Model optimisation with the Cylc workflow engine: application to wave hindcast calibration

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Outline

- What is model optimisation?
- How can this be automated?
- Task scheduling in complex forecast systems - Cylc
- A Cylc optimisation suite: Cyclops V1.0
- Application to a wave hindcast
- Potential applications and future developments

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Model parameter tuning

- A numerical model will generally have parameters that can be adjusted, and which affect the model outputs
- If the model has *M* adjustable parameters $(x_1, x_2, x_3, \ldots, x_M)$, each time we run the model we can evaluate some error metric *f* that gives a single "score" for the model.
- For example

$$f = RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i^{model} - y_i^{measured}\right)^2}$$

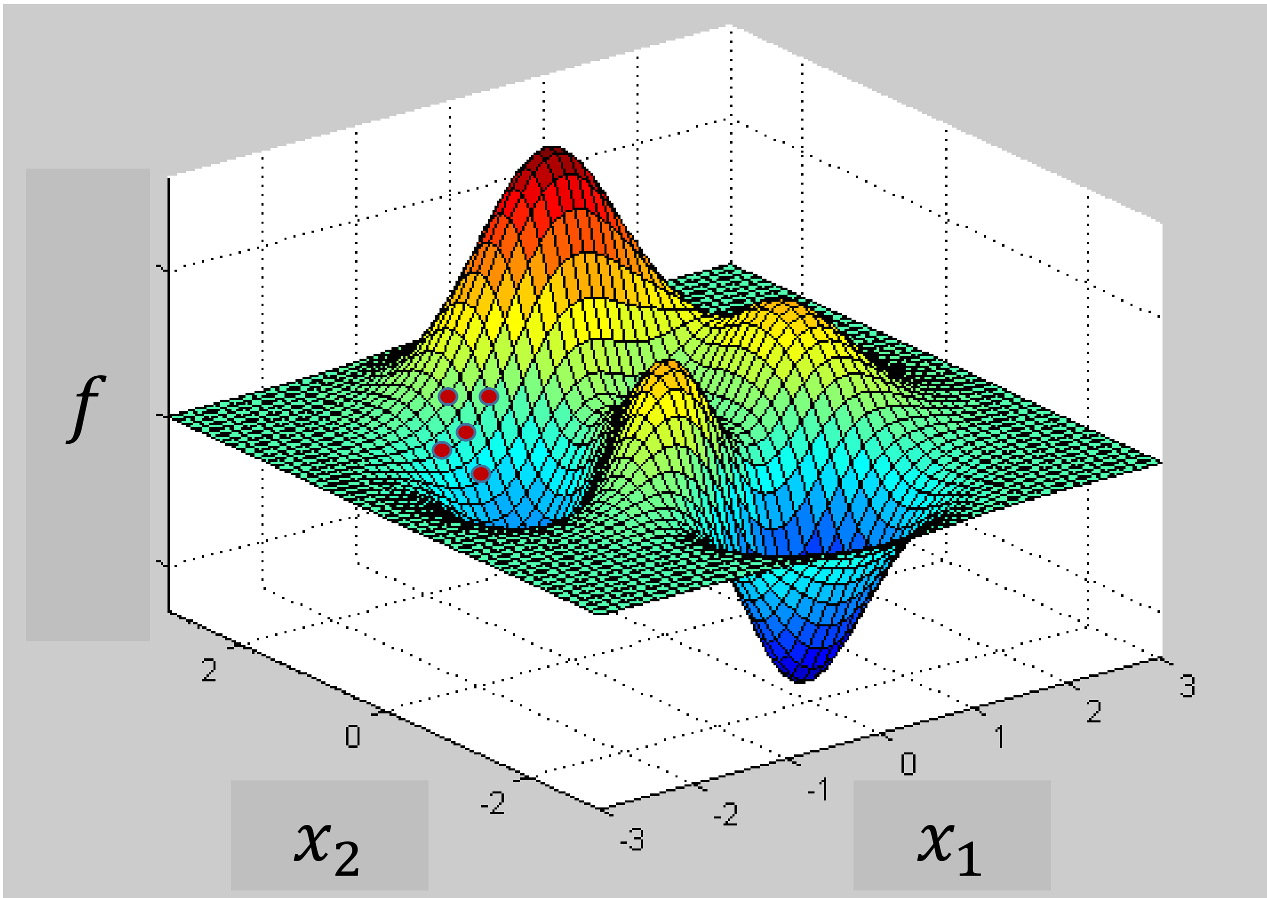
- The aim is to find a set of parameters that makes that error metric $f(x_1, x_2, x_3, \ldots, x_M)$ as small as possible

The objective function

2 parameter example

How does f vary with x_1 and x_2?

How can we find the optimal x_1 and x_2 as efficiently as possible?



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Algorithms for nonlinear optimisation

Global:

- **DIRECT: Dividing RECTangles (Jones et al., 1993)**
- **DIRECT-L: Dividing RECTangles, locally optimised (Gablonsky and Kelley, 2001)**
- **DIRECT-L-RAND: a slightly randomised variant of DIRECT-L (Johnson, 2014)**
- **CRS: Controlled Random Search (Hendrix et al., 2001)**
- **CRS2: Controlled Random Search (Price, 1983)**
- **CRS2-LM: Controlled Random Search with Local Mutation (Kaelo and Ali, 2006)**
- **MLSL: Multi-Level Single-Linkage (Rinnooy Kan and G. T. Timmer, 1987)**
- **ISRES: Improved Stochastic Ranking Evolution Strategy (Runarsson and Yao, 2005)**
- **ESCH: Evolutionary algorithm (da Silva Santos et al., 2010)**

