Statistical model checking for ODE models: challenges and applications to Environment modeling

G. Ardourel, G. Cantin, **Benoît Delahaye**, D. Julien, F. Khochman . . .
16/09/2024 Day on Probabilities

Outline

- Context: Natural systems, ODEs, ...

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- SMC for ODE models

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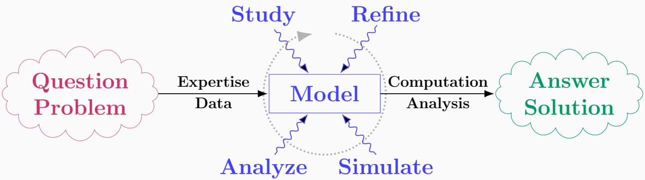
- Abstraction of ODE systems
- Applications
- Perspectives and future work

Context

Science of Models

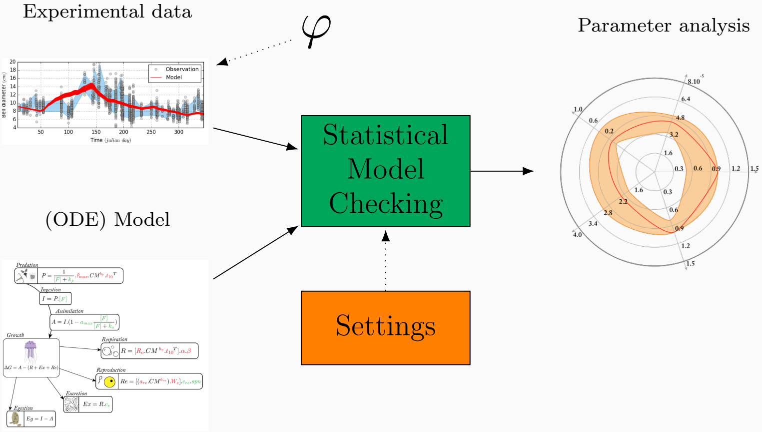


Motivations

Provide mathematical **guarantees** and **tools** for building and analyzing models

- usable by any scientist;
- answering real-life questions.

Example: Calibration of a jellyfish model[1]



[1] [Ramondec et al. 2020] Probabilistic modeling to estimate jellyfish ecophysiological properties and size distribution. *Scientific Reports*

Formal verification of ODE models

System

Formal verification of ODE models

System

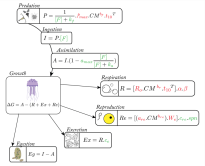
φ

Property

Formal verification of ODE models

System

(ODE) Model



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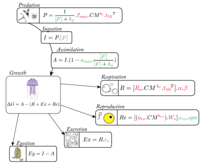
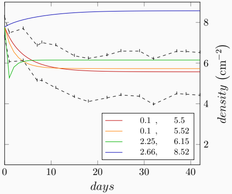


Set of traces



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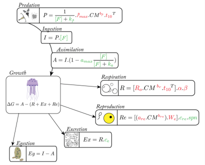

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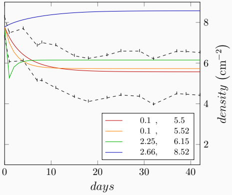

Some models may be verified directly (automata, graphs...).

φ

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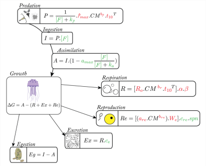

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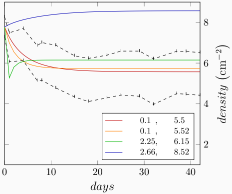

Sometimes we can only analyze traces of the model.

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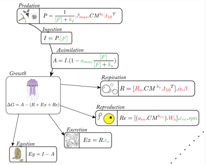

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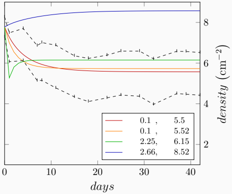
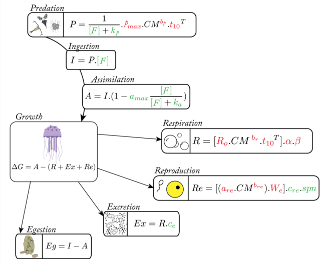


If Model ∼ Traces
⇒ Checking φ on the traces is equivalent to checking it on the model.

φ

Property

Why Probabilistic models?



Uncertainty and variability

- Several experiments

  $\Rightarrow$ data uncertainty.
- Family of systems

  $\Rightarrow$ parameters variability.

Statistical Model Checking for ODE models

SMC: answering “how good is a model?”

The Monte-Carlo procedure:

1. Randomly generate N samples $(\sigma_1, \ldots, \sigma_N)$ from the model M.
2. Check whether the sample i satisfies the property φ.
   $X_i = 1 \Leftrightarrow \sigma_i \models \varphi$
3. Compute the estimator $\hat{p} = \frac{\sum X_i}{N}$.

