiffs of results.

The script is the code we used to fit the datasets, and do simulations to validate the model. By mimicking this code, you can fit your own data! Fitting is done by running the function temp\_fit\_heating\_fixedrate.m with your data and the matrix that describes the experiment (on\_wells), and the parameters of best fit will be produced.