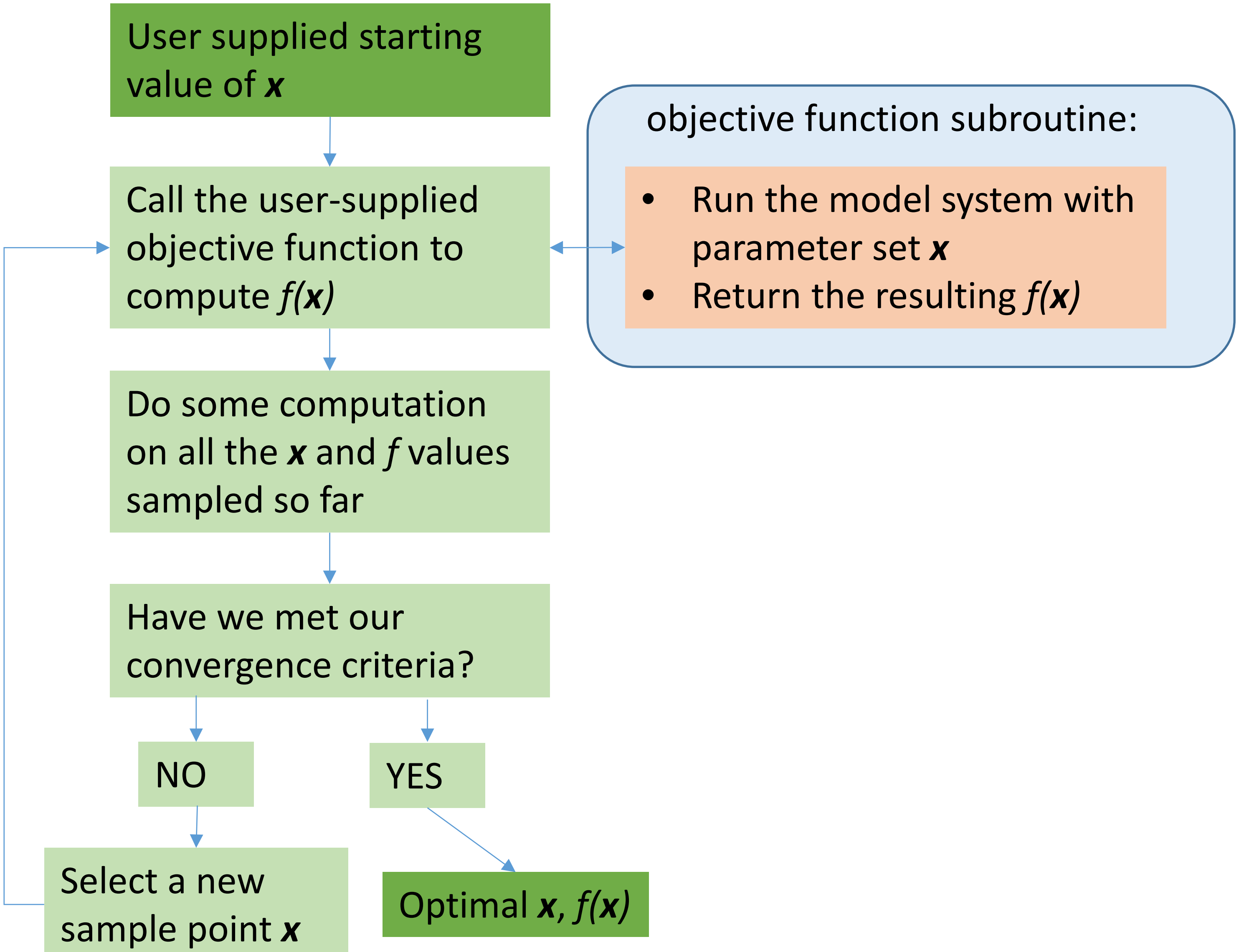
Local:

- **COBYLA: Constrained Optimization BY Linear Approximations (Powell, 1994)**
- **BOBYQA: Bounded Optimization BY Quadratic Approximation (Powell, 2009)**
- **NEWUOA: Unconstrained Optimization (Powell, 2004)**
- **NEWUOA-BOUND: a bounded variant of NEWUOA (Johnson, 2014)**
- **PRAXIS: Principal Axis (Brent, 1972)**
- **Nelder-Mead Simplex (Nelder and Mead, 1965)**
- **Sbplx: Nelder-Mead applied on a sequence of subspaces (Rowan, 1990)**

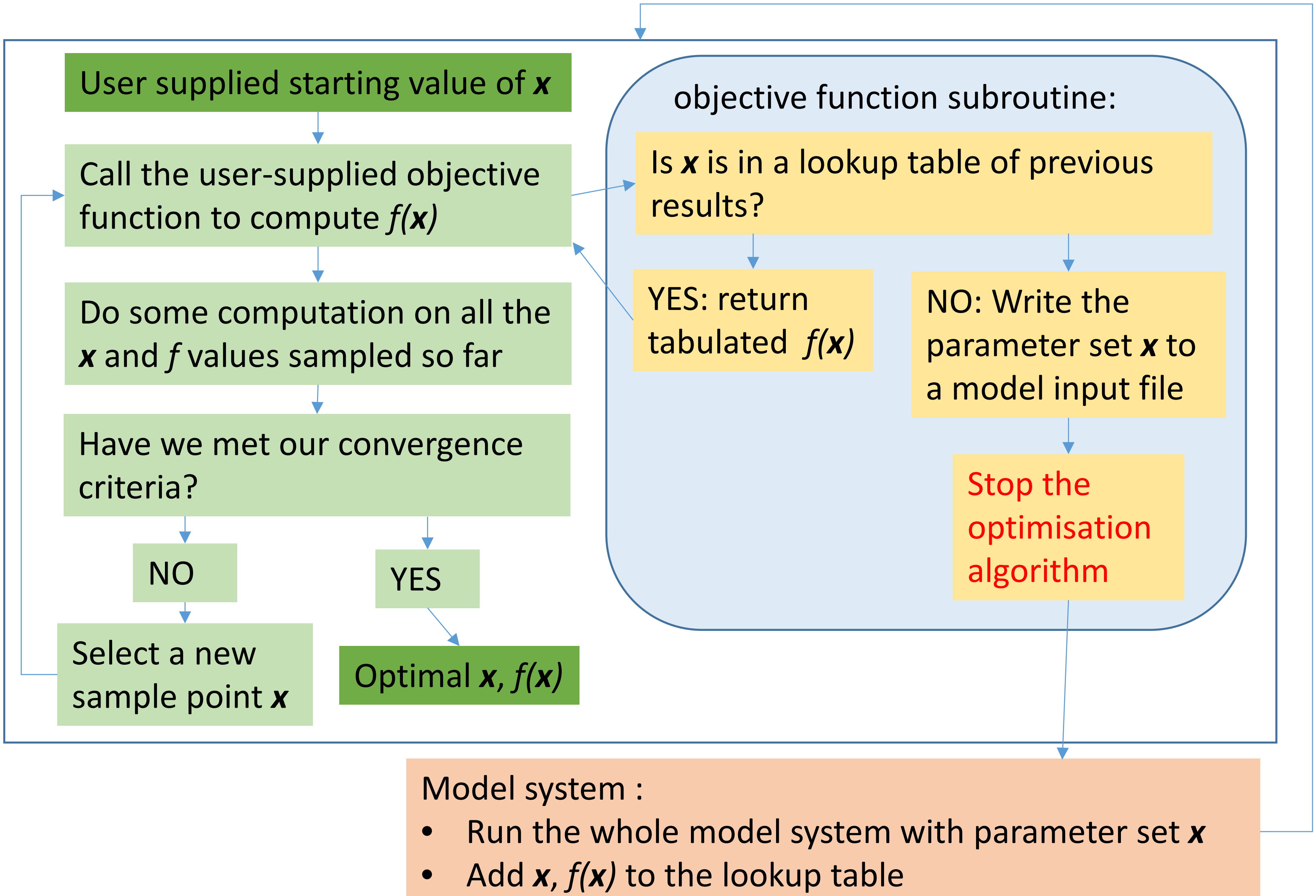
Nlopt nonlinear optimisation toolbox (Johnson, 2014)
http://ab-initio.mit.edu/nlopt