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Central Limit Theorem

- $\hat{p} \sim \mathbb{E}(X)$ $\Rightarrow \hat{p}$ is a good estimation of $p = \mathbb{P}(M \models \varphi)$.
- **precision α, risk θ.**

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Application to ODE models

[Liu et al. 2019] Statistical Model Checking-Based Analysis of Biological Networks.

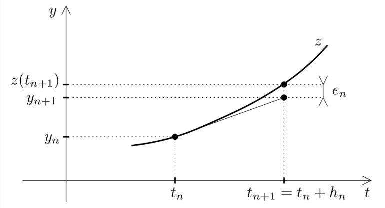
Automated Reasoning for Systems Biology and Medecine

Parameter analysis of ODE models with variability.

Problem: Approximations

Model $\not\approx$ Traces

Approximation error stacks up at each step: $\varepsilon = \max_n e_n$
$\Rightarrow$ SMC estimation does not apply to the original ODE model.



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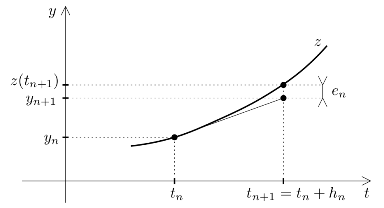

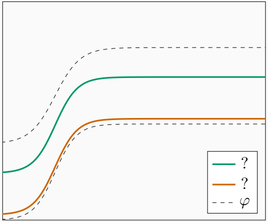

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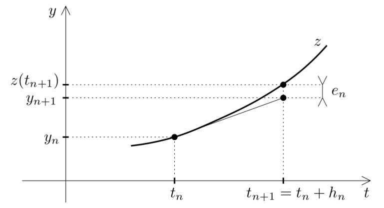

Solution: Safety margins

Proposition

If we can bound the approximation error ε on the value space, then we can define new properties $\varphi_- =$ "$\varphi - \varepsilon$" and $\varphi_+ =$ "$\varphi + \varepsilon$" to check.

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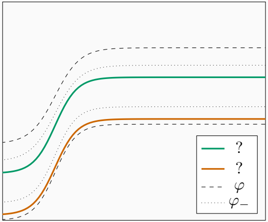

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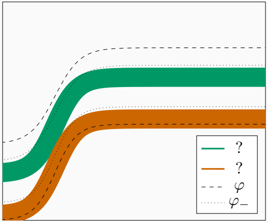

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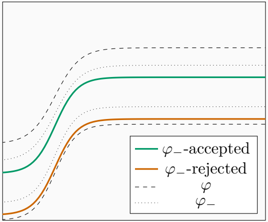

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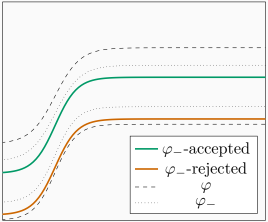

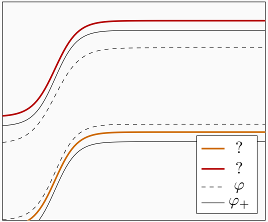

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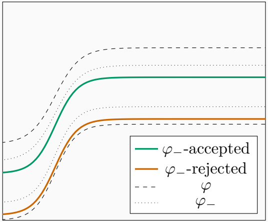

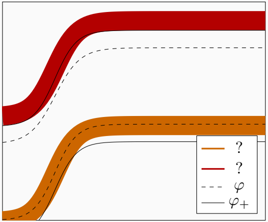

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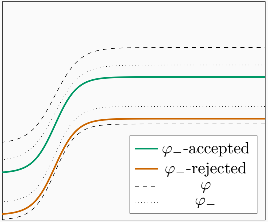

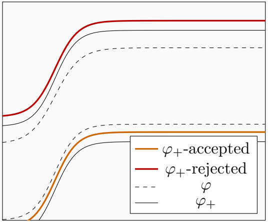

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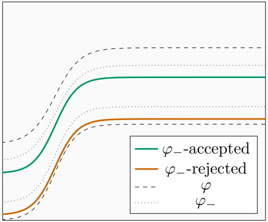

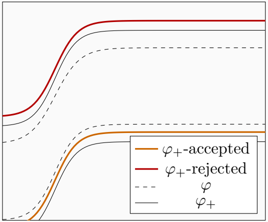

Guarantees: global risk ξ and precision α

Usual SMC

- $n = \frac{\log(2/\xi)}{2\alpha^2}$ simulations.

$\Rightarrow \mathbb{P}(p \in [\hat{p} - \alpha, \hat{p} + \alpha]) \geq 1 - \xi$

In our case (for each property)

- SMC risk $\theta = 1 - \sqrt{1 - \xi} < \xi$
- $n' = \frac{\log(2/\theta)}{2\alpha^2} > n$ simulations

$$\Rightarrow \mathbb{P}(p_- \in [\hat{p}_- - \alpha, \hat{p}_- + \alpha]) \geq 1 - \theta, \quad \mathbb{P}(p_+ \in [\hat{p}_+ - \alpha, \hat{p}_+ + \alpha]) \geq 1 - \theta$$

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Main Theorem

After performing $N = 2 \times n'$ simulations, the following statements hold:

- $\mathbb{P}(p \in [\hat{p}_- - \alpha, \hat{p}_+ + \alpha]) \geq 1 - \xi$;
- $\mathbb{P}(|\hat{p}_- - \hat{p}_+| \leq 3\alpha) \geq 1 - \xi$.

