Supplementary Material 1

1.1 Workflow example: Workflow 11 including calls audit log code

```
% Workflow 11 - PROTECH phytoplankton model uncertainty analysis using the
% GLUE method and a Limits of Acceptability approach
%
% This workflow is part of the CURE Toolbox
%
% This script provides an example application of the extended Generalized
% Likelihood Uncertainty Estimation (GLUE)including Limits of Acceptability
%(LoA)(see help GLUE_LoA.m for more details about the Uncertainty Analysis
% method and references).
%
%
*****************************************************************************************************
***********
% **** See See Section 7.10,7.12,7.13 and Box 7.1 Beven, 2009: Evironmental Modelling - An
Uncertain Future. **
% **** London : Routledge. 310 p. ISBN: 978-0-415-45759-0.
****************************************************
%
*****************************************************************************************************
***********
%
% MODEL AND STUDY AREA
% The simulation model used is PROTECH, a lake algal comunity structure
% model and the example is for Lake Windermere (north west UK) for 2008.
% See Reynolds et al 2001 for an decription of the model. In this case
% the model is in executable form. Simulations are required to be within
% the specified LoA for 3 variables: Chlorophyll, R-Type algae and CS-type
% algae for absolute acceptance of simulations.  In addition simulations
% are weighted by their goodness of fit to chlorophyll concentrations using
% a trapezoidal fuzzy measure at each observation timestep.
%
% Reynolds C.S., Irish A.E. & Elliott J.A. (2001). The ecological basis for
% simulating phytoplankton responses to environmental change (PROTECH).
% Ecological Modelling, 140, 271-291.
%
% Page, T., Smith, P.J., Beven, K.J., Jones, I.D., Elliott, J.A., Maberly,
% S.C., Mackay, E.B., De Ville, M., Feuchtmayr, H., 2017. Constraining
% uncertainty and process-representation in an algal community lake model
% using high frequency in-lake observations Ecological Modelling.357,1-13.
%
% In the workflow below, modelling decisions amnd assumptions are made
% explicit and are written to a log file of a user specified name (appened
% with current date)

clear all; close all
format long g
% Set up project
proj = 'PROTECH_GLUE_LOA'; proj2 = 'Projects';
if~exist(['Projects\',proj])
    mkdir('Projects\',proj)
end

% Flags %%%%%%%%%
plots = 1 % flag for plots to be plotted

Proj_flag = 2; % Project log file 1 = enter INITIAL info; 2 = EDIT info; 3 = OFF

DT = clock; DTstamp = [num2str(DT(1)),'-',num2str(DT(2)),'-',num2str(DT(3)),'-',num2str(DT(4)),'-
',num2str(DT(5))];
if Proj_flag > 1
    flnme = [proj2, '/', proj, '/', proj, '_Test_log_', DTstamp, '.txt']; % log file name
    fileID = fopen(flnme,'w');
end
```

```
my_dir = pwd ;% use the 'pwd' command if you have already setup the Matlab
% current directory to the CURE directory. Otherwise, you may define
% 'my_dir' manually by giving the path to the CURE directory.
% Set current directory to 'my_dir' and add paths for required sub-folders
cd(my_dir);
addpath('util');addpath('visualization');addpath('GLUE');

% Write project audit log (from dialog box or file depending on flag)
fileID = CURE_GUI(proj, proj2, Proj_flag,flnme);

%*************************************************************************
% NOTE:  In this example simulations have been pre-run because run times are
% significant. The output files are read in below
%*************************************************************************
% set up header for automatic writes to audit log

N = 1000;

fprintf(fileID,['_______________________________________________________________' ,'\n' ,'\n']);
fprintf(fileID,['AUTOMATIC ENTRIES' '\n']);
fprintf(fileID,['_______________________________________________________________' ,'\n' ,'\n']);
fprintf(fileID,['Number of simulations   ' num2str(N) '\n' '\n']);



% number of uncertain parameters [epsw Pf Nf Sif Kz wwf]
M  = 6 ;

X_Labels = {'epsw ','Pf ','Nf ','Sif ', 'Kz ', 'wwf '} ;
fprintf(fileID,['Parameters chosen for analysis   ' X_Labels{:} '\n' '\n']);

DistrFun  = 'unif'  ; % Parameter distribution
fprintf(fileID,['Parameter Distribution Chosen  =  ' DistrFun '\n' '\n']);
% ****NOTE par5 (kz) must be =< 0.4 for model stability****
xmin = [0.15  0.5 0.5 0.5 0.05 0.05] ; % minimum values
xmax = [0.35  2.5 1.5 1.5 0.4 0.6] ; % maximum value
fprintf(fileID,['Minimum/Maximumparameter values  =  ' '\n' num2str(xmin) '\n' num2str(xmax) '\n'
'\n']);

% % Save these ranges to the input file used by the PROTECH executable
% GPout = nan(length(xmin),2); GPout(1,1) = N;
% GPout(2:length(xmin)+1,1) = xmin;
% GPout(2:length(xmin)+1,2) = xmax;

% load in observed chlorophyll, species and Limits of Acceptability files
ch_obs = load('example\PROTECH\INPUT_WSB_2008\WSB_CHL_OBS_2008.csv');
obsCSR = load('example\PROTECH\INPUT_WSB_2008\CSR.csv');
chl_LOA = load('example\PROTECH\INPUT_WSB_2008\WSB2008LOA.txt');
CS_LOA = load('example\PROTECH\INPUT_WSB_2008\WSB2008LOA_CS.txt');
R_LOA = load('example\PROTECH\INPUT_WSB_2008\WSB2008LOA_R.txt');
% copy limits of acceptability to log folder
copyfile('example\PROTECH\INPUT_WSB_2008\WSB2008LOA.txt',[my_dir '/' 'Projects/' proj])
copyfile('example\PROTECH\INPUT_WSB_2008\WSB2008LOA_CS.txt',[my_dir '/' 'Projects/' proj])
copyfile('example\PROTECH\INPUT_WSB_2008\WSB2008LOA_R.txt',[my_dir '/' 'Projects/' proj])

%%%%%%%%%%%%%%%%%%%% OPEN RESULTS FILES %%%%%%%%%%%%%%%%%%%%%%


ch_ts = load('example/PROTECH/OUTPUT_WSB_2008/pre-run1/chlrec.out');


% % plot all Chlorophyll timeseries
% if plots == 1
%     figure(1)
%     plot(ch_ts','r:')
%     hold on
%     plot(ch_obs(:,1), ch_obs(:,2), 'k-o')
%     hold on
%     plot(ch_obs(:,1), chl_LOA(:,1), 'k-o')
%     hold on
%     plot(ch_obs(:,1), chl_LOA(:,2), 'k-o')
```

```
%     title('All simulated Chlorphyll timeseries')
%     xlabel('Days 2008')
%     ylabel('Chl (mg/m^-^3)')
% end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% GLUE-LoA %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Find acceptable ('behavioural') simulations using the 'GLUE_LoA' function
% (see help GLUE_LOA.m for more details after typing addpath('GLUE') *****)

% calculate goodness of fit weighting (fuzzy measure)for all simulations
%fprintf(fileID,['Goodness of fit to chlorophyll concentrations used in addition to absolute LoA
- calculated using trapezoidal fuzzy measure' '\n' '\n']);

wtg = zeros(length(ch_obs(:,1)),N); % initialise array
for ii = 1: length(ch_obs(:,1))
    wtg(ii,:) = trapmf(ch_ts(:,ch_obs(ii,1))',[chl_LOA(ii,1) ch_obs(ii,2)...
        ch_obs(ii,2) chl_LOA(ii,2)] );
end
GLF = sum(wtg); % Sum generalised likelihoods (weightings).

% Timesteps for first observed variable used as LoA
TS = ch_obs(:,1);

% Set up test of second and third set of LoA
% Requirement to adequately simulate algal species community structure
% for estimating risk from cyanobactera.
% second LoA is approximated using CS-type species; species 3 and 4 (of 8)
% third LoA is approximated using R-type species; species 1, 2 and 6 (of 8)

% load in the required simulated species files

sp1_ts = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\1_spec.out');
sp2_ts = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\2_spec.out');
sp3_ts = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\3_spec.out');
sp4_ts = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\4_spec.out');
sp6_ts = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\6_spec.out');

TS2 = obsCSR(:,1);
TS3 = TS2; % In this case observed timesteps for LoA2 & LoA3 are the same
cs_ts = sp3_ts+sp4_ts; % sum CS species (chlorophyl equivalents)
r_ts = sp1_ts+sp2_ts+sp6_ts; % sum R species (chlorophyl equivalents)

% Specify weighted percentiles to be returned from GLUE-LoA
% default is 0.05 0.5 0.95 if unspecified
Pc = [0.025 0.5 0.975];

% Call GLUE-LoA
[idx1, id_LOA, Pcnts] = GLUE_LOA(N, GLF',chl_LOA,ch_ts,TS,Pc,CS_LOA,cs_ts,...
    TS2,R_LOA,r_ts,TS3);

% change idx to logical
idx = logical(idx1);

%%%%%%% VISUALIZATION OF RESULTS

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Plot ACCEPTABLE time series LoA1 :
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
if plots == 1;figure(32);
    h = plot(ch_ts(idx(:,1)==1,:)','LineWidth',0.5);
    hold on;
    hi = plot(ch_obs(:,1), ch_obs(:,2), 'ro', 'Markersize', 10);
    hold on
    hj = plot(ch_obs(:,1), chl_LOA, 'go', 'Markersize', 10);
    legend([h(1),hi(1),hj(1)],{'individual acceptable Chl simulations (LoA 1)', 'Chl observed',
'LoA'})
    xlabel('timestep (days)'); ylabel('Chl (mg/m^-^3)')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'ch_loa1'], 'jpg' );
end
```

```
if plots == 1
    % Load in the parameter file
    Xrec = load('example\PROTECH\OUTPUT_WSB_2008\pre-run1\OUTPARfacs.out')

    figure(25)
    scatter_plots(Xrec,GLF',[],'Fuzzy Wtg',X_Labels,idx(:,1)==1)
    legend('All','Acceptable')
    suptitle('GLUE acceptable simulations (LoA 1)')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'dottyloa1'], 'jpg' );
    % Plot the number of acceptable simulations based upon the LoA for the
    % timesteps over the evaluation period
    figure(45)
    subplot(2,1,1);plot(ch_ts'); tx = axis; tx(4) = 100;
    hold on
    plot(ch_ts(idx(:,1)==1,:)','k')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,2), 'k-','userdata', 'LoA')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,1), 'k-','userdata', '')
    ylabel('Chl (mg/m^-^3)')
    subplot(2,1,2);bar(TS,sum(id_LOA(:,:,1)')/N*100); axis(tx);