- Versions in C, python
- Implements many algorithms
- We want derivative-free, bounded optimisation
- Requires the user to write a subroutine to evaluate the objective function

Schematic of an optimisation algorithm



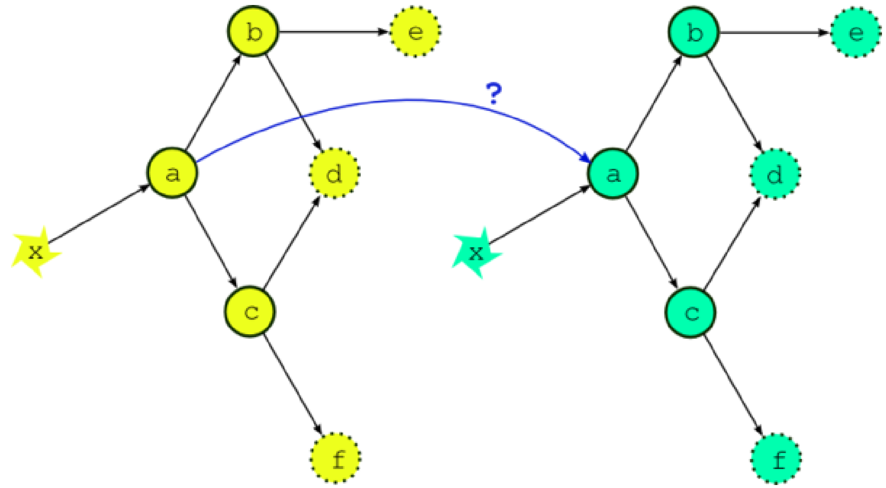
Schematic of an optimisation algorithm – with generic objective function

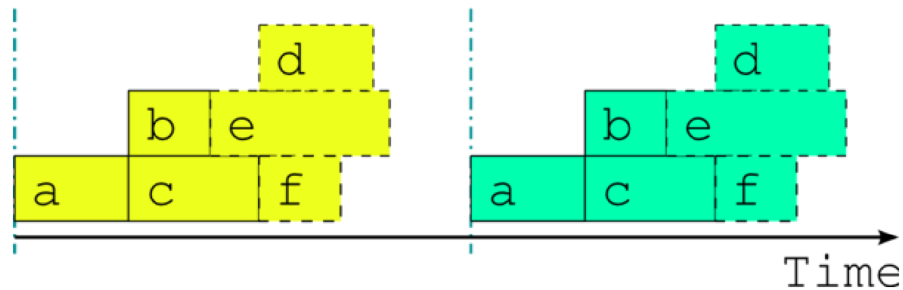


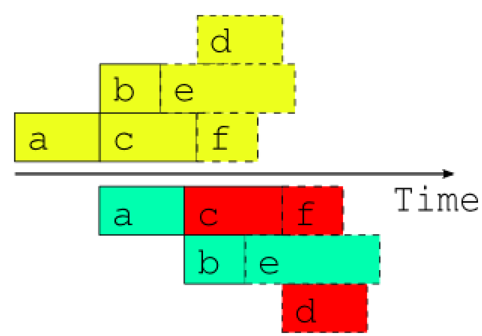
REPEAT UNTIL THE OPTIMISATION CODE COMPLETES

The Cylc workflow engine

- Developed by Hilary Oliver (NIWA) and collaborators (NIWA, UKMO,…)
- Handles the scheduling of inter-dependent computing tasks repeated over multiple cycles (e.g. in an operational forecast system)
- Configures task scheduling via dependency graphs
- Allows for tasks from multiple cycles to run simultaneously while respecting inter-cycle dependencies
- Used at:
  - NIWA (NZ)
  - UK Met Office
  - NRL Marine Meteorology Division (USA)
  - Max Planck Institute for Meteorology (Germany)
  - Bureau of Meteorology (Australia)
  - GFDL (NOAA/Princeton University, USA)
  - …







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Application to a wave hindcast

- Wavewatch v4.18 with either Tolman & Chalikov (1996) or Ardhuin et al (2010) source term parameterisation
- Global domain at 1° × 1° spatial resolution
- Input wind and sea ice concentration fields from the ERA-Interim Reanalysis (1979-2016)
- Error metric: normalised RMSE of significant wave height compared with collocated altimeter data (from the IFREMER database), spatially averaged (between 61°S and 61°N)

