OSTRICH Crash-Course
@ University of Waterloo

Juliane Mai

November 16, 2018

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Today's Outline

a. Introduction to Calibration

b. Introduction of OSTRICH toolbox

c. Single-objective calibration with DDS algorithm

↷ Exercise C_1

d. Multi-objective calibration with PA-DDS algorithm

↷ Exercise C_2

e.* Calibration using multiple cores (Parallel DDS/ PA-DDS)

↷ Exercise C_3 & C_4

Overview of Model Analysis Methods

Identification of
Model Deficits

Overview of Model Analysis Methods

Identification of
Model Deficits

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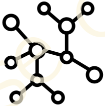
Reduction of
Model Complexity



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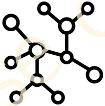

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Efficient
Model Calibration

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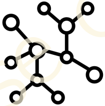

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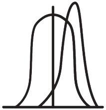
Estimation of
Model Uncertainty



Designed by Vecteezy

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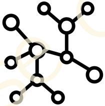

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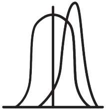

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Introduction of Calibration

– Example: Soil moisture data –

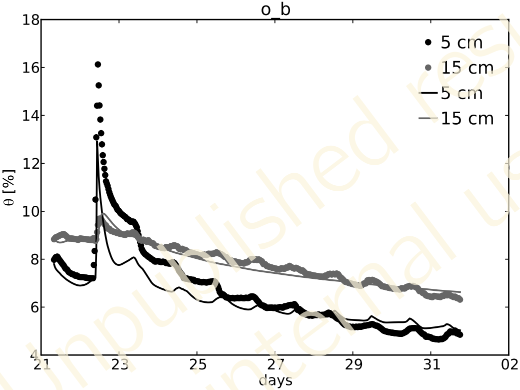

Figure: Observed and modeled soil moisture of an irrigation experiment in two depths. SCE was used to infer soil physics parameters. (Arndt Piayda @ UFZ Leipzig)

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Introduction of Calibration

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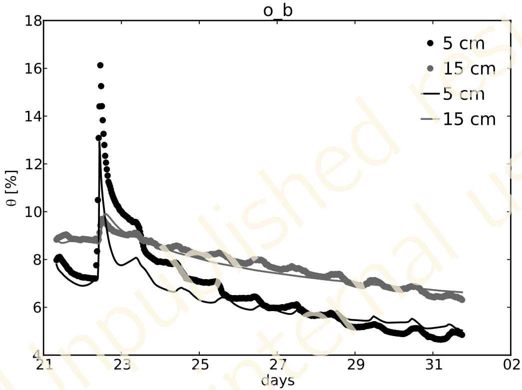

Cheap model

Dense data

No data error given

Multiple objectives

Different magnitude

Figure: Observed and modeled soil moisture of an irrigation experiment in two depths. SCE was used to infer soil physics parameters. (Arndt Piayda @ UFZ Leipzig)

Introduction of Calibration

– Example: Tree population and evolution –

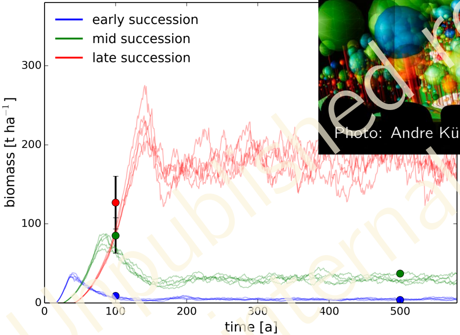

Photo: Andre Künzelmann

Figure: Observed and modeled tree populations (biomass) of three different species over 500 years. (Edna Rödig, Sebastian Lehmann @ UFZ Leipzig)

Introduction of Calibration

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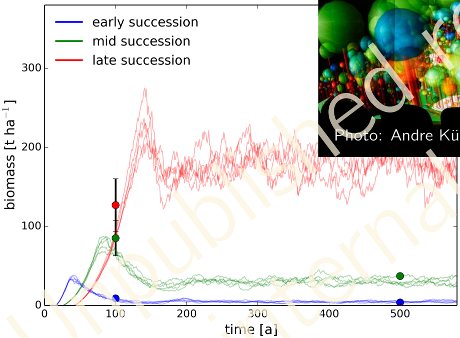

Data error known

Expensive model

Sparse data

Multiple objectives

Figure: Observed and modeled tree populations (biomass) of three different species over 500 years. (Edna Rödig, Sebastian Lehmann @ UFZ Leipzig)

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Introduction of Calibration

– Example: Cellular dynamics –

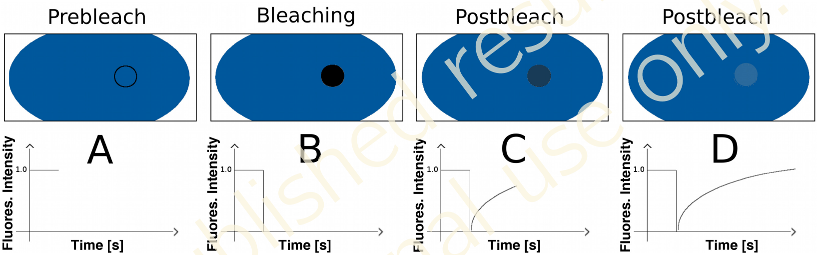

Figure: Experiment of Fluorescence Recovery After Photobleaching to determine diffusion and reaction rates in living cells (Juliane Mai @ UFZ Leipzig)

Introduction of Calibration

– Example: Cellular dynamics –

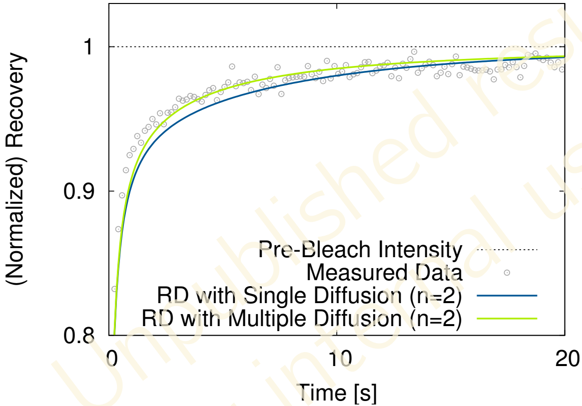

Figure: Fitting semi-analytical model functions to a biological measurements (Juliane Mai @ UFZ Leipzig)