    hold on; h = plot(TS,0.0,'r^');% identify observation timesteps
    legend([h(1)],{'Observation Timsteps'})
    ylabel('Acceptable LOA1 (%)')
    suptitle('GLUE acceptable simulations LoA 1')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'loa1_TS'], 'jpg' );
end

% plot acceptable simulations for CS species

figure(33)
h = plot(obsCSR(:,1),obsCSR(:,4),'ro', 'Markersize', 10);
hold on
hi = plot(obsCSR(:,1),CS_LOA,'go', 'Markersize', 10);
hold on
hj = plot(1:365,sp3_ts(idx(:,1)==1,:)+sp4_ts(idx(:,1)==1,:));
legend([h(1),hi(1),hj(1)],{'CS Type Species observed',  'LoA','individual acceptable CS
simulations (LoA 1)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('CS Type Species - acceptable simulations LoA 1')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'CS_loa1'], 'jpg' );

% plot acceptable simulations for R species
figure(34)
h = plot(obsCSR(:,1),obsCSR(:,5),'ro','Markersize', 10);
hold on
hi = plot(obsCSR(:,1),R_LOA,'go','Markersize', 10);
hold on
hj = plot(1:365,sp1_ts(idx(:,1)==1,:)+sp2_ts(idx(:,1)==1,:)+...
    sp6_ts(idx(:,1)==1,:));
legend([h(1),hi(1),hj(1)],{'R Type Species observed',  'LoA','individual acceptable R simulations
(LoA 1)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('R Type Species - acceptable simulations LoA 1')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'R_loa1'], 'jpg' );


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Plot ACCEPTABLE time series LoA1 & LoA 2:
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
if plots == 1;
    figure(35);
    h = plot(ch_obs(:,1), ch_obs(:,2), 'ro','Markersize', 10);
    hold on
    hi = plot(ch_obs(:,1), chl_LOA, 'go','Markersize', 10);
    hold on
    hj = plot(ch_ts(idx(:,1)==1 & idx(:,2) ==1,:)');
    xlabel('timestep (days)'); ylabel('Chl (mg/m^-^3)')
```

```
    legend([h(1),hi(1),hj(1)],{'Chl observed',  'LoA','individual acceptable Chl simulations (LoA
1 & 2)'})
    title('GLUE acceptable simulations LoA 1 & LoA 2')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'ch_loa1_2'], 'jpg' );
end


if plots == 1
    figure(26)
    scatter_plots(Xrec,GLF',[],'Fuzzy Wtg',X_Labels,(idx(:,1) == 1 &...
        idx(:,2) == 1))
    legend('All','Acceptable')
    suptitle('GLUE acceptable simulations LoA 1 & LoA 2')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'dottyloa1_2'], 'jpg' );
    % Plot the number of acceptable simulations based upon the LoA for the
    % timesteps over the evaluation period
    figure(46)
    subplot(3,1,1);plot(ch_ts'); tx = axis; tx(4) = 100;
    hold on
    plot(ch_ts(idx(:,1)==1 & idx(:,2) ==1,:)','k')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,2), 'k-','userdata', 'LoA')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,1), 'k-','userdata', '')
    ylabel('Chl (mg/m^-^3)')
    subplot(3,1,2);bar(TS,sum(id_LOA(:,:,1)')/N*100); axis(tx);
    ylabel('Acceptable LoA1 (%)')
    hold on; h = plot(TS,0.0,'r^');% identify observation timesteps
    legend([h],{'Observation Timsteps'})
    subplot(3,1,3);bar(TS2,sum(id_LOA(1:length(TS2),:,2)')/N*100); axis(tx);
    ylabel('Acceptable LoA2 (%)')
    hold on; h = plot(TS2,0.0,'r^');% identify observation timesteps
    legend([h(1)],{'Observation Timsteps'})
    xlabel('Timestep')
    suptitle('GLUE acceptable simulations LoA 1 & LoA 2')

    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'loa1_2_TS'], 'jpg' );
end

% plot acceptable simulations for CS species LoA1 and LoA2
figure(36)
h = plot(obsCSR(:,1),obsCSR(:,4),'ro','Markersize', 10);
hold on
hi = plot(obsCSR(:,1),CS_LOA,'go','Markersize', 10);
hold on
hj = plot(1:365,sp3_ts(idx(:,1) == 1 & idx(:,2) == 1,:)+sp4_ts(idx(:,1) ==...
    1 & idx(:,2) == 1,:));
legend([h(1),hi(1),hj(1)],{'CS Type observed',  'LoA','individual acceptable CS Type simulations
(LoA 1 & 2)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('CS Type Species')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'CS_loa1_2'], 'jpg' );
% plot acceptable simulations for R species  LoA1 and LoA2
figure(37)
h = plot(obsCSR(:,1),obsCSR(:,5),'ro','Markersize', 10);
hold on
hi = plot(obsCSR(:,1),R_LOA,'go','Markersize', 10);
hold on
hj = plot(1:365,sp1_ts(idx(:,1) == 1 & idx(:,2) == 1,:)+...
    sp2_ts(idx(:,1) == 1 & idx(:,2) == 1,:)+...
    sp6_ts(idx(:,1) == 1 & idx(:,2) == 1,:));
legend([h(1),hi(1),hj(1)],{'R Type observed',  'LoA','individual acceptable R Type simulations
(LoA 1 & 2)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('R Type Species')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'R_loa1_2'], 'jpg' );

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Plot ACCEPTABLE time series LoA1, LoA2 & LoA 3:
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
if plots == 1;figure(30);
    h = plot(ch_obs(:,1), ch_obs(:,2), 'ro','Markersize', 10);
    hold on
    hi = plot(ch_obs(:,1), chl_LOA, 'go','Markersize', 10);
    hold on
    hj = plot(Pcnts(:,1:length(Pc)),'k','LineWidth',1.5);
    hold on
    hk = plot(ch_ts(idx(:,1)== 1 & idx(:,2) == 1 & idx(:,3) == 1,:)');
    xlabel('timestep (days)'); ylabel('Chl (mg/m^-^3)')
    legend([h(1),hi(1),hj(1), hk(1)],{'Chl observed',  'LoA','individual acceptable Chl
simulations (LoA 1, 2 & 3)'})
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'ch_loa1_2_3'], 'jpg' );
end

if plots == 1
    figure(27)
    scatter_plots(Xrec,GLF',[],'Fuzzy Wtg',X_Labels,(idx(:,1)==1 &...
        idx(:,2) ==1 & idx(:,3) == 1))
    legend('All','Acceptable')
    suptitle('GLUE acceptable simulations LoA , LoA 2 & LOA 3')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'dotty_loa1_2_3'], 'jpg' );
    % Plot the number of acceptable simulations based upon the LoA for the
    % timesteps over the evaluation period

    figure(47)
    subplot(4,1,1);plot(ch_ts'); tx = axis; tx(4) = 100;
    hold on
    plot(ch_ts(idx(:,1)==1 & idx(:,2)==1 & idx(:,3) == 1,:)','k')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,2), 'go','userdata', 'LoA')
    hold on
    plot(ch_obs(:,1), chl_LOA(:,1), 'go','userdata', '')
    ylabel('Chl (mg/m^-^3)')
    subplot(4,1,2);bar(TS,sum(id_LOA(1:length(TS),:,1)')/N*100); axis(tx);
    hold on; h = plot(TS,0.0,'r^');% identify observation timesteps
    legend([h(1)],{'Observation Timsteps'})
    ylabel('Acceptable LoA1 (%)')
    subplot(4,1,3);bar(TS2,sum(id_LOA(1:length(TS2),:,2)')/N*100); axis(tx);
    hold on; h =  plot(TS2,0.0,'r^');% identify observation timesteps
    legend([h(1)],{'Observation Timsteps'})
    ylabel('Acceptable LoA2 (%)')
    subplot(4,1,4);bar(TS3,sum(id_LOA(1:length(TS3),:,3)')/N*100); axis(tx);
    hold on; h = plot(TS3,0.0,'r^');% identify observation timesteps
    legend([h(1)],{'Observation Timsteps'})
    ylabel('Acceptable LoA3 (%)')
    xlabel('Timestep')
    suptitle('GLUE acceptable simulations LoA , LoA 2 & LoA 3')
    saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'TS_loa1_2_3'], 'jpg' );
end

% plot acceptable simulations for CS species based on all 3 LoA
figure(38)
h = plot(obsCSR(:,1),obsCSR(:,4),'ro', 'Markersize', 10);
hold on
hi = plot(obsCSR(:,1),CS_LOA,'go', 'Markersize', 10);
hold on
hj = plot(Pcnts(:,length(Pc)+1:2*length(Pc)),'k','LineWidth',1.5);
hold on
hk = plot(1:365,sp3_ts(idx(:,1)==1 & idx(:,2) ==1 & idx(:,3) == 1,:)+...
    sp4_ts(idx(:,1)==1 & idx(:,2) ==1 & idx(:,3) == 1,:));
legend([h(1),hi(1),hj(1),hk(1)],{'CS Type observed',  'LoA','Percentiles','individual acceptable
CS Type simulations (LoA 1, 2 & 3)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('Acceptable simulations LoA 1, 2 & 3 - CS Type Species')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'CS_loa1_2_3'], 'jpg' );

% plot acceptable simulations for R species
figure(39)
h = plot(obsCSR(:,1),obsCSR(:,5),'ro', 'Markersize', 10);
```

```
hold on
hi = plot(obsCSR(:,1),R_LOA,'go', 'Markersize', 10);
hold on
hj = plot(Pcnts(:,2*length(Pc)+1:3*length(Pc)),'k','LineWidth',1.5);
hold on
hk = plot(1:365,sp1_ts(idx(:,1)==1 & idx(:,2) ==1 & idx(:,3) == 1,:)+...
    sp2_ts(idx(:,1)==1 & idx(:,2) ==1 & idx(:,3) == 1,:)+...
    sp6_ts(idx(:,1)==1 & idx(:,2) ==1 & idx(:,3) == 1,:));
legend([h(1),hi(1),hj(1),hk(1)],{'R Type observed',  'LoA','Percentiles','individual acceptable R
Type simulations (LoA 1, 2 & 3)'})
ylabel('Chl (mg/m^-^3)')
xlabel('Timestep')
title('Acceptable simulations LoA 1, 2 & 3 - R Type Species')
saveas( gcf, [my_dir '/' 'Projects/' proj '/' 'R_loa1_2_3'], 'jpg' );


% plot 2D correlations for acceptable simulations (idx = 3)
C = ones(sum(sum(sum(idx')==3')),1);% this sets the symbols to a single colour
figure(22)
scatter_plots_interaction(Xrec(sum(idx')==3',:),C,[],X_Labels)
suptitle('2D Parameter Correlation - acceptable par values')


disp(['Number of simulations     =     ' num2str(N)])
disp(['Number of acceptable simulations LoA 1     =     ' ...
    num2str(sum(idx(:,1)))])
disp(['Number of acceptable simulations LoA 1 & 2     =     ' ...
    num2str(sum(idx(:,1) == 1 & idx(:,2) ==1))])
disp(['Number of acceptable simulations LoA 1, 2 & 3     =     ' ...
    num2str(sum(idx(:,1) == 1 & idx(:,2) ==1 & idx(:,3) ==1))])

% fprintf(fileID,['Number of acceptable simulations LoA 1     =     ' ...
%     num2str(sum(idx(:,1))) '\n']');
% fprintf(fileID,['Number of acceptable simulations LoA 1 & 2     =     ' ...
%     num2str(sum(idx(:,1) == 1 & idx(:,2) ==1)) '\n']');
% fprintf(fileID,['Number of acceptable simulations LoA 1, 2 & 3     =     '...
%     num2str(sum(idx(:,1) == 1 & idx(:,2) ==1 & idx(:,3) ==1)) '\n']');

% fclose(fileID); fclose('all');

fprintf(fileID,['RESULTS' '\n' 'Number of acceptable simulations     =     '...
    num2str(sum(idx(:,1))) '\n']');

fclose('all');
```

