

# **RCaN**

## **Supplementary Material**

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### **1 Introduction**

1. Goals: an example of a RCaN study : a sequence of RCaN-commands, their input, their output and their interpretation.
2. The case study: the Barents sea (main text).
3. The RCaN file has been previously built. It is attached.
4. All following commands in joined R script.
5. A first run with all main steps.
6. A second run after removing some constraints
7. Comparisons between both runs and interpretation

### **2 Preliminary: R Environment**

A few libraries are to be loaded.

```
> library(RCaN) #the main package  
> library(ggplot2) #to draw results  
> library(coda) #to explore mcmc  
> library(dplyr) #to manipulate data frame
```

```
> library(xtable) #to create latex tables  
> library(xlsx) # to import excel files
```

### 3 The RCaN file

Parameters, observations and constraints have been gathered in an Excel file with a specific structure.

```
> setwd('/Users/christianmullon/gitC/article_supporting')
> NAMEFILE <- 'BarentsSeaReconstructions_01_02_21.xlsx'
> # NAMEFILE <- 'CaN_template_minis.xlsx'
```

### **3.1 Components**

	Component	Inside	AssimilationE	Digestibility	OtherLosses
1	PP	0.00	0.00	0.65	0.00
2	Hzoo	1.00	1.00	0.90	8.40
3	Ozoo	1.00	1.00	0.90	5.50
4	Benthos	1.00	0.94	0.60	1.50
5	PelF	1.00	0.90	0.90	2.85
6	DemF	1.00	0.93	0.85	1.65
7	MM	1.00	1.00	0.00	5.50
8	Birds	1.00	0.84	0.00	60.00
9	Fisheries	0.00	0.00	0.00	0.00
10	NorSeaZoo	0.00	0.00	0.00	0.00

Table 1: Components

### **3.2 Fluxes**

### **3.3 Observations**

### **3.4 Constraints**

	Flux	From	To	Trophic
1	PP_Hzoo	PP	Hzoo	1.00
2	PP_Ozoo	PP	Ozoo	1.00
3	PP_Benthos	PP	Benthos	1.00
4	Hzoo_Ozoo	Hzoo	Ozoo	1.00
5	Hzoo_PelF	Hzoo	PelF	1.00
6	Ozoo_Ozoo	Ozoo	Ozoo	1.00
7	Ozoo_PelF	Ozoo	PelF	1.00
8	Ozoo_DemF	Ozoo	DemF	1.00
9	Ozoo_MM	Ozoo	MM	1.00
10	Ozoo_Birds	Ozoo	Birds	1.00
11	Benthos_Benthos	Benthos	Benthos	1.00
12	Benthos_DemF	Benthos	DemF	1.00
13	PelF_PelF	PelF	PelF	1.00
14	PelF_DemF	PelF	DemF	1.00
15	PelF_MM	PelF	MM	1.00
16	PelF_Birds	PelF	Birds	1.00
17	DemF_DemF	DemF	DemF	1.00
18	DemF_MM	DemF	MM	1.00
19	NorSeaZoo_Hzoo	NorSeaZoo	Hzoo	0.00
20	NorSeaZoo_Ozoo	NorSeaZoo	Ozoo	0.00
21	PelF_Fisheries	PelF	Fisheries	0.00
22	DemF_Fisheries	DemF	Fisheries	0.00
23	MM_Fisheries	MM	Fisheries	0.00
24	Ozoo_Fisheries	Ozoo	Fisheries	0.00

Table 2: Fluxes

	Year	Prod_Sat	Hzoo_Biomass	Ozoo_Biomass	Pelagics
1	1988.00		25432.12	24275.61	428.28
2	1989.00		31987.20	16130.85	864.52
3	1990.00		23027.73	7481.54	5831.66
4	1991.00		21188.34	16833.36	7288.56
5	1992.00		27314.02	7940.31	5152.50
6	1993.00		37612.31	11880.41	799.64
7	1994.00		72438.19	22699.62	203.94
8	1995.00		57941.78	23526.60	195.66
9	1996.00		38465.04	24633.25	504.21
10	1997.00		43364.75	19153.71	912.15