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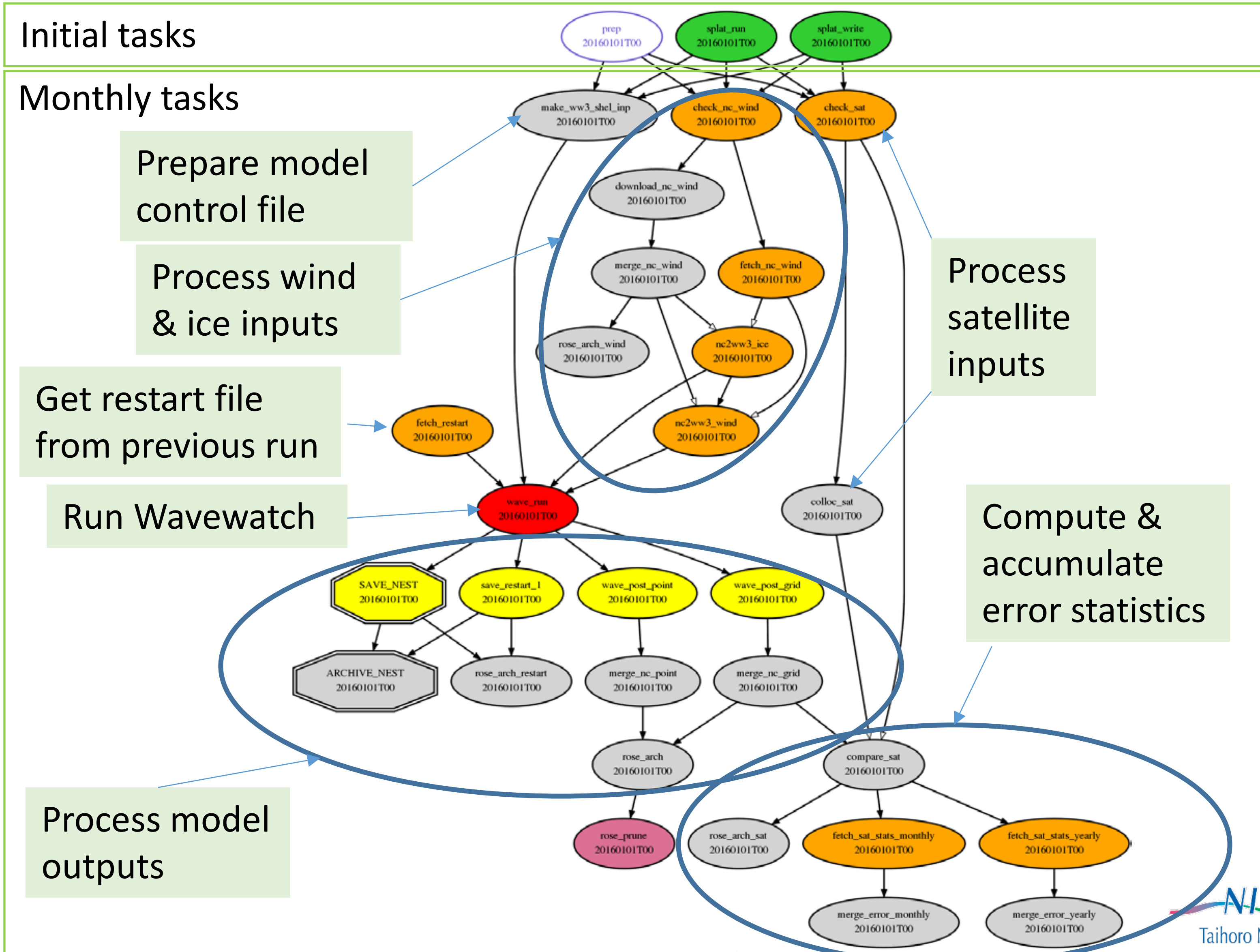
Cylc dependency graph example: wave hindcast suite



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A Cylc optimisation suite

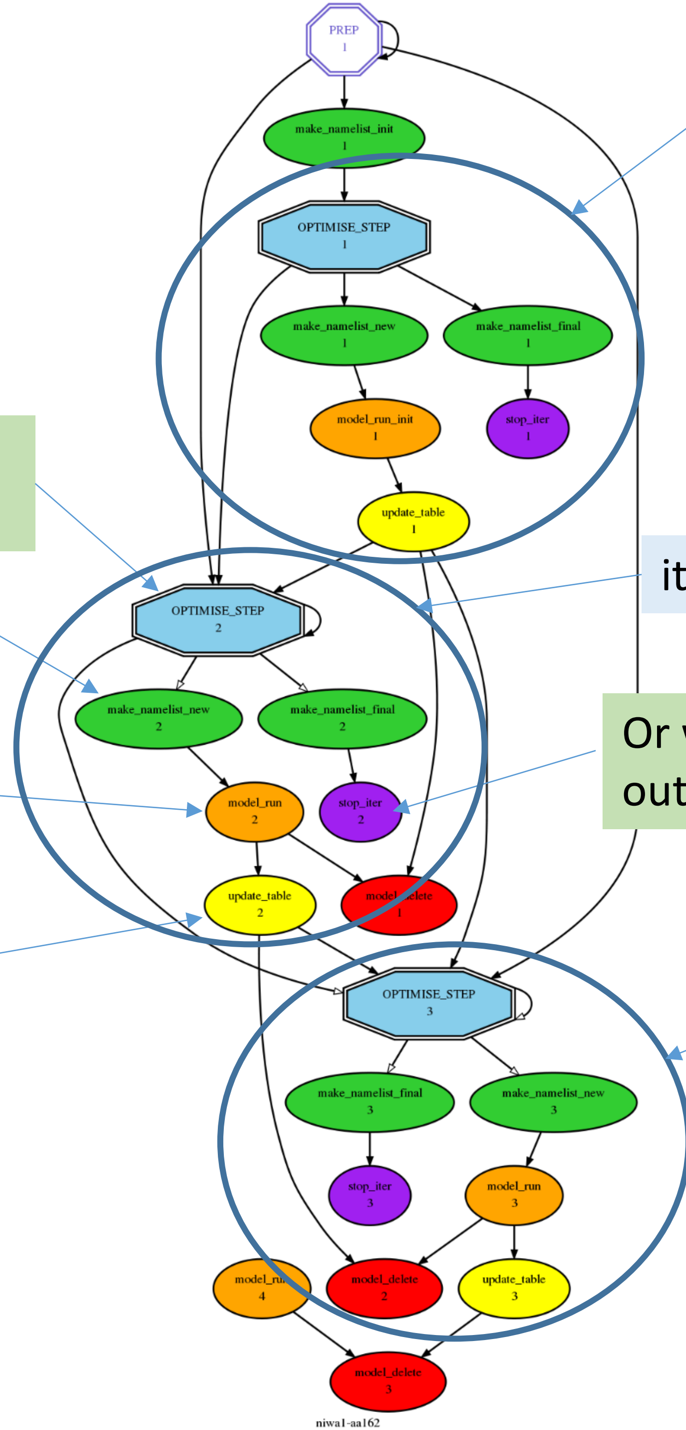
- Instead of cycling on time, use integer cycling, on iteration number