1.2 Audit Log associated with Workflow 11

MODELLING CONDITION LOG FOR PROJECT: PROTECH_GLUE_LOA 18-Jul-2022 16:54:25

AIM OF STUDY:

Identification of modelling uncertainties prior to development of forecasting version of model

MODEL NAME:

PROTECH

STUDY LOCATION:

Windermere

MODEL ALTERNATIVES CONSIDERED:

None

MODEL STRUCTURE OPTIONS:

Thermal structure of lake driven by daily observed temperature profiles

Daily timestep used

Constant lake depth used

MODEL EMULATOR CONSIDERED?

No

ASSUMPTIONS AND ADDITIONAL NOTES/COMMENTS

Algal species chosen to represent community

1 Oscillatoria

2 Asterionella

3 Anabaena

4 Aphanizomenon flos-aquae

5 Paulschulzia tenera

6 Melosira

7 Monoraphidium

8 Cryptomonas

MODELLING UNCERTAINTIES GENERAL

PRIMARY UNCERTAINTIES (MODEL STRUCTURE):

The model is a 1-dimensional representation of the lake and hence implicitly mixes laterally each model layer at each timestep. The daily timestep leads to uncertainties associated with sub-daily dynamics: e.g. temporary weak stratified periods which allow higher algal growth than may be expected given daily data.

PRIMARY UNCERTAINTIES (PARAMETERS):

Underwater light: aleatory (including variability in light extinction) and epistemic (related to lake mixing assumptions etc.) but treated as aleatory.

PRIMARY UNCERTAINTIES (INPUTS):

Nutrient inputs: epistemic & aleatory but treated as aleatory.

PRIMARY UNCERTAINTIES (CONSTRAINING OBSERVATIONS):

Chlorophyll-a observations are relaively well-known compared to the algal "count" data. The algal species conts are best treated as proportions of species in a relative way as absolute concentrations of individual species are difficult to eatimate from these data. Both datasets are only measured at weekly or fortnightly frequency such that between observation dynamics will be missed.

PRIMARY UNCERTAINTIES (OTHER):

Uncertainties assumed negligible given magnitude of primary uncertainties

Negligible Uncertainty 1: Hydrological fluxes and assumed dynamic steady-state (lake input = lake output & depth constant)

Negligible Uncertainty 2: No significant sediment-derived nutrient sources)

Negligible Uncertainty 3: Chosen algal species are an adequate representation of community structure)

Negligible Uncertainty 4: Physical and bathymetric parameters known and treated deterministically.

OBSERVATIONS FOR MODEL CONSTRAINT

SPECIFY THE OBSERVATIONS AVAILABLE FOR MODEL CONSTRAINT?

Chlorophyll-a concentrations; proportions of R-type functional species; CS-type functional species; CS-type functional species

WHAT ARE SPECIFIC UNCERTAINTIES ASSOCIATED WITH EACH VARIABLE (ALEATORY)

Chlorophyll a observations: sampling error associated with the integrated water samples themselves, analytical error associated with the laboratory-based chlorophyll measurement: estimated to be +/- 8WHAT ARE SPECIFIC UNCERTAINTIES ASSOCIATED WITH EACH VARIABLE (EPISTEMIC)

The uncertainty associated with spatial heterogeneity is more difficult to estimate and varies over time (Elliott and Defew, 2012) and between species (e.g. wind-blown cyanobacteria species can be particularly heterogeneous: George and Heaney, 1978); we estimated the overall error to be in the order of +/-25BASIS FOR ASSESSING GOODNESS OF FIT:

GLUE-LoA and Fuzzy Weightings.