Introduction of Calibration

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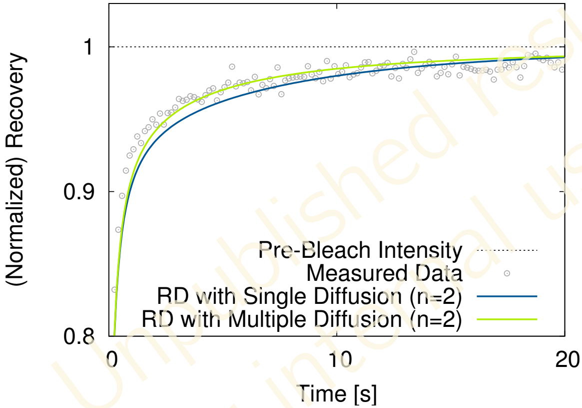

Cheap model

Dense data

Data error known

Model unknown

Over-parametrization

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Introduction of Calibration

– Example: Soil temperatures & moisture –

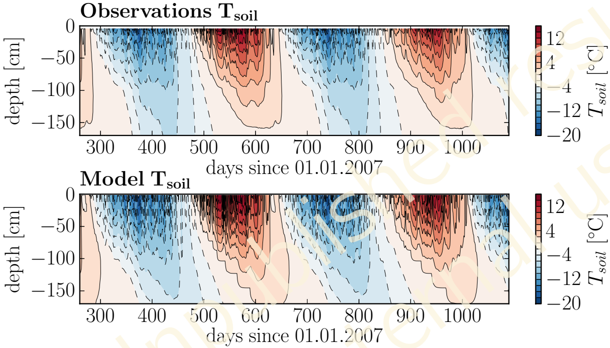

Figure: Calibrating WECan under permafrost conditions in Tianshuihai, China (Matthias Cuntz, Ute Wollschläger @ UFZ, Leipzig)

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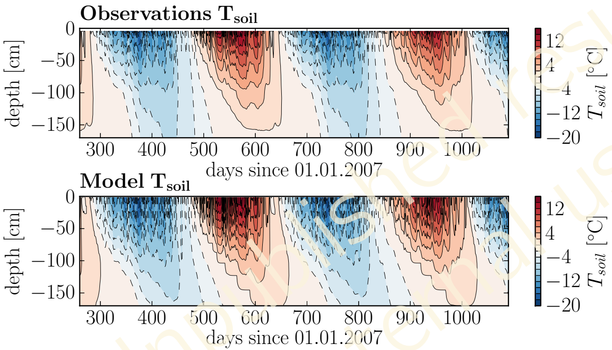

Expensive model

Multiple objectives

Spatio-temporal data

Irregular data

Data error not known

Figure: Calibrating WECan under permafrost conditions in Tianshuihai, China (Matthias Cuntz, Ute Wollschläger @ UFZ, Leipzig)

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Introduction of Calibration

– Example: Evapotranspiration –

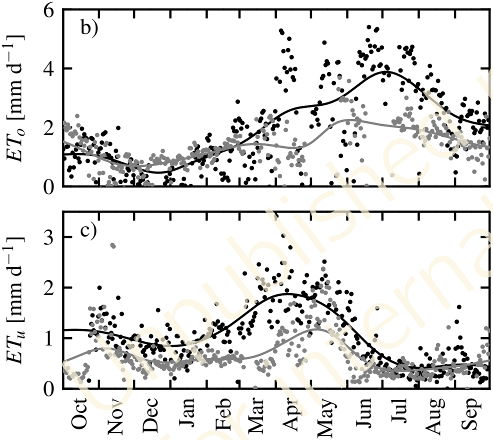

Figure: Smoothing daily sum of (b) ecosystem and (c) understorey ET using `kernel_regression`. (Arndt Piayda @ UFZ, Leipzig)

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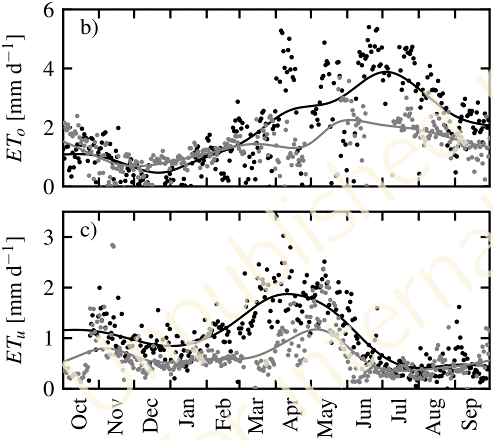

Dense data

Model not of interest

noisy data

Bin-width not known

Figure: Smoothing daily sum of (b) ecosystem and (c) understorey ET using `kernel_regression`. (Arndt Piayda @ UFZ, Leipzig)

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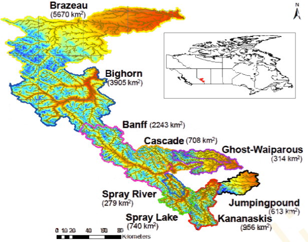
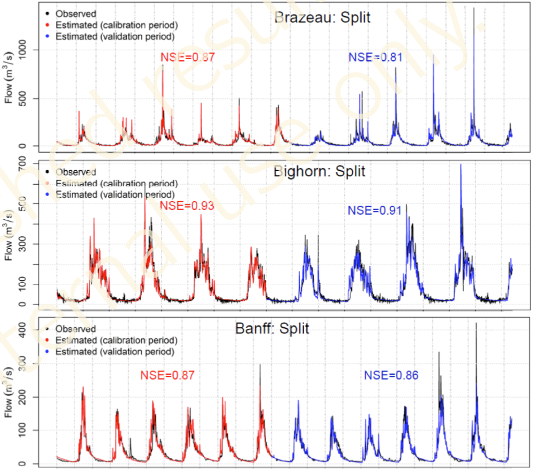
Introduction of Calibration
– Example: Streamflow modeling –





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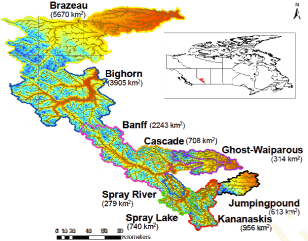

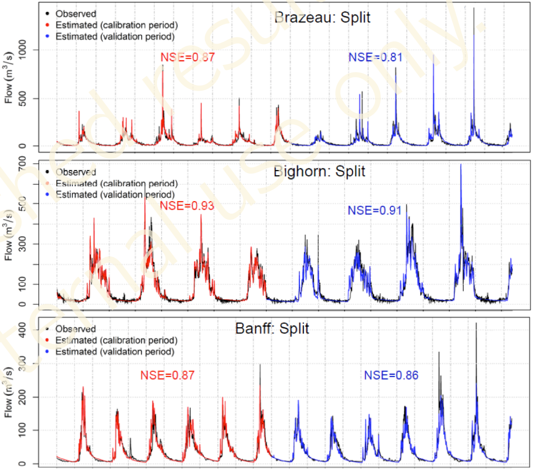

Dense data

Few parameters

Integral data

Data error unknown

Outliers

Multiple stations

Raven

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Introduction of Calibration

Minimize discrepancy between modeled variables and observations

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Introduction of Calibration

Minimize discrepancy between
modeled variables and observations

sounds easy, but:

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Introduction of Calibration

Minimize discrepancy between
modeled variables and observations

sounds easy, but:

- depends on model (version)
- depends on research question
- depends on location
- depends on budget
- depends on data availability
- ...