Run the optimisation algorithm to pick the next parameter set

Create a model input file with the requested parameter set

Start a new copy of the model suite

Update the lookup table with the result



iteration 1

iteration 2

Or write some final outputs and stop

iteration 3

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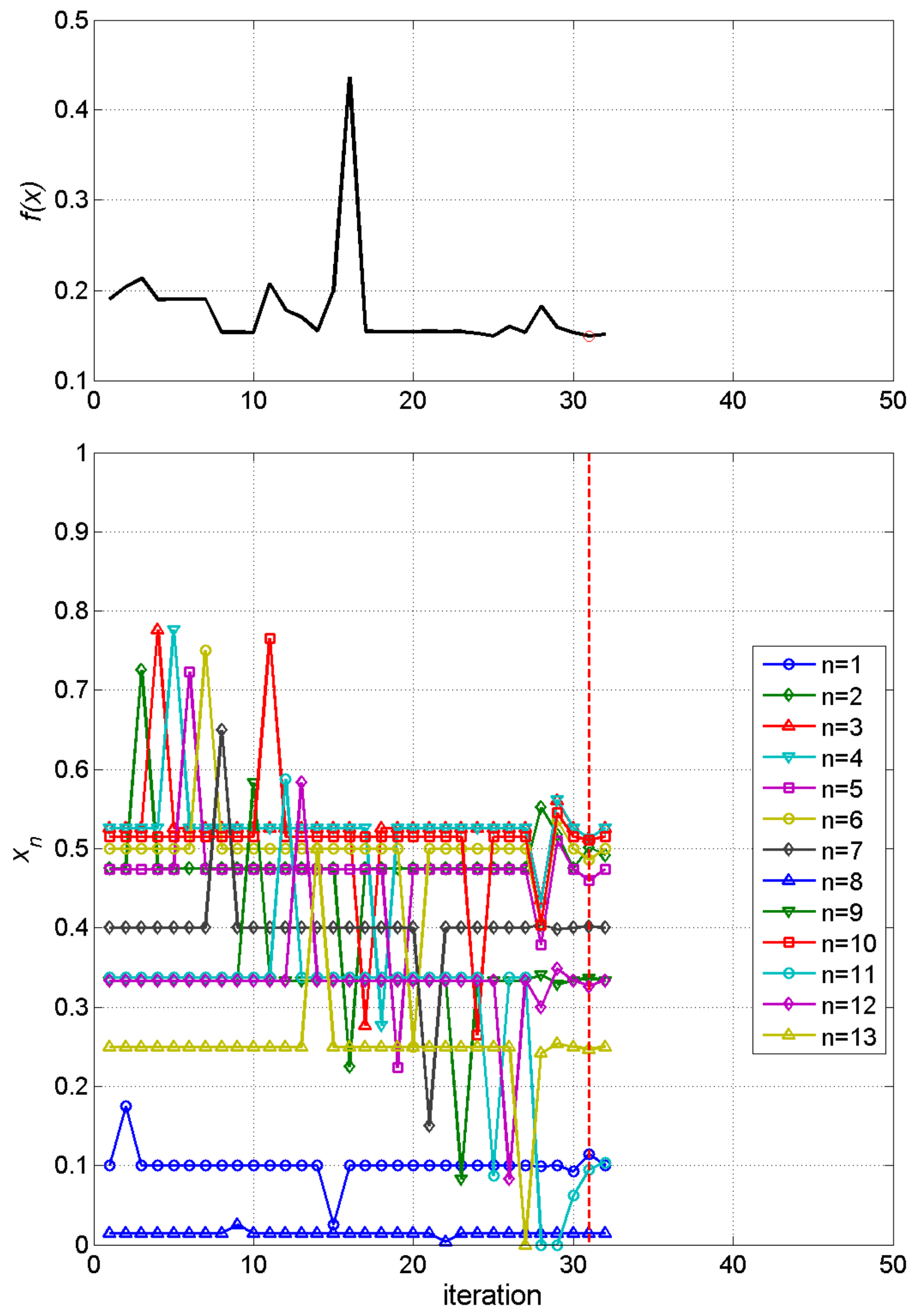
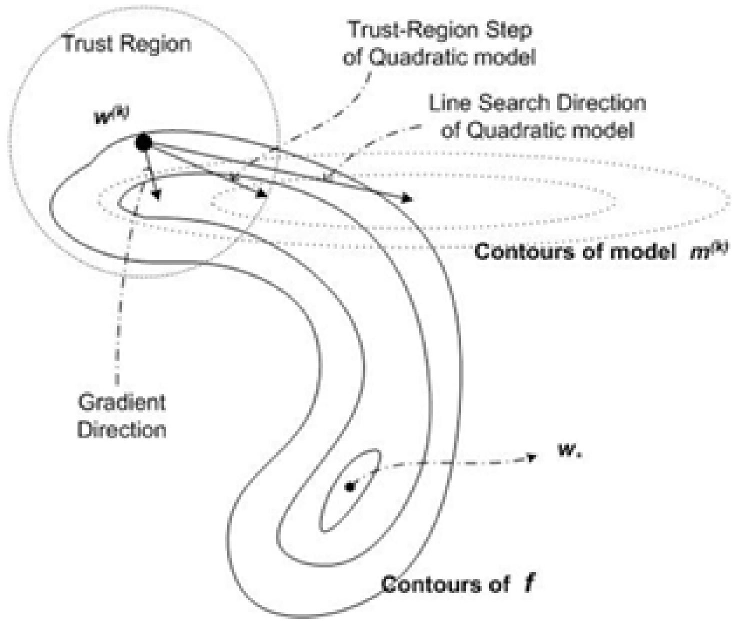
Evolution of the optimisation (ST2, 3 months)

- ST2 Tolman & Chalikov (1996) parameterisation
- 13 adjustable parameters:
  - o 6 from the wind input term
  - o 6 from the dissipation terms
  - o 1 for DIA nonlinear interaction strength
- Calibration run from Feb-Apr 1997
- Stopping criteria: < 2% change in *f* or ***x***
- Error metric reduced from:
  0.1901 (initialised with Tolman & Chalikov defaults), to
  0.1495 (after 33 iterations)



Algorithm:
BOBYQA (Bounded Optimisation By Quadratic Approximation)
A LOCAL trust-region method (Powell 2009)