Files containg LoA values copied to log folder

LoA1 = chlorophyll

LoA2 = R-type (species 1,2 and 6)

LoA1 = CS-type (species 3 and 4)

METHOD FOR COMBINATION OF MULTI-VARIABLE GOODNESS OF FIT:

Goodness of fit to chlorophyll concentrations used in addition to absolute LoA - calculated using trapezoidal fuzzy measure and combined with equal weighting as uncertainty ranges provide individual confidence weightings.

ASSUMPTIONS AND ADDITIONAL NOTES/COMMENTS:

INPUT(S), DEPENDENCIES & SAMPLING

MODEL INPUT (BOUNDARY CONDITION) UNCERTAINTY (ALEATORY):

The input uncertainties were not the focus of this excercise as the PROTECH model was being developed for forecasting purposes within an Enseble Kalman Filter (EKF). In the EKF the model inputs were updated as part of the data assimilation.

MODEL INPUT (BOUNDARY CONDITION) UNCERTAINTY (EPISTEMIC):

Not considered

UNCERT DISTRIBUTION(S) (ALEATORY):

Not considered

HOW ARE EPISTEMIC UNCERTAINTIES REPRESENTED?

Not considered

RATIONALE UNDERLYING DISTRIBUTIONS/SCENARIOS ETC. TO BE SAMPLED:

Not considered

DEPENDENCIES BETWEEN INPUTS :

None known or represented

ASSUMPTIONS AND ADDITIONAL NOTES/COMMENTS:

PARAMETERS, DEPENDENCIES & SAMPLING

CHOICE OF PARAMETERS TO SAMPLE & RATIONALE:

Uncertainty in model parameters (aleatory): Parameters chosen for analysis: epsw Pf Nf Sif Kz wwf . Parameters and ranges chosen from previous analyses.

PARAMETER UNCERTAINTY (ALEATORY):

Limits of Acceptability defined using observations and expert opinion including:

Sampling error

Spatial and temporal variability: incommensurability of point measurements

Knock-on effects during simulations

PARAMETER UNCERTAINTY (EPISTEMIC):

Implicit within parameter ranges but poorly known.

DEFINE METHOD FOR INCORPORATING PARAMETER DEPENDENCIES:

No dependencies represented.

AUTOMATIC ENTRIES

Number of simulations 1000

Parameters chosen for analysis epsw Pf Nf Sif Kz wwf

Parameter Distribution Chosen = unif

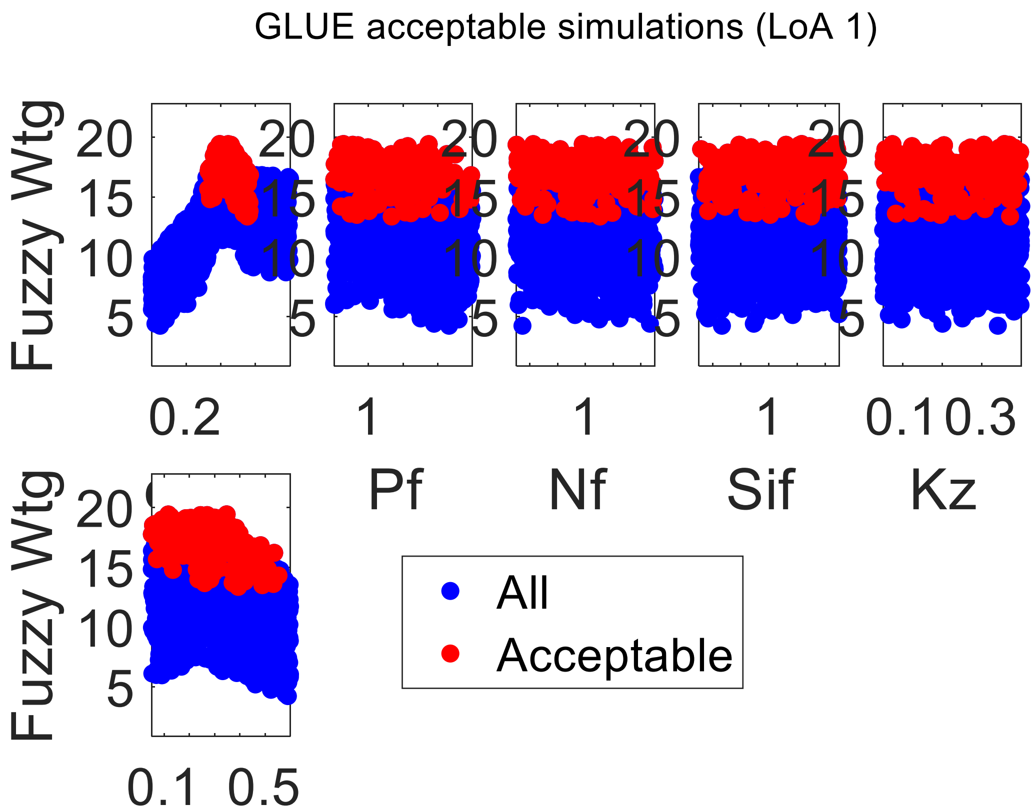
Minimum/Maximumparameter values =

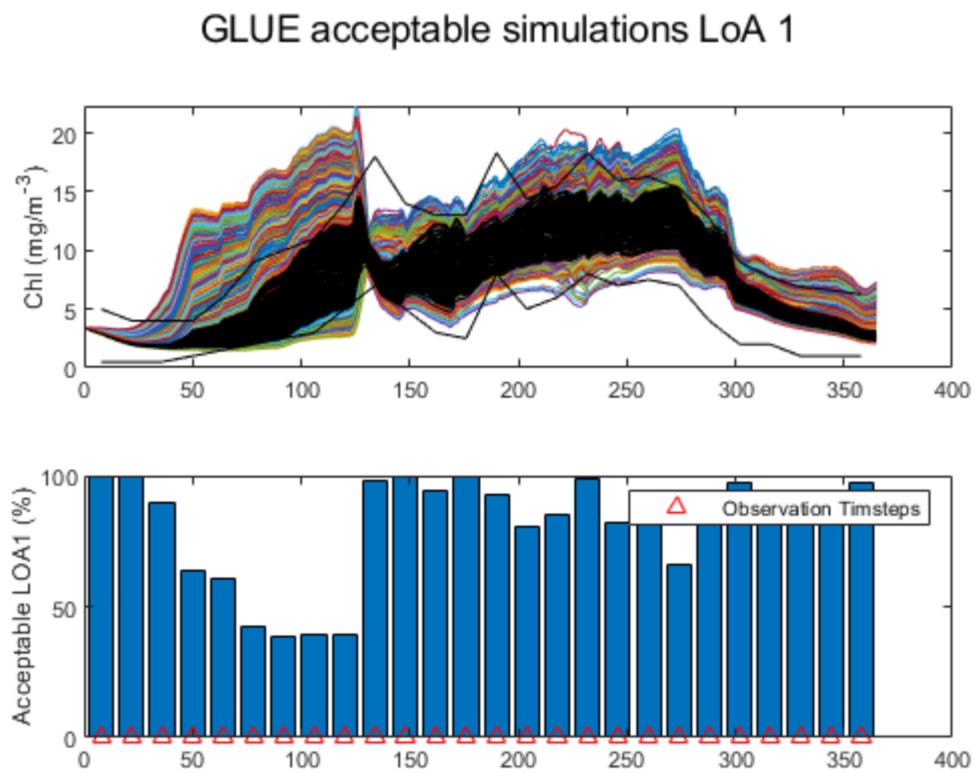
0.15	0.5	0.5	0.5	0.05	0.05
0.35	2.5	1.5	1.5	0.4	0.6