Table 3: Observations

	Id	Constraint
1	C01	PP_Hzoo + PP_Ozoo + PP_Benthos <= Prod_Sat * 1.5
2	C02	PP_Hzoo + PP_Ozoo + PP_Benthos >= Prod_Sat / 1.5
3	C03	PP_Hzoo + PP_Ozoo + PP_Benthos <= 2000000
4	C04	PP_Hzoo + PP_Ozoo + PP_Benthos >= 500000
5	C05	NorSeaZoo_Hzoo = 8 * 1600
6	C06	NorSeaZoo_Ozoo = 2 * 1600
7	C07	PelF_Fisheries >= Pel_landings

Table 4: Constraints

## 4 Building polytope

```
> begin <- Sys.time()
> POLYTOPE <- buildCaN(NAMEFILE)
> end <- Sys.time()
> end-begin

Time difference of 3.126441 mins

> summary(POLYTOPE)

      Length Class      Mode
components_param     10 data.frame list
species              7 -none-   character
fluxes_def           4 data.frame list
flow                 24 -none-   character
series               22 data.frame list
ntstep                1 -none-   numeric
data_series_name    21 -none-   character
constraints          5 data.frame list
H                     49 -none-   numeric
N                   168 -none-   numeric
A                  2009575 dgCMatrix S4
AA11                2009575 dgCMatrix S4
C                  49600 dgCMatrix S4
CA11                49600 dgCMatrix S4
v                     64 -none-   numeric
vAll                 64 -none-   numeric
L                  173600 dgCMatrix S4
b                     2593 -none-   numeric
bAll                 2593 -none-   numeric
symbolic_enviro     903 -none- environment
```

## 5 Structure of polytope

The polytope is defined by two pairs of a matrix and a vector.  $F$  being the vector of all flows at all timesteps, first one ( $A, b$ ) is an equality  $A.F = b$ , second one ( $C, v$ ) is an eqality  $C.F \leq v$ . For the Barents sea, we have:

```
> dim(POLYTOPE$a)
[1] 2593 775

> length(POLYTOPE$b)
[1] 2593

> dim(POLYTOPE$c)
```

```
[1] 64 775  
> length(POLYTOPE$v)  
[1] 64
```

## 6 Checking polytope

As it is defined in the RCaN file for the Barents' sea, the polytope is non-empty and bounded:

```
> checkPolytopeStatus(POLYTOPE)  
[1] "polytope ok"
```

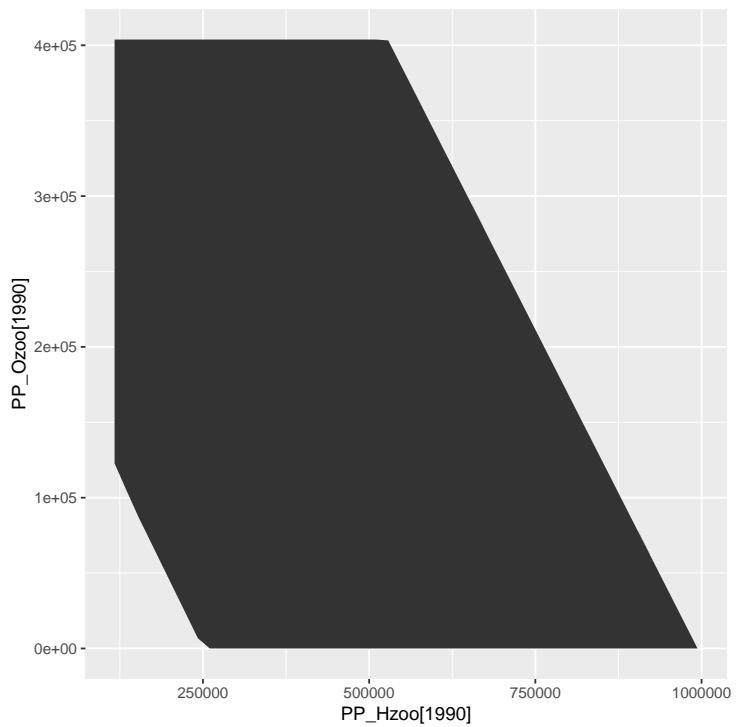
Limits of the Barents' sea polytope in all dimensions are obtained with getAllBoundsParam:

```
> BOUNDS <- getAllBoundsParam(POLYTOPE, progressBar = FALSE)  
> summary(BOUNDS)
```

param	lowerbound	upperbound
Length:775	Min. : 0.0	Min. : 0
Class :character	1st Qu.: 0.0	1st Qu.: 2667
Mode :character	Median : 0.0	Median : 8629
	Mean : 12566.2	Mean : 311440
	3rd Qu.: 906.5	3rd Qu.: 86908
	Max. :448256.5	Max. :7983360