Introduction of Calibration

Minimize discrepancy between
modeled variables and observations

sounds easy, but:

- depends on model (version)
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- depends on location
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- ...

There's no recipe!
It's an art!
Be creative!

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Introduction of Calibration

– Main components: Objective function –

discrepancy measure = objective function

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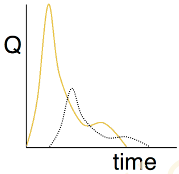

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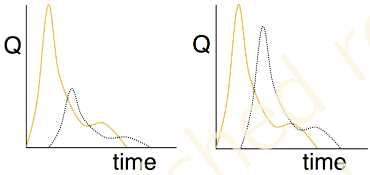

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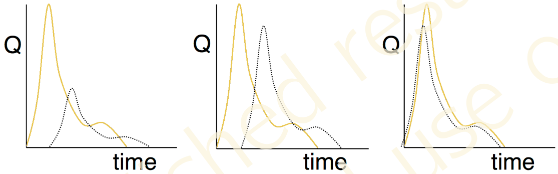

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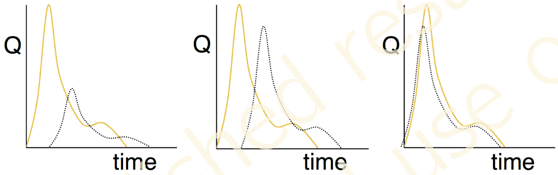

including:

- distance metric
  e.g., absolute error, squared difference, . . .
- combining multiple objectives
  e.g., bias, mean, variance, NSE, percent bias, . . .
- data error/ uncertainty handling
  e.g., likelihood, error model, . . .
- weighting of time steps/ multiple spatial units
  e.g., equal weighting, area weighting, seasonal weighting, . . .

Introduction of Calibration

– Main components: Identification of parameters and their ranges –

- identify parameters

  also: go through model code and find hidden hard-coded parameters
- define type of parameter distribution

  uniform distribution, Gaussian distribution, or any other distribution
- identify parameters of parameter distribution

  i.e., min/max for uniform, mean and variance for Gaussian distribution through literature review, iterative approach, physical or numerical boundaries

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↷ defines search domain for calibration

↷ the larger the domain, the harder/longer the search

↷ the smaller the domain, the more likely not to find global optimum

↷ find a balance

↷ revise your parameter space after first calibration runs

Introduction of Calibration

– Main components: Sampling of new candidates –

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Manual calibration

Automatic calibration

Introduction of Calibration

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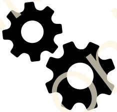

Manual calibration | **Automatic calibration**

- **subjective** choice of parameters and parameter ranges
- time willing to wait for answer (budget) is **subjective**

Introduction of Calibration

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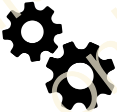
- **subjective** decision on selection of new candidates; random sampling very inefficient
- quality of result highly dependent on modeler mood, patience, curiosity

Introduction of Calibration

– Main components: Sampling of new candidates –

Manual calibration



Automatic calibration

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- time willing to wait for answer (budget) is **subjective**

Manual calibration:

- **subjective** decision on selection of new candidates; random sampling very inefficient
- quality of result highly dependent on modeler mood, patience, curiosity

Automatic calibration:

- **objective** generation of new candidates by algorithm: $\curvearrowright$ *core of algorithm!*
- subjective choice of calibration method and its algorithmic parameters

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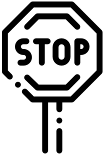
Introduction of Calibration
– Main components: Stopping criteria –



depends on calibration method
some approaches are:

- budget (= max. number of model evaluations) has been reached
- max. computing time has been elapsed
- independent (ensemble) parameter sets are similar enough
- improvement of objective function has not (significantly) changed over last iterations

Introduction to Calibration

– Main components: Analysis of calibration results –

don't trust blindly but analyze the calibration results by:

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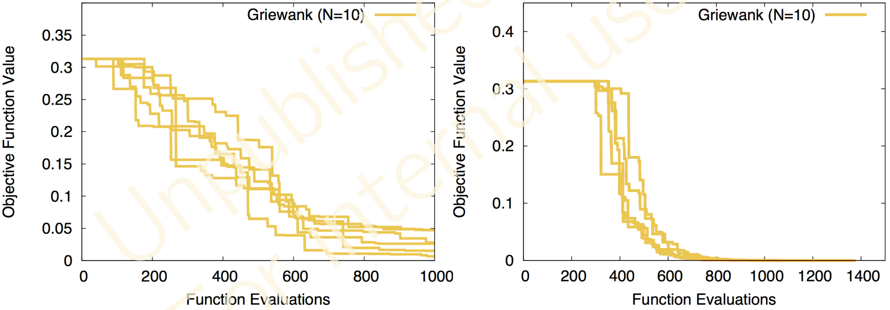
don't trust blindly but analyze the calibration results by:

- ✓ comparing results of independent calibration runs (multi-start)
  - ↷ helps to detect if algorithm ended up in local optimum



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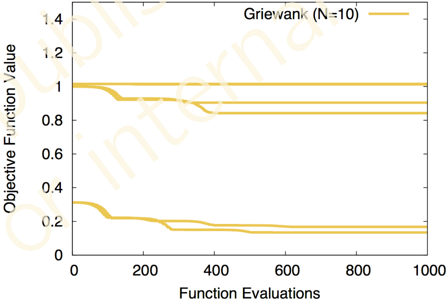