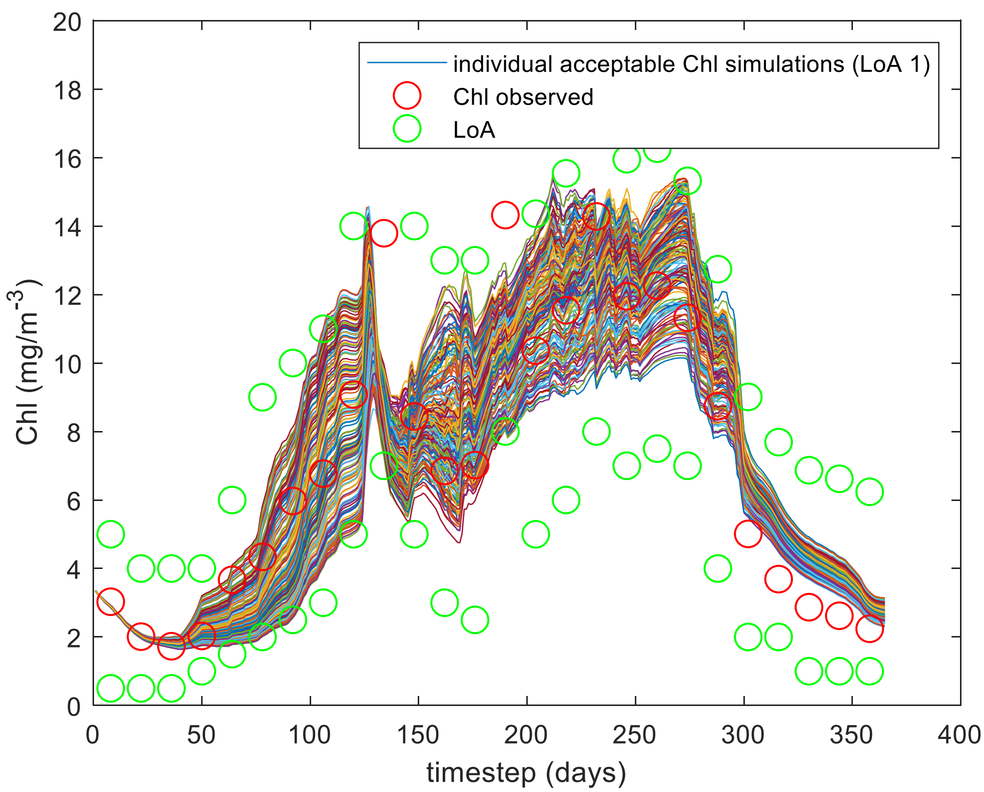
RESULTS

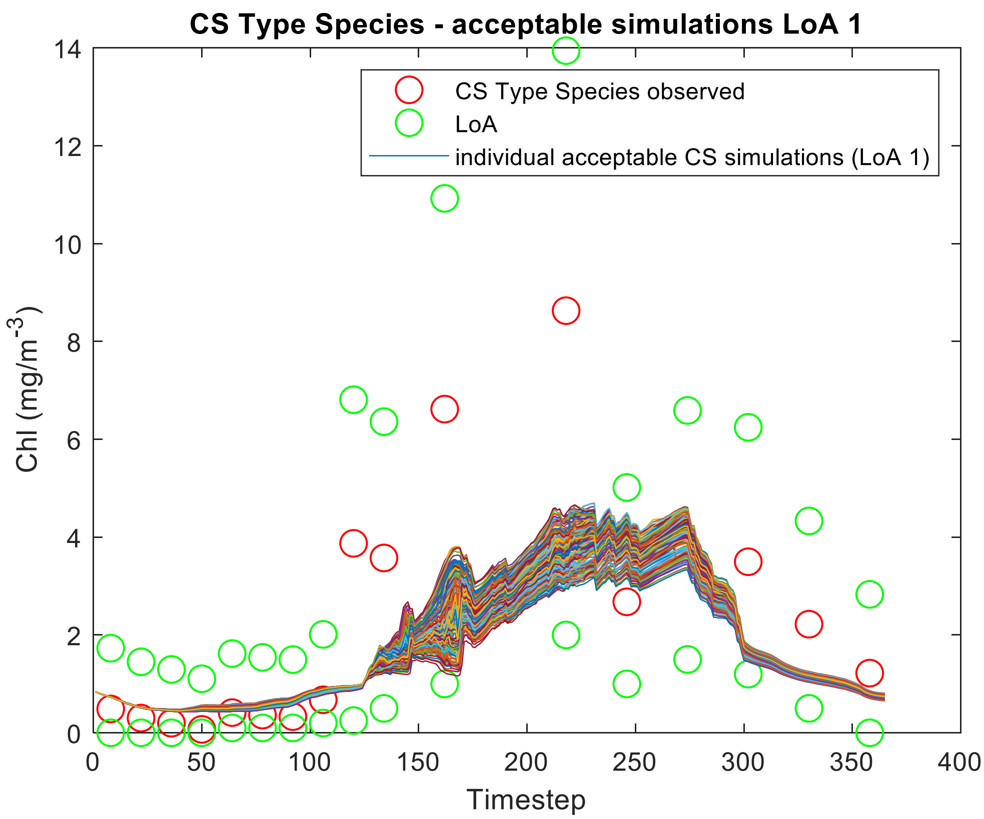
Number of acceptable simulations = 171

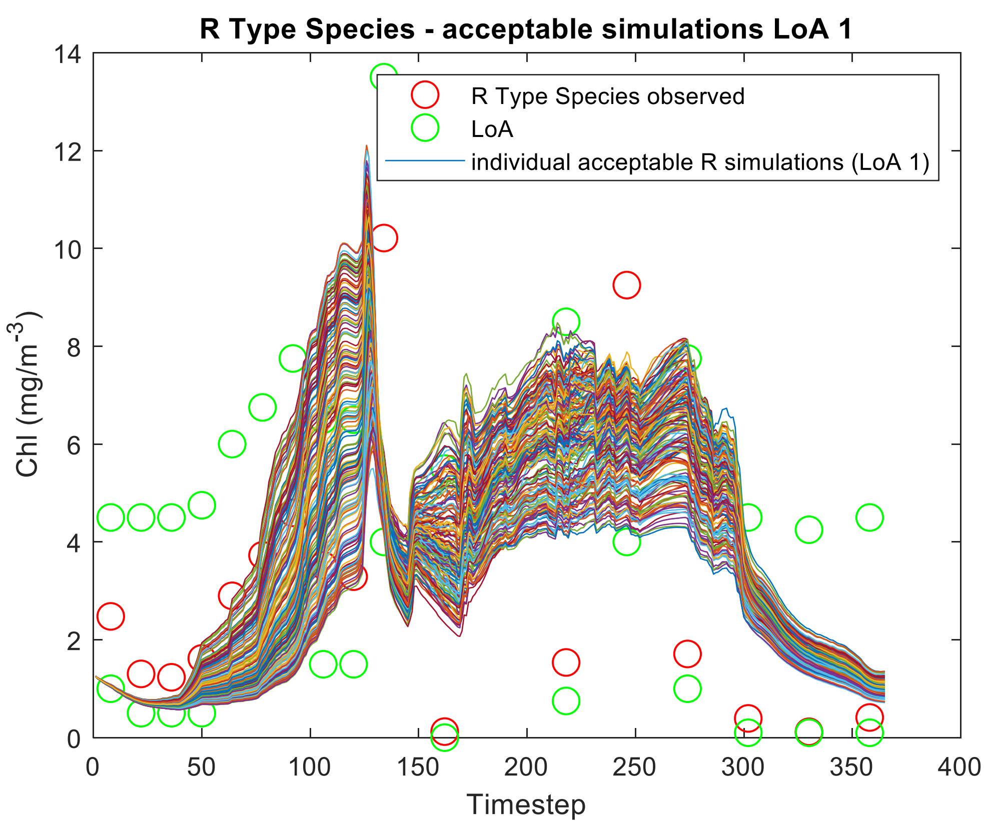
1.3 Figures associated with Workflow 11



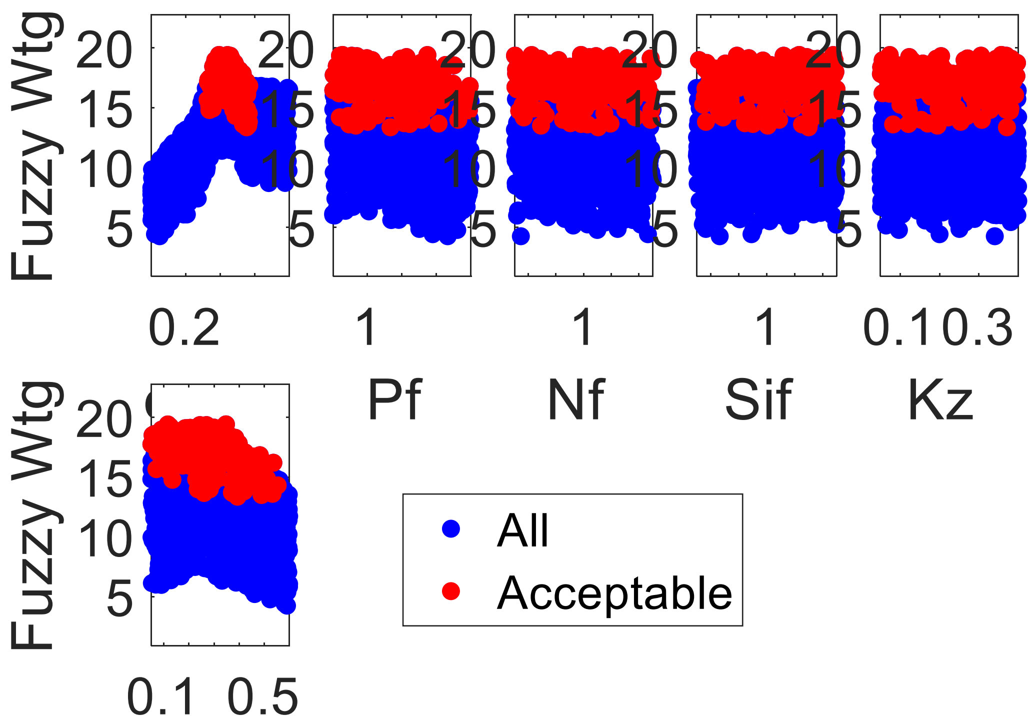

GLUE acceptable simulations LoA 1
Chl (mg/m^-3)
Acceptable LOA1 (%)
Observation Timsteps
0
50
100
150
200
250
300
350
400


individual acceptable Chl simulations (LoA 1)
Chl observed
LoA
Chl (mg/m^-3)
timestep (days)
0
50
100
150
200
250
300
350
400