Function plotPolytope2D allows seeing the polytope in the plane defined by two parameters. In its first two dimensions, for the second 1990, the Barents sea polytope dimensions appears as.

```
> fluxX <- paste(FLUXES[1,1], '[1990]', sep="")  
> fluxY <- paste(FLUXES[2,1], '[1990]', sep="")  
> plotPolytope2D(POLYTOPE, c(fluxX, fluxY), progressBar=FALSE)
```



## 7 Sampling polytope

### 7.1 Sampling

```
> begin = Sys.time()
> SAMPLE <- sampleCaN(POLYTOPE,
+                         N=100, thin=100,
+                         nchain=2,
+                         ncore=2)
> end=Sys.time()
> end-begin
```

Time difference of 13.5143 mins

## 7.2 Convergence

Using coda.

```
> nchain(SAMPLE$mcmc)  
[1] 2  
> # summary(SAMPLE$mcmc)
```

Gelman diagnostics. Gelman and Rubin (1992) propose a general approach to monitoring convergence of MCMC output in which  $m > 1$  parallel chains are run with starting values that are overdispersed relative to the posterior distribution. Convergence is diagnosed when the chains have ‘forgotten’ their initial values, and the output from all chains is indistinguishable. The gelman.diag diagnostic is applied to a single variable from the chain. It is based a comparison of within-chain and between-chain variances, and is similar to a classical analysis of variance.

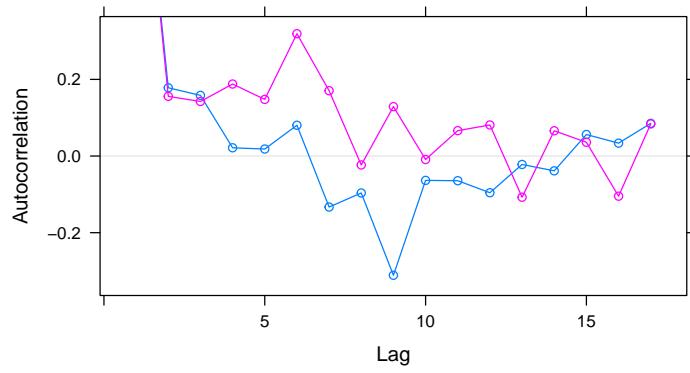
```
> fluxY <- paste(FLUXES[2,1], '[1990]', sep="")  
> gelman.diag(SAMPLE$mcmc[,fluxY])
```

Potential scale reduction factors:

	Point est.	Upper C.I.
[1,]	1.02	1.12

Autocorrelation function

```
> fluxZ <- paste(FLUXES[3,1], '[1990]', sep="")  
> thinned_SAMPLE <- window(SAMPLE$mcmc, thin=2)  
> thin(thinned_SAMPLE)  
  
[1] 2  
  
> acfplot(thinned_SAMPLE[,fluxZ])
```