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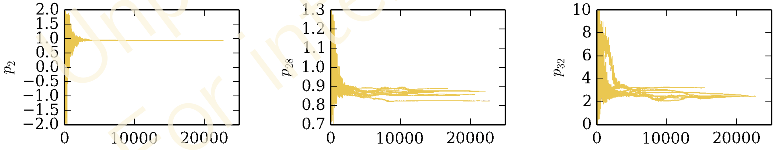
- ✓ testing different initial guesses (first parameter set)
  - ↷ helps to detect if algorithm ended up in local optimum
- ✓ analyzing how parameter values develop over course of calibration
  - ↷ helps to identify insensitive/ unidentifiable parameters
  - ↷ you might be able to identify parameter dependencies/ interactions



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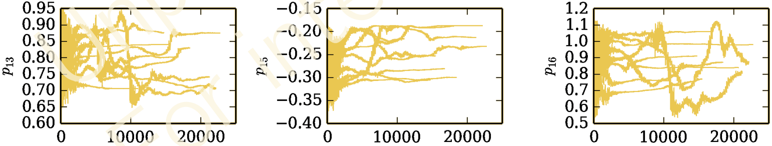

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- ✓ analyzing final parameter values
  - ↷ if values are at parameter boundary, revise the parameter search domain

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- ✓ analyzing final parameter values
  - ↷ if values are at parameter boundary, revise the parameter search domain
- ✓ checking (visually) match of optimal model run and observations
  - ↷ helps to see if objective function is suitable

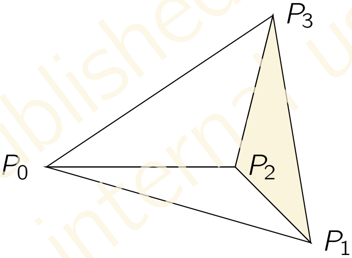
Introduction of Calibration

Some algorithms ...

Introduction of Calibration

– Algorithms: Nelder-Mead algorithm –

- method described by Nelder and Mead[1] and open-source[2]
- simplex = $(N+1)$ points in search space
- simplex is transformed over time

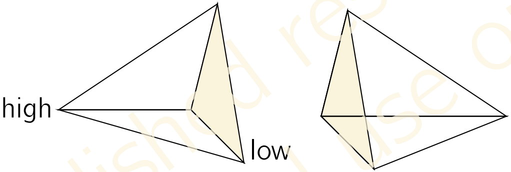


[1] Nelder, J.A., and Mead, R. 1965, Computer Journal, vol. 7, pp. 308–313.
[2] Numerical Recipes Fortran 77, Chap. 10.4, pp. 402-406.

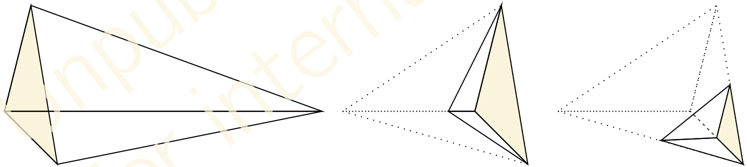
Introduction of Calibration

– Algorithms: Nelder-Mead algorithm –

possible simplex transformations:



(a) initial simplex (b) reflection



(c) reflection & expansion (d) contraction (e) multiple contraction

Introduction of Calibration
– Algorithms: Nelder-Mead algorithm –

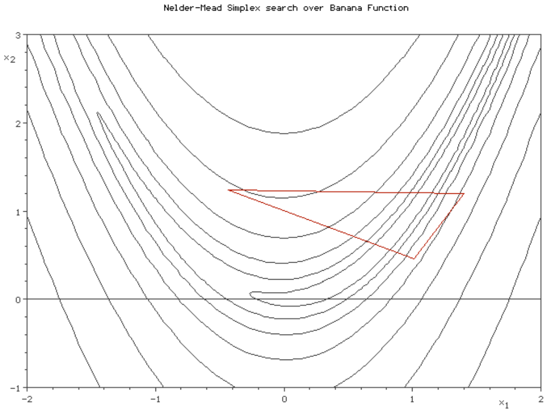


Figure: Nelder-Mead scheme

Introduction of Calibration
– Algorithms: Nelder-Mead algorithm –

- no possibility to escape local minimum
- several independent runs using same initial guess lead to same results
- Nelder-Mead performance depends on quality of initial guess
- use another optimization method to get good initial guess

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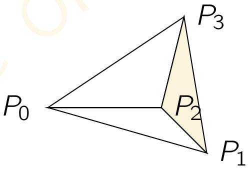
Introduction of Calibration

– Algorithms: Shuffled Complex Evolution (SCE) –

- introduced by Duan et al.[1]
- idea: multi-start Nelder-Mead with shuffeling of parameter sets after a number of evolution steps
- tuning parameters of SCE:
  - number of complexes
  - number of points in each complex
  - number of evolution steps before shuffling
  - number of points in sub-complex
  - ...



[1] Duan QY, Gupta VK, and Sorooshian S 1993, J. Opt. Theory and App., vol. 76, pp. 501-521.

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Introduction of Calibration

– Algorithms: Dynamically Dimensioned Search (DDS) –

- DDS algorithm described by Tolson & Shoemaker:

WATER RESOURCES RESEARCH, VOL. 43, W01413, doi:10.1029/2005WR004723, 2007

Dynamically dimensioned search algorithm for computationally efficient watershed model calibration

Bryan A. Tolson[1] and Christine A. Shoemaker[2]

Received 10 November 2005; revised 25 May 2006; accepted 31 August 2006; published 17 January 2007.

- Stochastic global optimization algorithm – a direct search method
- Originally designed for automatic calibration of environmental simulation models:
  - **Simple to implement** & no parameter-tuning needed
  - Generate calibrated model in **modeller's time frame**
  - Calibration objective is to **find good or acceptable solutions**, not globally optimal solution

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Introduction of Calibration

– Algorithms: Dynamically Dimensioned Search (DDS) –

STEP 1. Define DDS setup parameters for D dimensional problem

- neighborhood perturbation size parameter r ($r = 0.2$)
- maximum # of function evaluations, m

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STEP 2. Evaluate objective function at initial solution

STEP 3. Randomly select a subset of the D decision variables for perturbation from the current best solution

- size of subset decreases as maximum function eval. limit m approached

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Introduction of Calibration

– Algorithms: Dynamically Dimensioned Search (DDS) –

STEP 1. Define DDS setup parameters for D dimensional problem

- neighborhood perturbation size parameter r ($r = 0.2$)
- maximum # of function evaluations, m

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- perturbations beyond decision variable boundary reflected

UNIVERSITY OF WATERLOO

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STEP 6. Update function evaluation counter, $i = i + 1$, and check stopping criterion:

- IF $i = m \mapsto$ STOP
  ELSE repeat STEP 3.