<Trust-Region method>

Gradient
Stable
Slow, learning rate

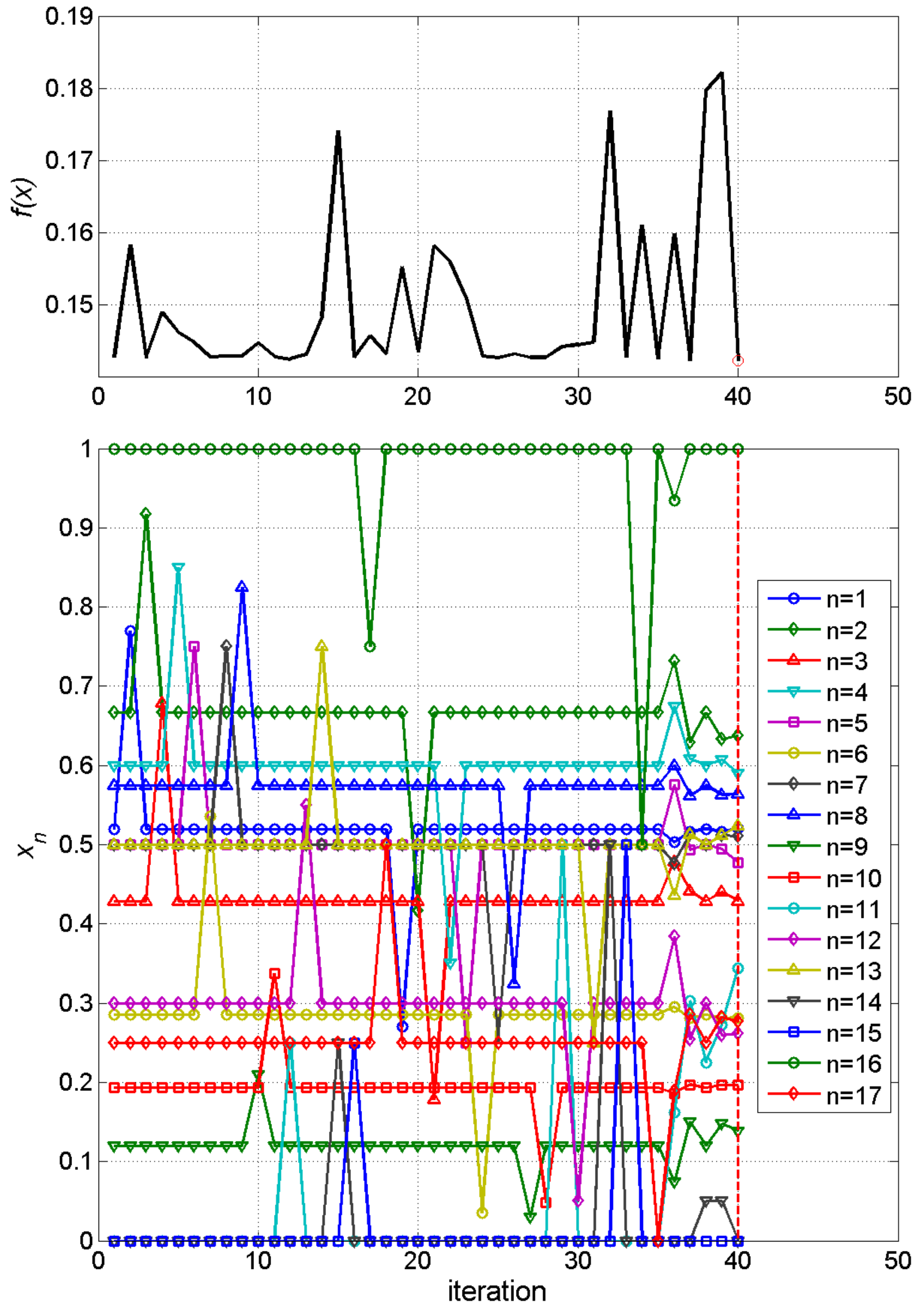
Trust-Region method
Fast & Stable

Newton
Fast
Unstable, complexity, learning rate

A trust-region method finds a direction and a step size in an efficient and reliable manner with the help of a quadratic model of the objective function.

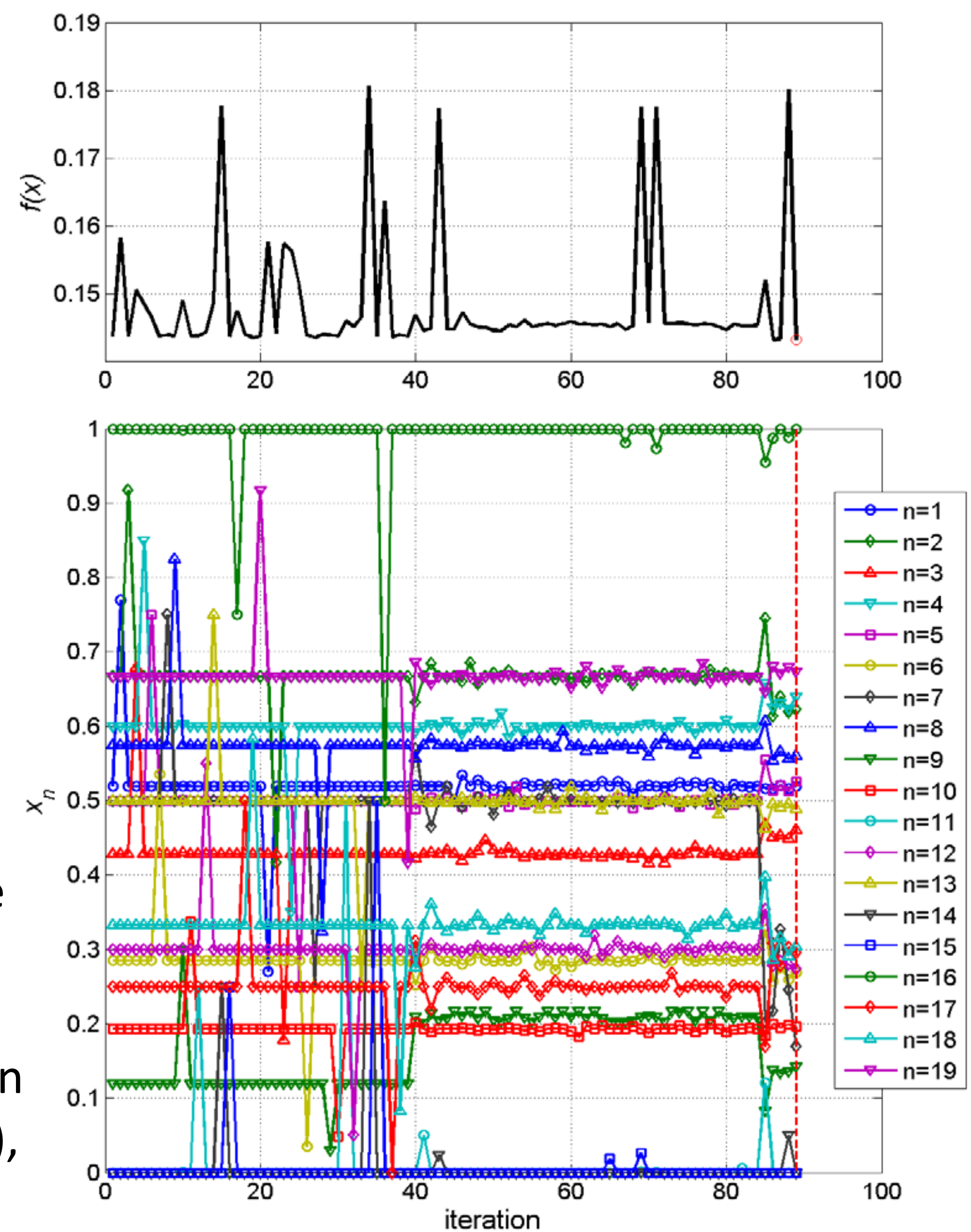
Evolution of the optimisation (ST4, 3 months)