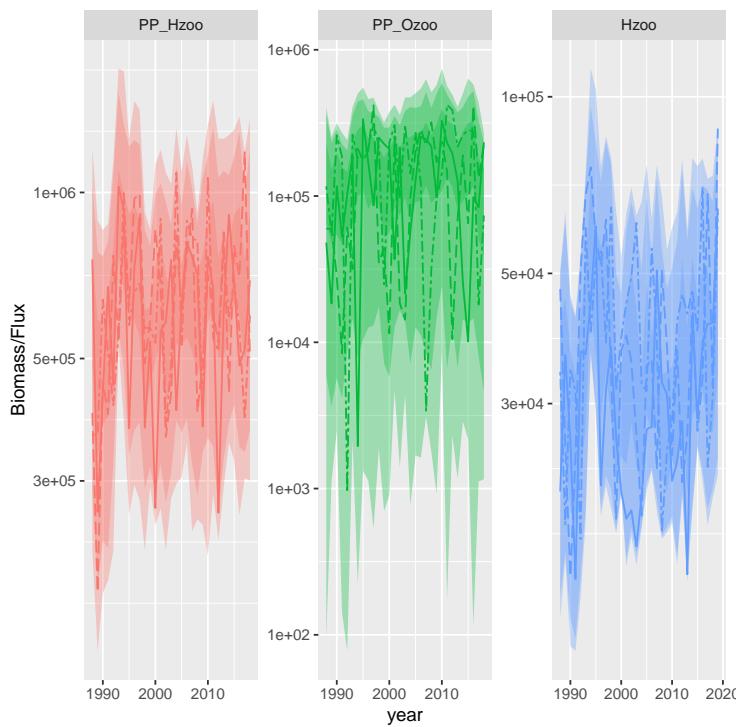
### 7.3 Dynamics

For several variables or flux, plots of sampled dynamics.

```
> fluxX <- FLUXES[1,1]
> fluxY <- FLUXES[2,1]
> compA <- COMPONENTS[2,1]
> compB <- COMPONENTS[3,1]
> c(fluxX,fluxY,compA)

[1] "PP_Hzoo" "PP_Ozoo" "Hzoo"

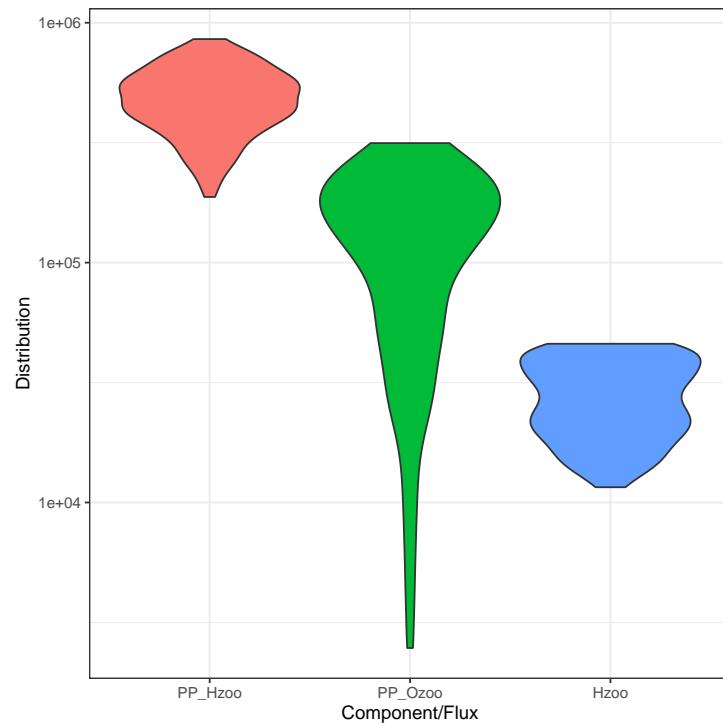
> g <- ggSeries(SAMPLE, c(fluxX,fluxY,compA), TRUE)
> g + scale_y_log10() + guides(color = FALSE, fill = FALSE)
```



## 7.4 Distribution

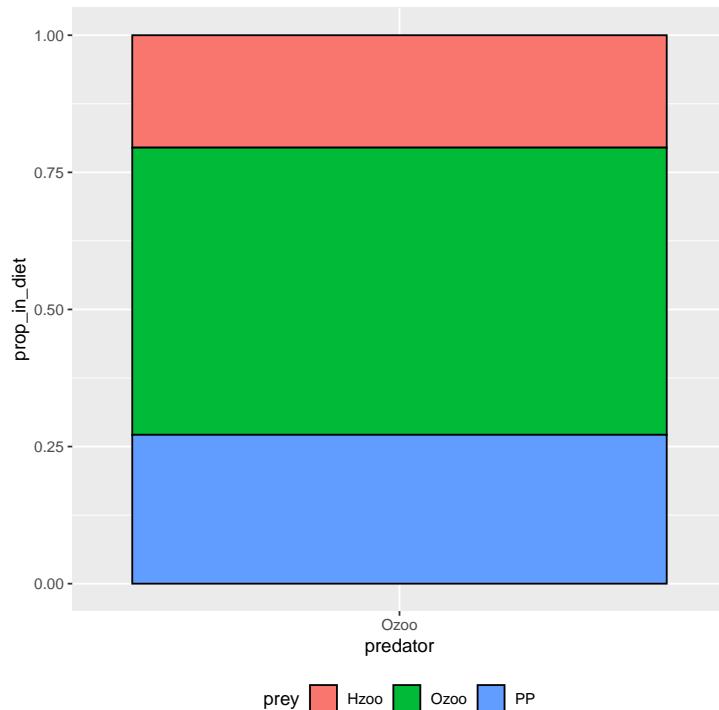
For a component or a flux, for a year, the distribution of sampled values.

```
> ggViolin(SAMPLE,c(fluxX,fluxY,compA),year=1990,TRUE)
```