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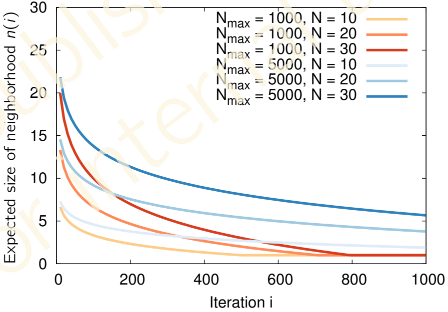
Introduction of Calibration

– Algorithms: Dynamically Dimensioned Search (DDS) –

Expected number of parameters n changed during an iteration depends on current iteration i, budget N_{max} and total number of parameters N:

$$n(i) = \text{Max}\left[N \cdot (1 - \frac{\ln(i)}{\ln(N_{max})}), 1\right]$$



Introduction of Calibration

– Algorithms: Pareto-Archived Dynamically Dimensioned Search (PA-DDS) –

Introduction of Calibration

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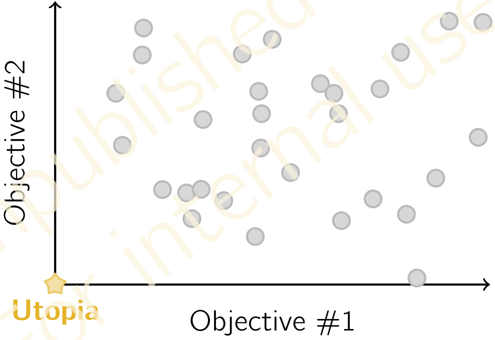
Fundamental multi-objective concept is **non-dominance** in objective function space



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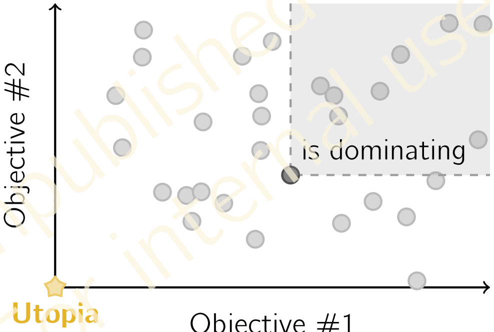

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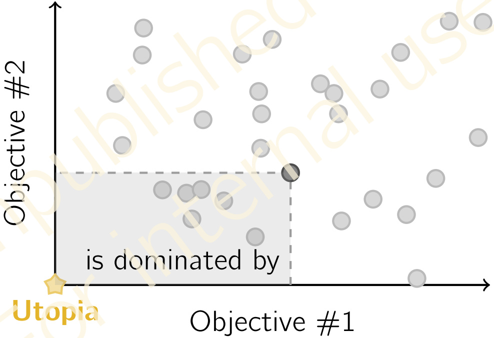

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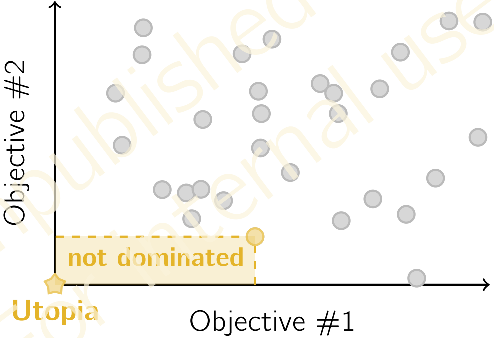

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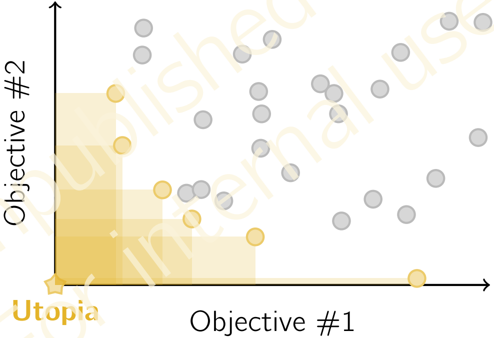

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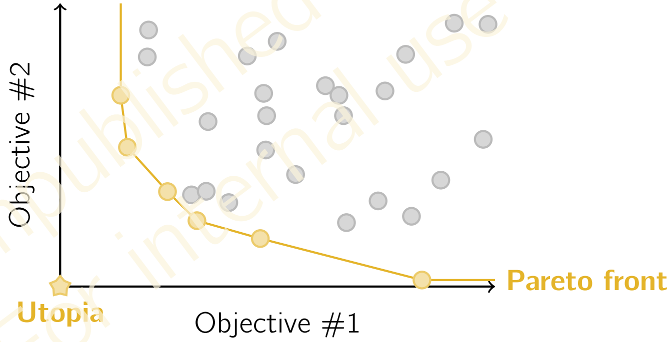

Introduction of Calibration

– Algorithms: Pareto-Archived Dynamically Dimensioned Search (PA-DDS) –

How to create new candidate solution?

- algorithm specific

Introduction of Calibration

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Introduction of Calibration

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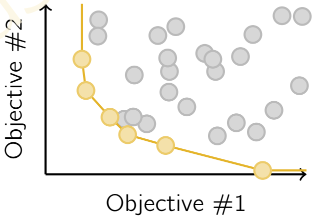

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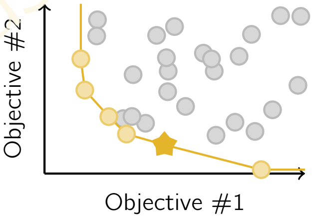

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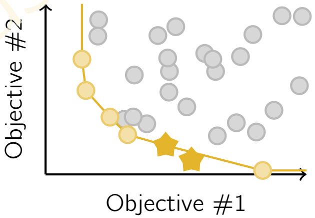

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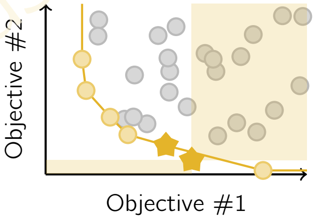

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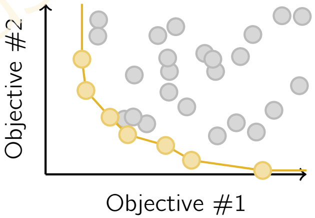

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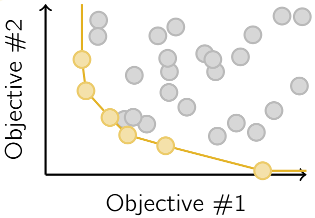