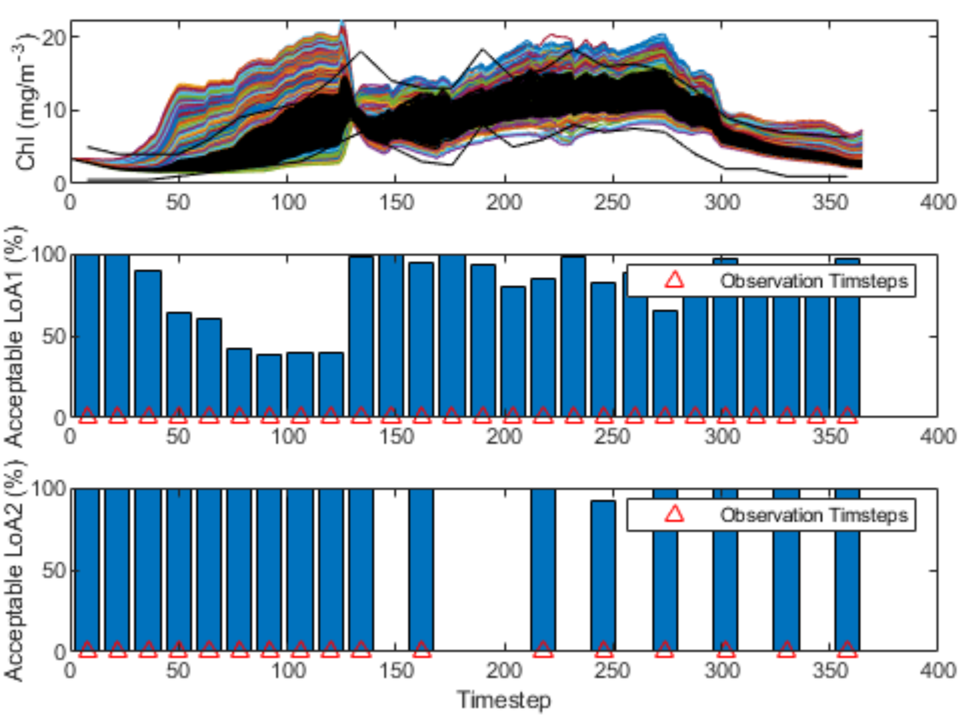

CS Type Species - acceptable simulations LoA 1
CS Type Species observed
LoA
individual acceptable CS simulations (LoA 1)
Chl (mg/m-3)
Timestep
0
2
4
6
8
10
12
14
0
50
100
150
200
250
300
350
400


R Type Species - acceptable simulations LoA 1
R Type Species observed
LoA
individual acceptable R simulations (LoA 1)
Chl (mg/m-3)
Timestep
0
2
4
6
8
10
12
14
0
50
100
150
200
250
300
350
400

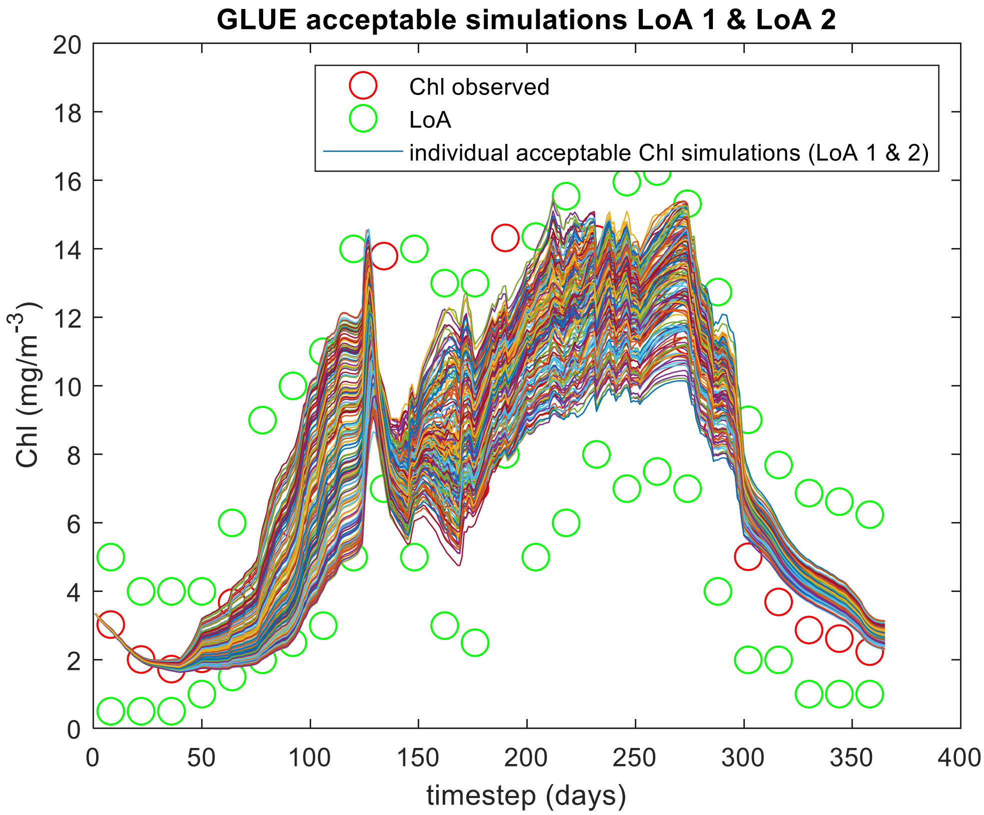
GLUE acceptable simulations LoA 1 & LoA 2



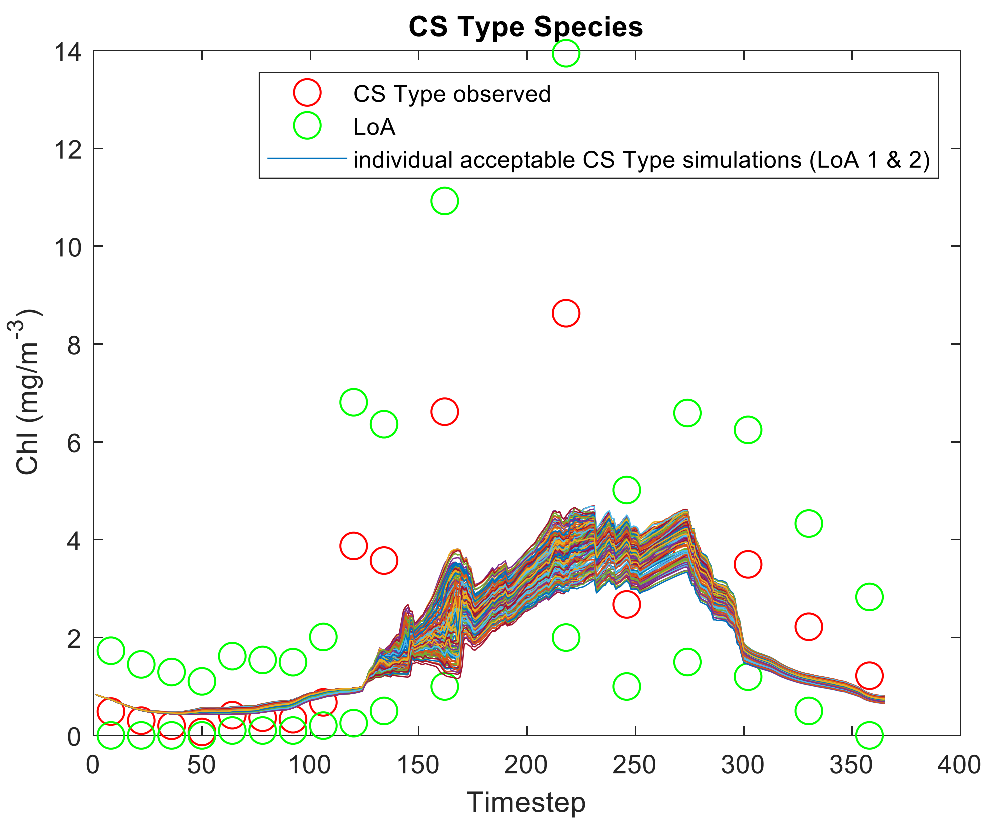
GLUE acceptable simulations LoA 1 & LoA 2