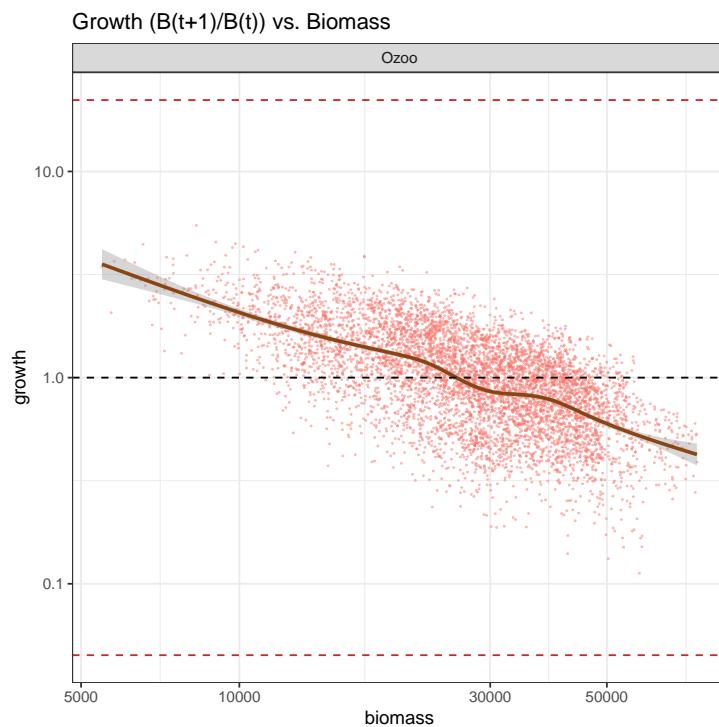
## 7.5 Diet relationships

```
> ggDiet(SAMPLE, compB)
```



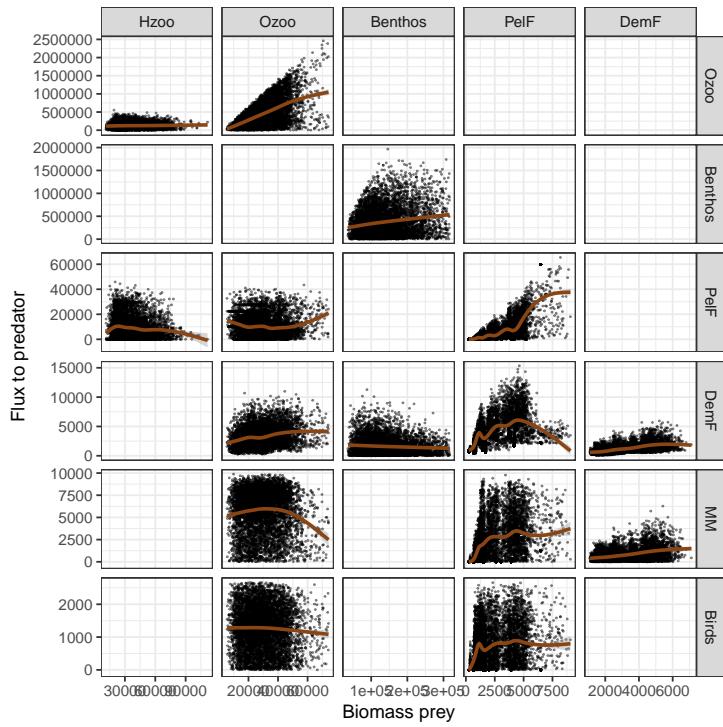
## 7.6 Growth

```
> ggGrowth(SAMPLE, compB)
```