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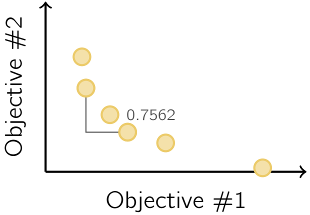

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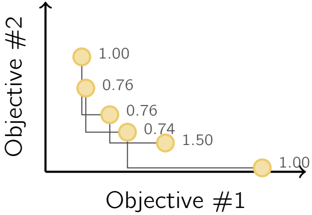

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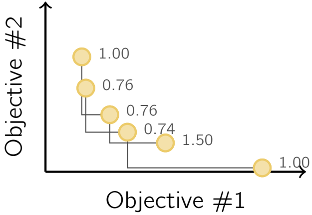

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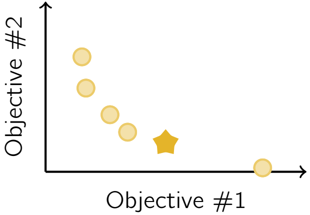

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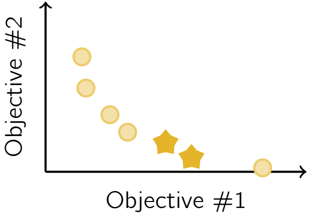

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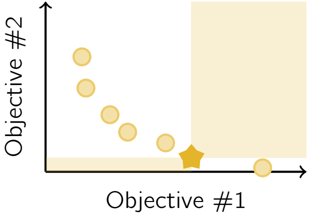

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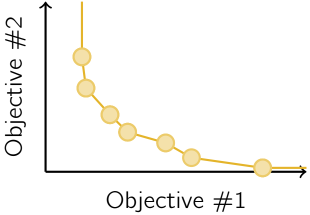

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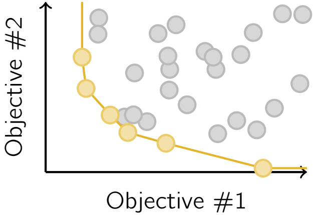

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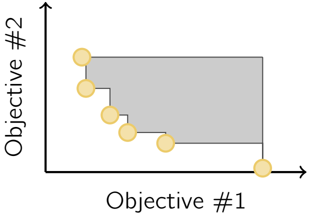

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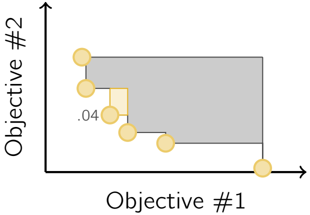

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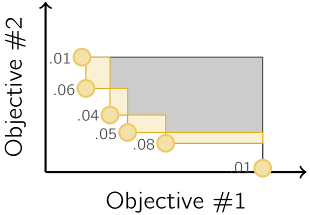

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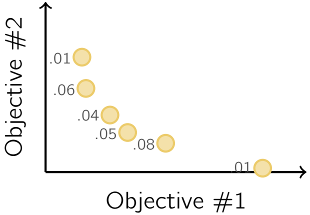

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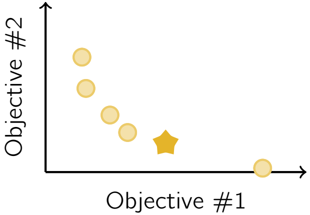

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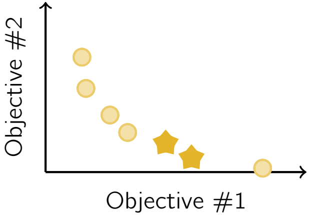

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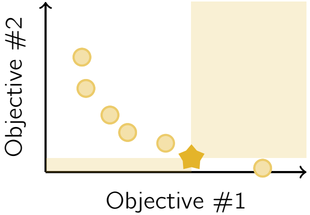

UNIVERSITY OF WATERLOO

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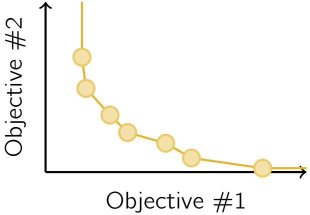

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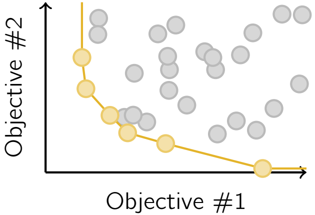

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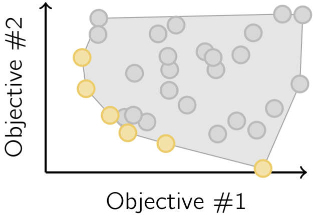

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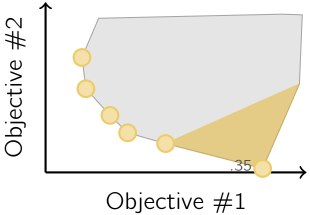

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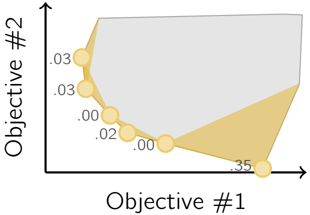

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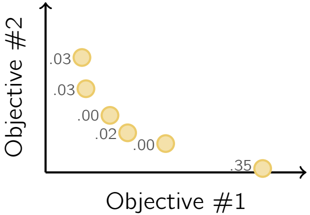

Introduction of Calibration

– Algorithms: Pareto-Archived Dynamically Dimensioned Search (PA-DDS) –

How to create new candidate solution?

- algorithm specific
- PA-DDS offers multiple options to select solution
  - Random
  - Crowding Distance CD: Asadzadeh & Tolson (2009) *Conf Gen & Evol Comp*
  - Hyper-volume contribution HVC: Asadzadeh & Tolson (2013) *Eng Opt*
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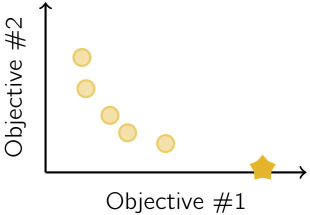

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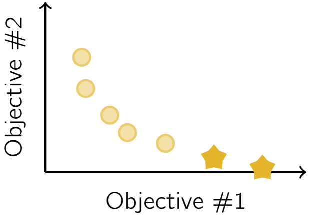

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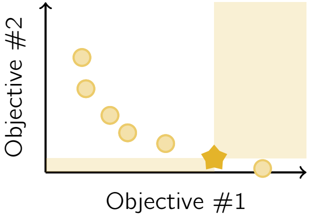

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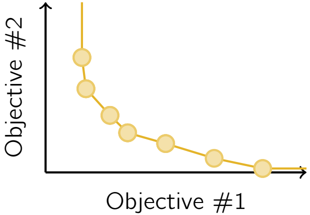
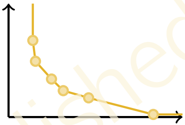
    - Choose Pareto solution based on CHC
    - Perturb associated parameter set and evaluate its objectives
    - Check non-dominance of new objective set
    - Update Pareto Front (if necessary)



Introduction of Calibration

– Algorithms: Pareto-Archived Dynamically Dimensioned Search (PA-DDS) –

Step 1. use MO **optimizer** to find multiple non-dominated (Pareto optimal) solutions



Step 2. modeler becomes **decision-maker**:
picking one of the above solutions as the final calibration solution (multi-criteria decision making)

Introduction of Calibration

And many more algorithms ...