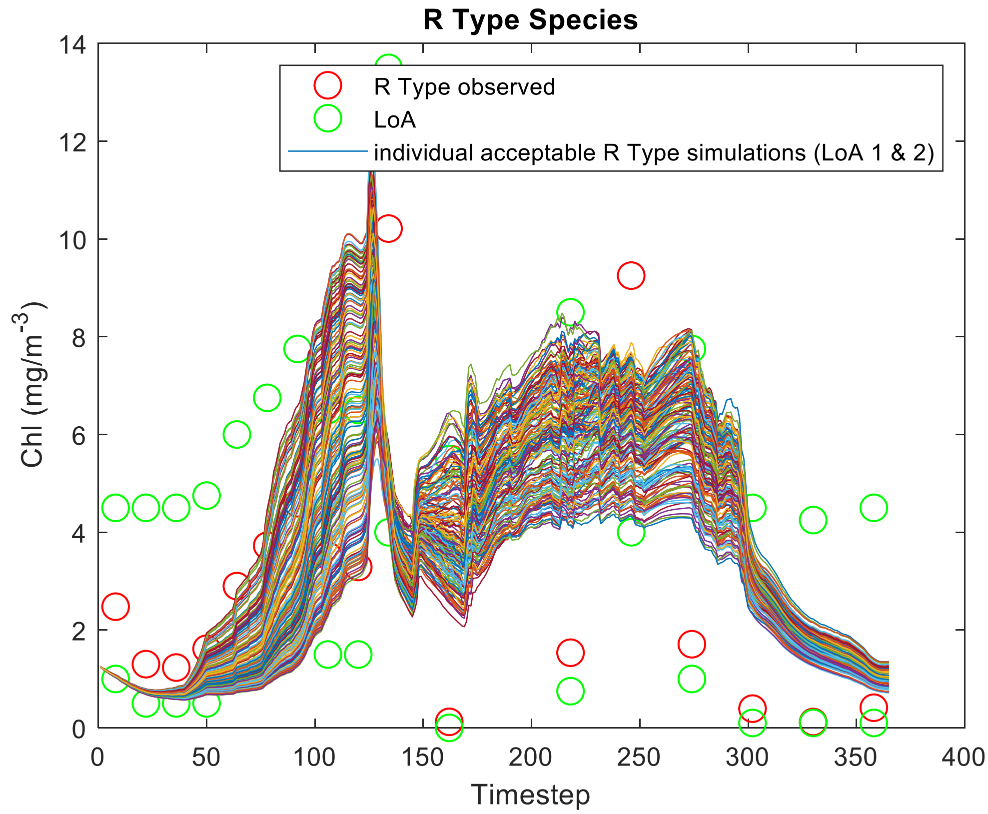


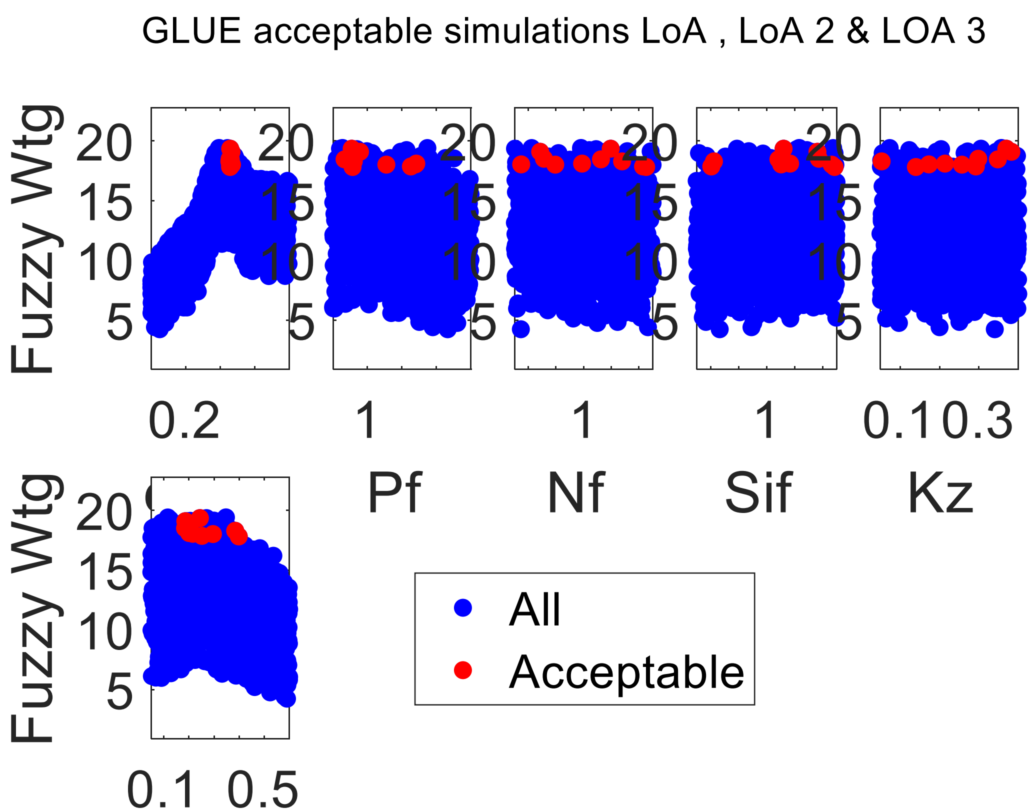
GLUE acceptable simulations LoA 1 & LoA 2