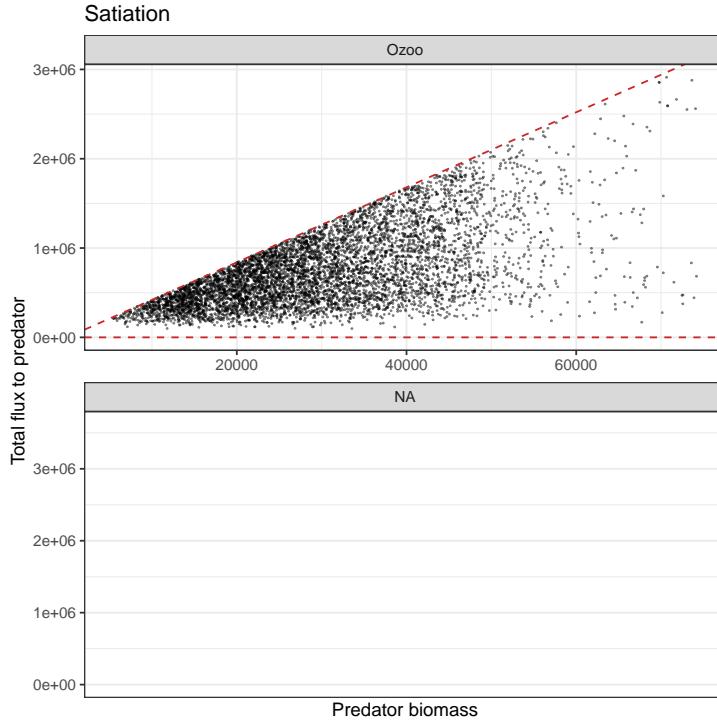
## 7.7 Trophic relation

```
> ggTrophicRelation(SAMPLE)
> # ggTrophicRelation(SAMPLE, compB)
```



## 7.8 Satiation

```
> ggSatiation(SAMPLE, compB)
```



## 8 Try and errors

### 8.1 Activating and desactivating constraint

```
> # deactivate constraints C02
> constA = CONSTRAINTS[2,1]
> constA

[1] "C02"

> POLYTOPEA <- toggleConstraint(POLYTOPE, constA)

[1] "deactivate inequality C02 : 1998" "deactivate inequality C02 : 1999"
[3] "deactivate inequality C02 : 2000" "deactivate inequality C02 : 2001"
[5] "deactivate inequality C02 : 2002" "deactivate inequality C02 : 2003"
[7] "deactivate inequality C02 : 2004" "deactivate inequality C02 : 2005"
[9] "deactivate inequality C02 : 2006" "deactivate inequality C02 : 2007"
[11] "deactivate inequality C02 : 2008" "deactivate inequality C02 : 2009"
[13] "deactivate inequality C02 : 2010" "deactivate inequality C02 : 2011"
[15] "deactivate inequality C02 : 2012" "deactivate inequality C02 : 2013"
[17] "deactivate inequality C02 : 2014" "deactivate inequality C02 : 2015"
[19] "deactivate inequality C02 : 2016" "deactivate inequality C02 : 2017"
[21] "deactivate inequality C02 : 2018"
```

```

> # deactivate constraints CO2 for year 1991
> checkPolytopeStatus(POLYTOPEA)
[1] "polytope ok"

```

## 8.2 Building and analyzing sample

```

> begin = Sys.time()
> SAMPLEA <- sampleCaN(POLYTOPEA,
+                           N=100, thin=100,
+                           nchain=2,
+                           ncore=2)
> end=Sys.time()
> end-begin

Time difference of 14.12087 mins

> fluxX <- FLUXES[1,1]
> fluxY <- FLUXES[2,1]
> compA <- COMPONENTS[2,1]
> compB <- COMPONENTS[3,1]
> c(fluxX,fluxY,compA)

[1] "PP_Hzoo" "PP_Ozoo" "Hzoo"

> g <- ggSeries(SAMPLEA, c(fluxX,fluxY,compA), TRUE)
> g + scale_y_log10() + guides(color = FALSE, fill = FALSE)

```