Introduction of Calibration

And many more algorithms ...

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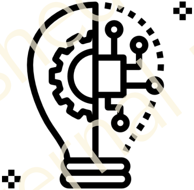
Introduction of Calibration

And many more algorithms ...



Introduction of OSTRICH

(Hydrologic) Model

RAVEN
GR4J
HBV
mHM
...

Optimizer

DDS
PA-DDS
Nelmin
SCE
...

Introduction of OSTRICH

(Hydrologic) Model $\xrightarrow{\text{Objective Function Value}}$ Optimizer

(Hydrologic) Model	Optimizer
RAVEN	DDS
GR4J	PA-DDS
HBV	Nelmin
mHM	SCE
...	...

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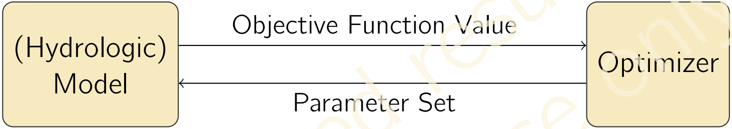

RAVEN	DDS
GR4J	PA-DDS
HBV	Nelmin
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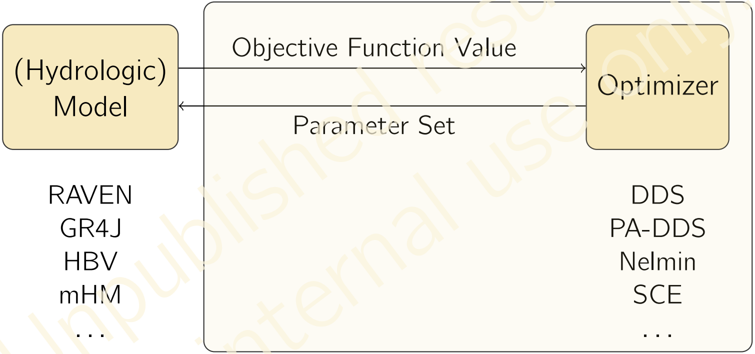
...	...

Introduction of OSTRICH



Framework provided by OSTRICH toolbox

Introduction of OSTRICH

Introduction of OSTRICH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OSTRICH - Optimization Software Toolkit
developed by L. Shawn Matott (University of Buffalo)
includes various optimization, sensitivity and uncert. analysis algorithms

webpage: `http://www.eng.buffalo.edu/~lsmatott/Ostrich/OstrichMain.html`
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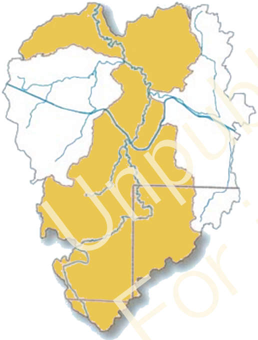
Introduction of OSTRICH

– Exercise C_1 –

- Irondequoit creek watershed (326 km^2) in New York State, USA draining into Lake Ontario
- Raven tutorial model using simple lumped model (GR4J)
- maximize Nash-Sutcliffe efficiency at outlet using DDS algorithm



Introduction of OSTRICH

– The setup file ostIn.txt –

```
# Optimization algorithm
ProgramType            [ DDS | PADDS | SCE | ... ]

# Objective function type
ObjectiveFunction      [ GCOP | WSSE ]

# Script that runs model
ModelExecutable        ./Ost-RAVEN.sh | Ost-RAVEN.bat

# Optional: Script that conserves model runs with
#           currently best parameter set
PreserveBestModel      ./save_best.sh | save_best.bat
```

Introduction of OSTRICH

– The setup file ostIn.txt –

```
# calibration will work in seq. and parallel mode
ModelSubdir processor_

# list all directories that contain information
# required to run model
BeginExtraDirs
  model
EndExtraDirs

# name of template files and their proper final
# name required by model
BeginFilePairs
  Irondequoit.rvp.tpl; Irondequoit.rvp
EndFilePairs
```

Introduction of OSTRICH

– The setup file ostIn.txt –

```
# parameter/ decision variable specification
BeginParams
   # param.  init.    low  high    tx_in  tx_ost  tx_out
    par_x1   random   0.01  2.5     none   none    none
    par_x2   random   −15    10     none   none    none
    par_x3   random    10   700     none   none    none
    par_x4   random     0     7     none   none    none
    par_x5   random     1    30     none   none    none
    par_x6   random     0     1     none   none    none
EndParams
```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Introduction of OSTRICH

– The setup file ostIn.txt –

```
# Specify the response variables in model output.
BeginResponseVars
  # name filename                keyword   line col token
  NSE   ./model/result.csv;  OST_NULL  1    4    ','
EndResponseVars

# (Optional) Modify response variables
BeginTiedRespVars
  NegNS 1 NS wsum -1.00
EndTiedRespVars

# Specify objective function
BeginGCOP
  CostFunction      NegNS
  PenaltyFunction  APM
EndGCOP
```

Introduction of OSTRICH

– The setup file ostIn.txt –

```
# (Optional) Random seed control
RandomSeed 123

# Algorithm should be last in this file
# --> Look up algorithm specific settings in manual
BeginDDSAlg
    PerturbationValue 0.20
    MaxIterations       50
    UseRandomParamValues
   # (optional) intialize DDS to parameter
   # values in initial model input files
    UseInitialParamValues
EndDDSAlg
```


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Introduction of OSTRICH

– Exercise C_1 –

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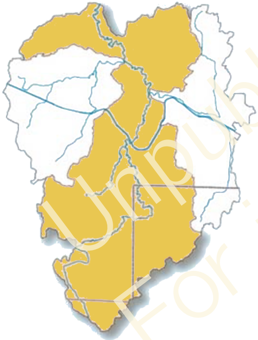

Walkthrough and tasks can be found on your exercise sheet C_1!