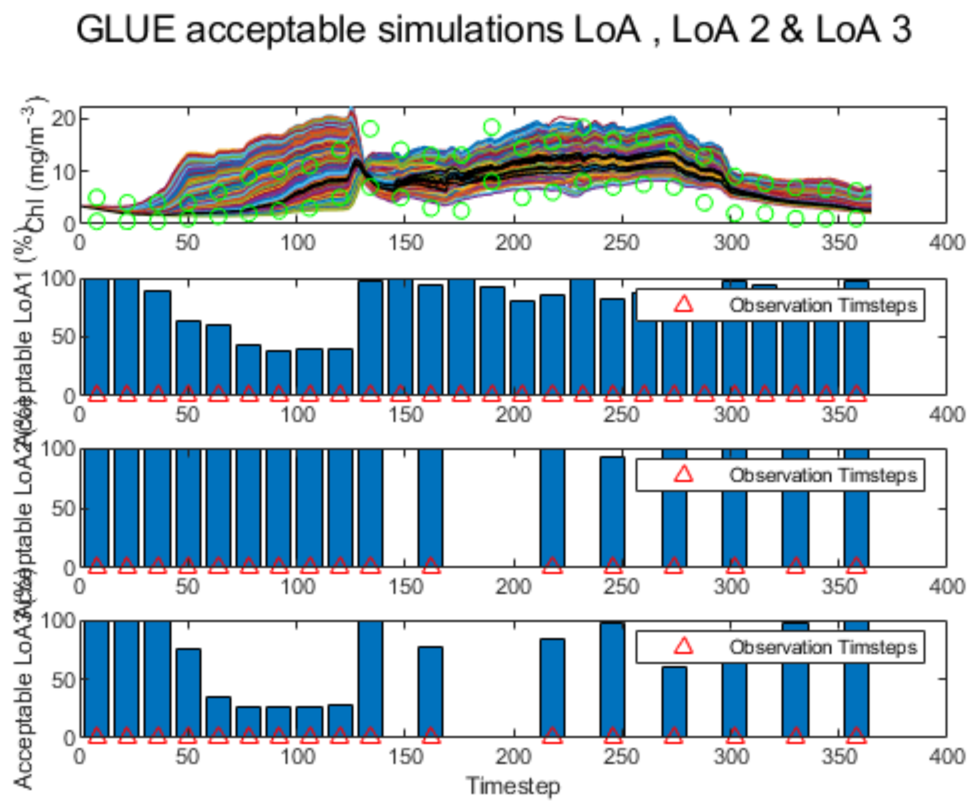


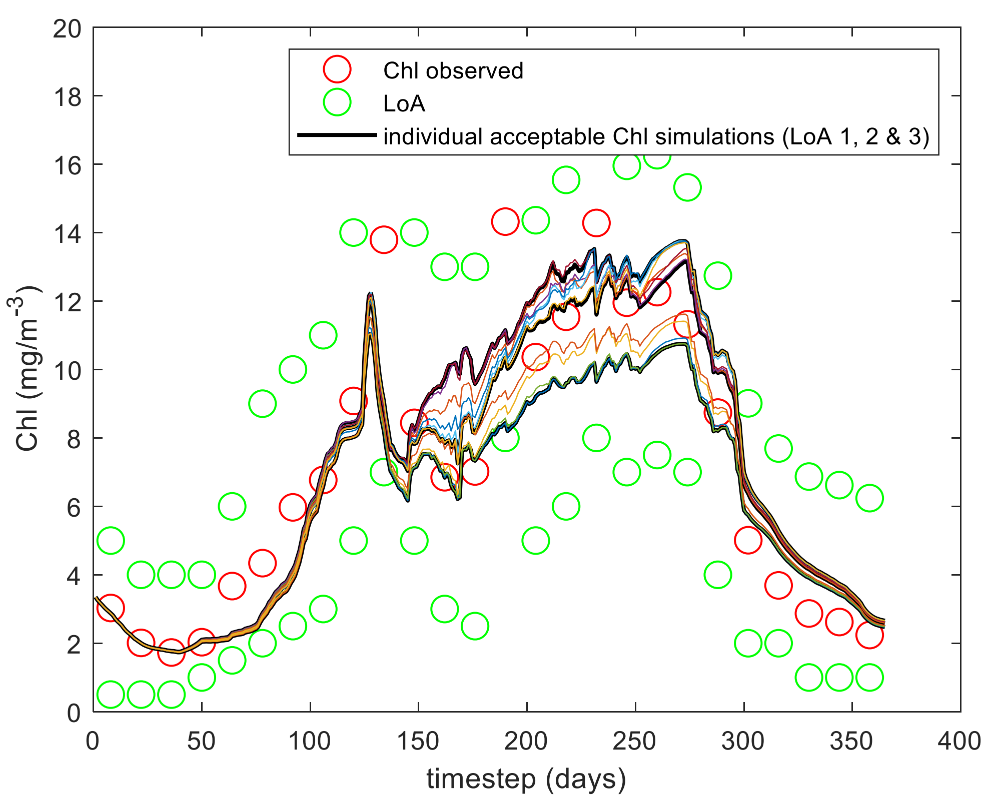
CS Type Species

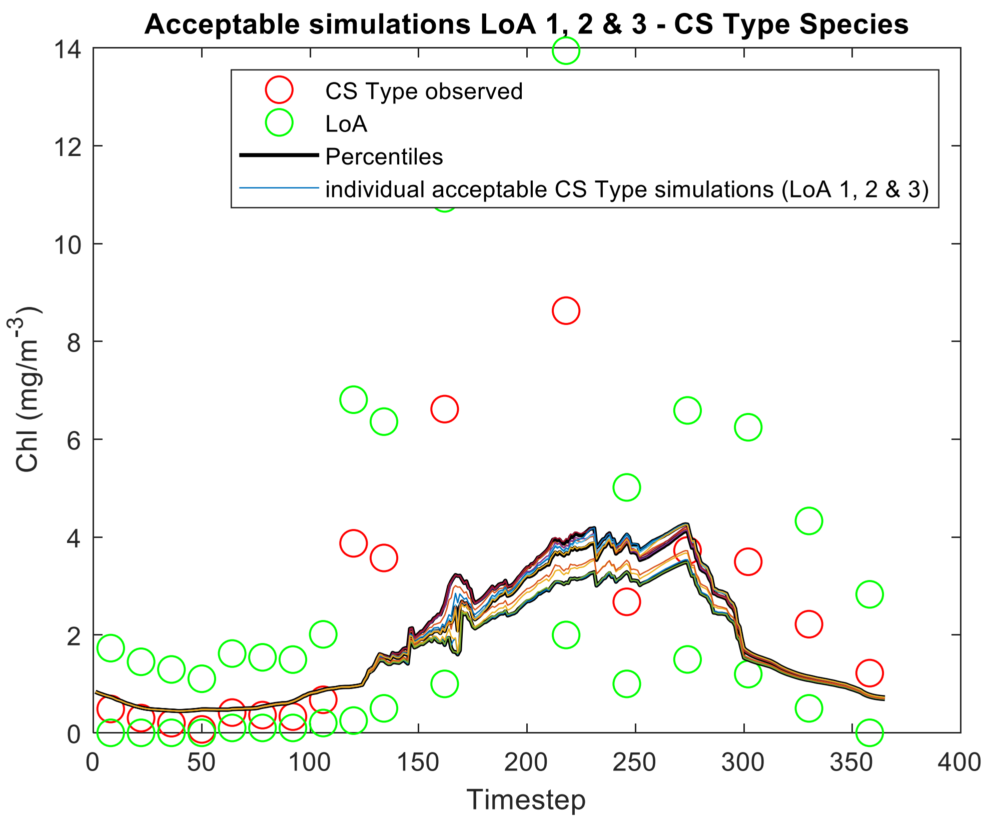



R Type Species
R Type observed
LoA
individual acceptable R Type simulations (LoA 1 & 2)
Chl (mg/m^-3)
Timestep
0
50
100
150
200
250
300
350
400
0
2
4
6
8
10
12
14

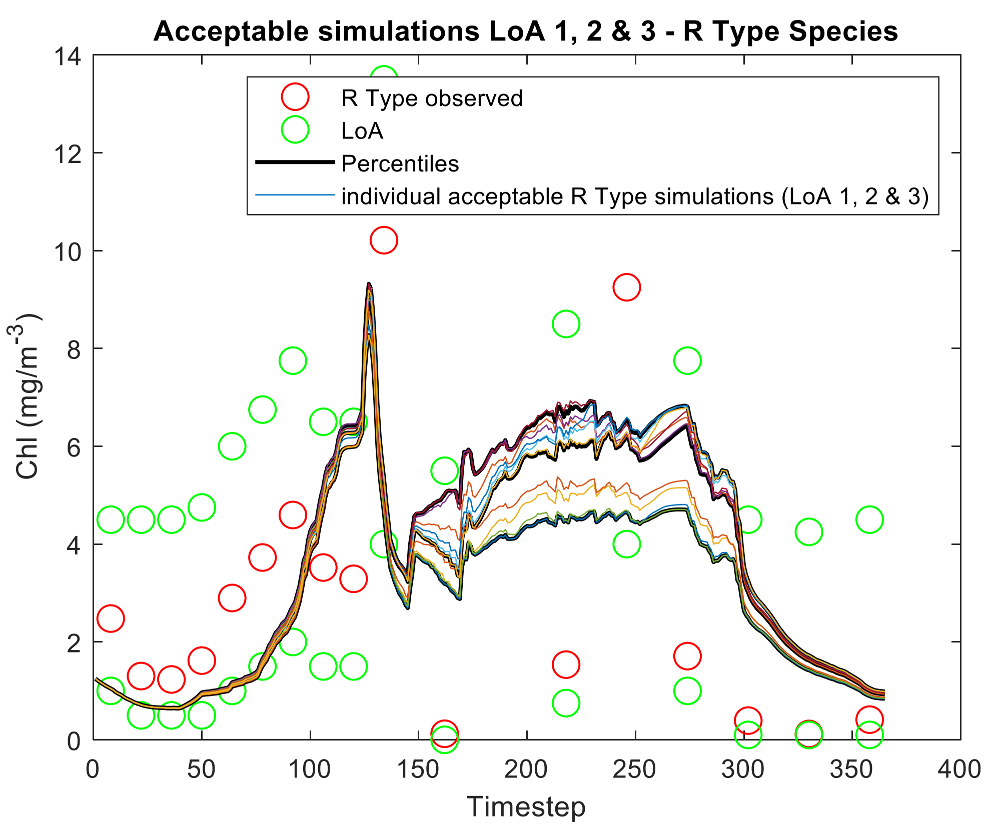

GLUE acceptable simulations LoA , LoA 2 & LOA 3
Fuzzy Wtg
20
15
10
5
0.2
1
Pf
1
Nf
1
Sif
0.1 0.3
Kz
Fuzzy Wtg
20
15
10
5
0.1 0.5
All
Acceptable


GLUE acceptable simulations LoA , LoA 2 & LoA 3
Chl (mg/m⁻³)
Acceptable LoA1 (%)
Acceptable LoA2 (%)
Acceptable LoA3 (%)
Observation Timsteps
Timestep


Chl observed
LoA
individual acceptable Chl simulations (LoA 1, 2 & 3)
Chl (mg/m⁻³)
timestep (days)



Acceptable simulations LoA 1, 2 & 3 - CS Type Species
CS Type observed
LoA
Percentiles
individual acceptable CS Type simulations (LoA 1, 2 & 3)
Chl (mg/m-3)
Timestep



Acceptable simulations LoA 1, 2 & 3 - R Type Species
R Type observed
LoA
Percentiles
individual acceptable R Type simulations (LoA 1, 2 & 3)
Chl (mg/m-3)
Timestep

2D Parameter Correlation - acceptable par values