- ST4 Ardhuin et al (2010) parameterisation
- 17 adjustable parameters:
    - o 8 from the wind input term (including swell)
    - o 8 from dissipation terms
    - o 1 for DIA nonlinear interaction strength
- Calibration run from Feb-Apr 1997
- Stopping criteria: < 2% change in *f* or ***x***
- Error metric reduced from:
  0.1427 (initialised with Ardhuin et al (2010) defaults (TEST441), to
  0.1422 (after 40 iterations)



Evolution of the optimisation (ST4 – 1 year)

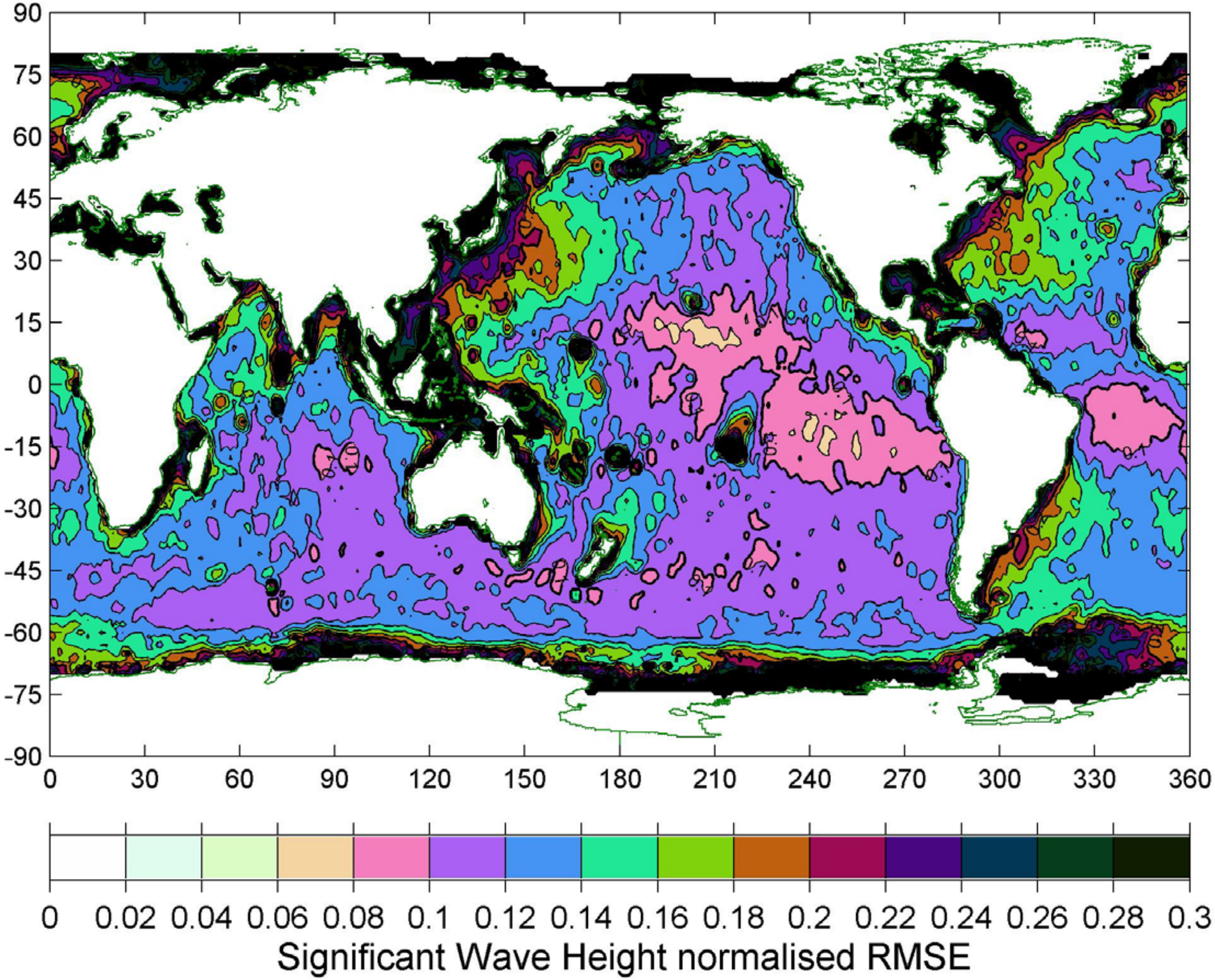
- ST4 Ardhuin et al (2010) parameterisation
- 19 adjustable parameters:
  - o 8 from wind input term (including swell)
  - o 8 from dissipation terms
  - o 1 for DIA nonlinear interaction strength
  - o 2 sea ice concentration thresholds
- Calibration run from Jan-Dec 1997
- Stopping criteria: < 0.1% change in *f* or ***x***
- Error metric reduced from:
  0.1436 (initialised with Ardhuin et al (2010) defaults (TEST441), to
  0.1431 (after 89 iterations)