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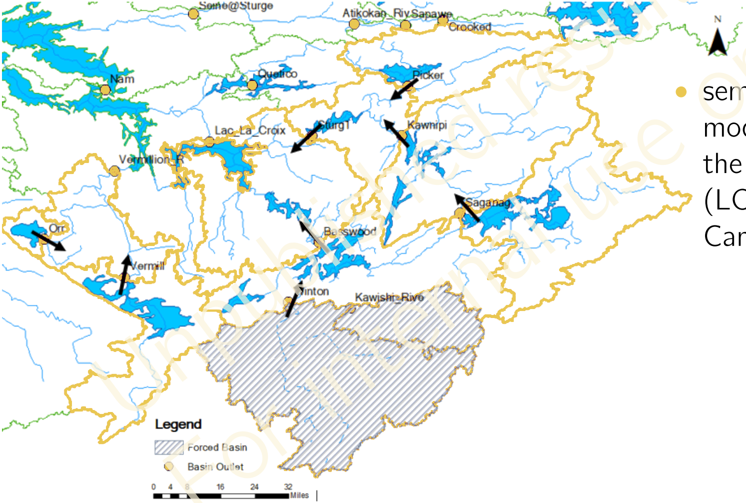
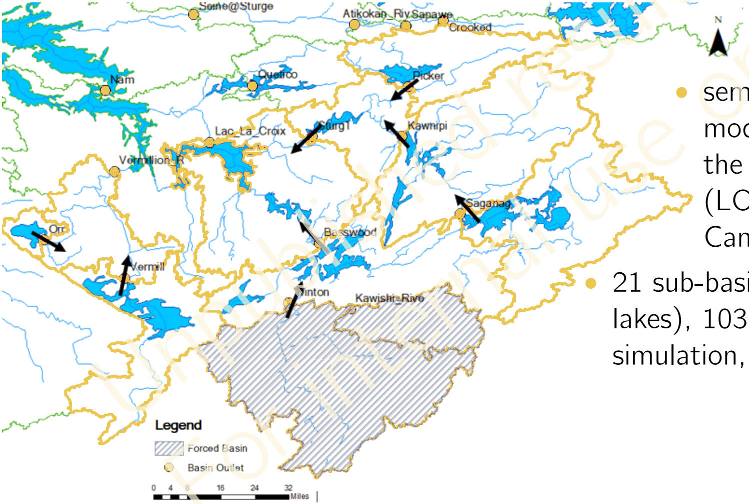
– Exercise C_2 –



- semi-distributed model of Lake of the Woods basin (LOWRL) in Canada

Introduction of OSTRICH

– Exercise C_2 –



- semi-distributed model of Lake of the Woods basin (LOWRL) in Canada
- 21 sub-basins (9 explicit lakes), 103 HRUs, 6 yr simulation, 128 parameter

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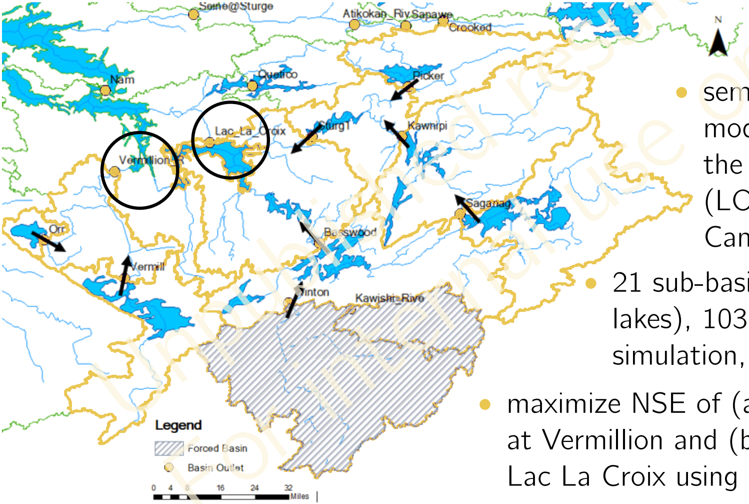
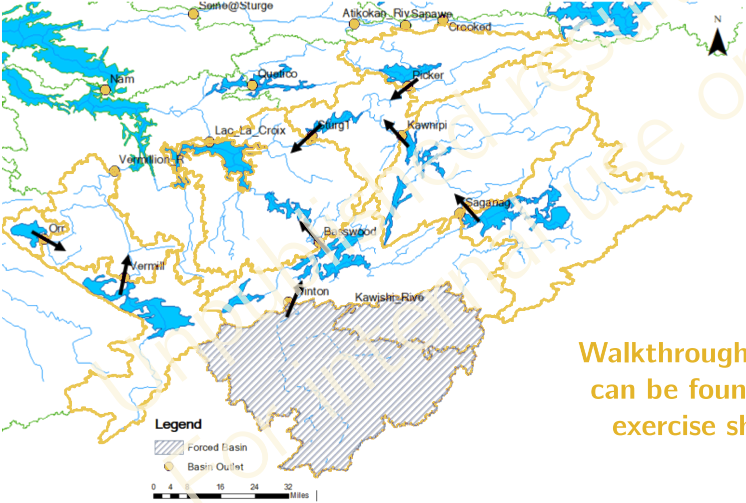
– Exercise C_2 –



- semi-distributed model of Lake of the Woods basin (LOWRL) in Canada
- 21 sub-basins (9 explicit lakes), 103 HRUs, 6 yr simulation, 128 parameter
- maximize NSE of (a) streamflow at Vermillion and (b) inflows to Lac La Croix using PA-DDS

Introduction of OSTRICH

– Exercise C_2 –



Walkthrough and tasks can be found on your exercise sheet C_2!

Introduction of OSTRICH

– Exercise C_3 and C_4 –

Sequential Calibration

Single objective

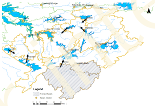
C_1

Irondequoit basin

DDS algorithm

Multiple objectives

C_2



LOWRL basin

PA-DDS algorithm

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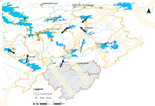
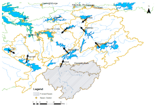
Introduction of OSTRICH

– Exercise C_3 and C_4 –

	Sequential Calibration	Parallel Calibration
Single objective	C_1  Irondequoit basin **DDS algorithm**	C_3  Irondequoit basin **Parallel DDS algorithm**
Multiple objectives	C_2  LOWRL basin **PA-DDS algorithm**	C_4  LOWRL basin **Parallel PA-DDS algorithm**