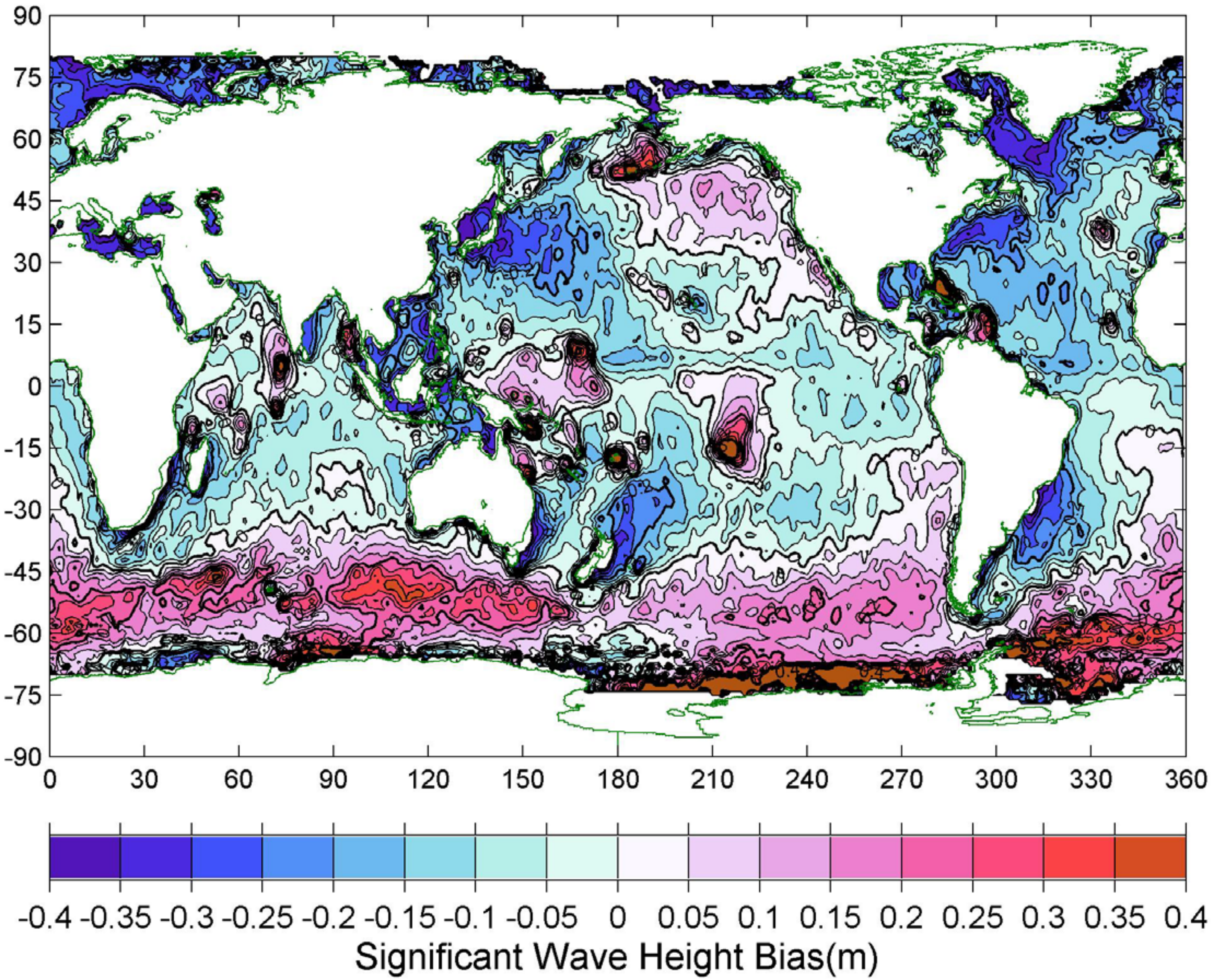
Parallel model simulations

- In the first part of the BOBYQA algorithm, a fixed sequence of parameter values is used, varying one dimension at a time, to form a quadratic model
- In that case, the next *x* value chosen does not depend on the values of *f* previously determined
- Hence we could run several model simulations in parallel
- This capability has been implemented in the Cylc optimisation suite.

Error statistics from the full hindcast – normalised RMS error in Hs



Error statistics from the full hindcast – bias in Hs



Summary

- Numerical models can be tuned/calibrated by solving a nonlinear optimisation problem
- There are many algorithms for this: some are good for “local” optimisation (getting to a nearby minimum as quickly as possible), some are good for a “global” solution (not missing a deeper minimum elsewhere)
- These usually require the user to supply a subroutine to evaluate the objective function.
- We have developed an optimisation tool based on the Cylc workflow engine, that uses a simple, generic objective function subroutine
- Hence it can be readily applied to optimise any model system that has been implemented as a Cylc suite, that accepts parameter values on startup, and returns an error metric on completion
- This has been applied to optimise a wave model hindcast against altimeter measurements.
- Published through zenodo (Cyclops-v1.0: https://doi.org/10.5281/zenodo.837907).

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Parameters for 12 month ST4 optimisation (SIN4, SNL1, MISC)

Parameter	Code variable	Initial	Lower bound	Upper bound	Final	Delta	n
	SIN4:						
z_u	ZWND	10.0					
α_0	ALPHA0	0.0095					
β_{max}	BETAMAX	1.52	1.0	2.0	1.5194	0.02498	1
p_{in}	SINTHP	2.0					
z_α	ZALP	0.006					
s_u	TAUWSHELTER	1.0	0.0	1.5	0.9339	0.2706	2
s_0	SWELLFPAR	1					
s_2	SWELLF	0.8	0.5	1.2	0.8224	0.0206	3
s_1	SWELLF2	-0.018	-0.03	-0.01	-0.01721	0.00064	4
s_3	SWELLF3	0.015	0.01	0.02	0.01526	0.00042	5
Re_c	SWELLF4	1.0×10^5	0.8×10^5	1.5×10^5	0.9888×10^5	0.2328×10^5	6
s_5	SWELLF5	1.2	0.8	1.6	0.9360	0.3974	7
s_6	SWELLF6	0.0					
s_7	SWELLF7	2.3×10^5	0.0	4.0×10^5	2.2433×10^5	0.7911×10^5	8
z_r	Z0RAT	0.04					
$z_{0.max}$	Z0MAX	0.0					
	SINBR	0.0					
	SNL1:						
C	NLPROP	2.5×10^7	2.4×10^7	2.8×10^7	2.5181×10^7	0.1191×10^7	17
	MISC:						
$\epsilon_{c,0}$	CICE0	0.25	0.15	0.45	0.2413	0.1285	18
$\epsilon_{c,n}$	CICEN	0.75	0.55	0.85	0.7521	0.2358	19
	FLAGTR	4					

Parameters for 12 month ST4 optimisation (SDS4)

Parameter	Code variable	Initial	Lower bound	Upper bound	Final	Delta	n
	SDS4:						
	SDSC1	0.0					
p	WNMEANP	0.5					
	FXPM3	4.0					
f_{FM}	FXFM3	9.9					
C_{ds}^{sat}	SDSC2	-2.2×10^{-5}	-2.5×10^{-5}	0.0	-2.1433×10^{-5}	0.0087×10^{-5}	9
C_{cu}	SDSCUM	-0.40344	-0.5	0.0	-0.40194	0.02145	10
B_0	SDSC4	1.0					
C_{turb}	SDSC5	0.0	0.0	1.2	0.0	-	11
δ_d	SDSC6	0.3	0.0	1.0	0.2736	0.0928	12
B_r	SDSBR	9.0×10^{-4}	8.0×10^{-4}	10.0×10^{-4}	8.9788×10^{-4}	0.0951×10^{-4}	13
	SDSBR2	0.8					
p^{sat}	SDSP	2.0					
	SDSISO	2					
C_{ds}^{BCK}	SDSBCK	0.0	0.0	0.2	0.0	-	14
	SDSABK	1.5					
	SDSPBK	4.0					
	SDSBINT	0.3					
C_{ds}^{HCK}	SDSHCK	0.0	0.0	2.0	0.0	-	15
Δ_θ	SDSDTH	80.0					
s_B	SDSCOS	2.0	0.0	2.0	2.0	0.0757	16
	SDSBRF1	0.5					
	SDSBRFDF	0					
	SDSBM0	1.0					
	SDSBM1	0.0					
	SDSBM2	0.0					
	SDSBM3	0.0					
	SDSBM4	0.0					
	WHITECAPWIDTH	0.3					

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