Bonus: extension to reward functions.

Parameterization and stability analysis

Parameterization

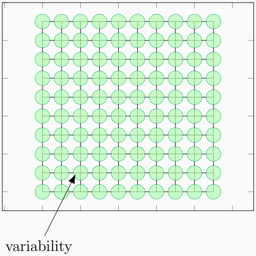
- Parameterization: Find parameter values λ for a generic model.

- Goal: Find good values for λ w.r.t. score $(\mathbb{E}(r))$ of φ-satisfaction.

- Any algorithm:
  - Local search: low execution time / superficial search;
  - **Global** search: more informative / higher execution time;
  - ...

What we do

1. Compute the grid of parameters.
2. Compute the score of each value.
3. Select the best value.



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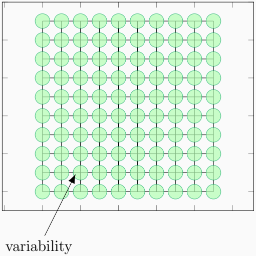

Reminder

It only works if we can bound the error ε!

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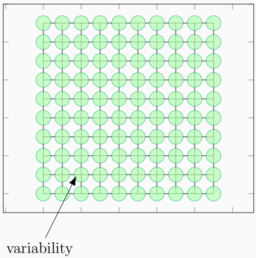

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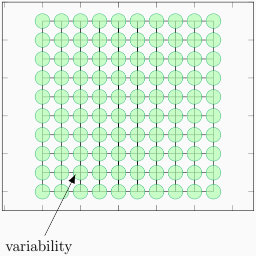

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Lemma 1

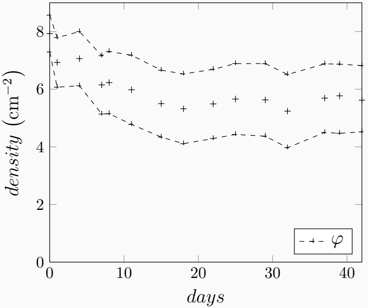
For any arbitrary $\varepsilon > 0$, there exists an integration step h such that

$$0 < \varepsilon_h < \varepsilon, \quad \forall \lambda.$$

POC: Aurelia Aurita[2]

Jellyfish species from the Adriatic Sea.

- $x'(t) = a \cdot x(t) \cdot \left(1 - \frac{x(t)}{b}\right)$
- $\varphi =$ data $\pm$ standard error



[2][Melica et al. 2014] Logistic density-dependent growth of an aurelia aurita polyps population. *Ecological Modeling*.

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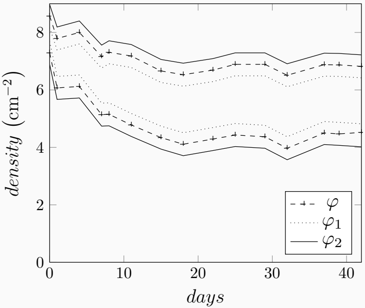

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Parameter analysis

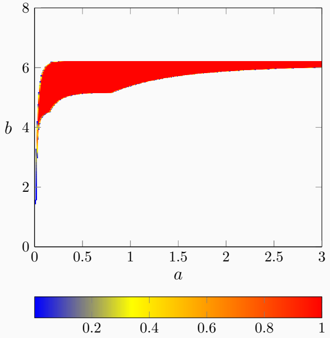

Fig. 1: Probability of staying in the tunnel.

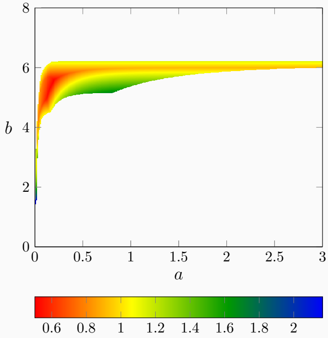

Fig. 2: Expected distance to data.

Stability

- Stability analysis: Find whether the trajectories of a generic model deviate from its initial condition x_0.

- Goal: Find good values for x_0 w.r.t. score $(\mathbb{E}(r))$ of stability.

- Any algorithm:
  - Local search: low execution time / superficial search;
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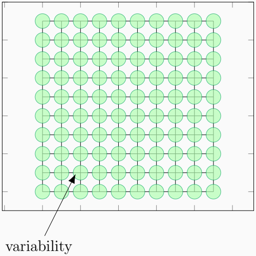
What we do

1. Grid of **initial conditions**.
2. Compute the score of each value.



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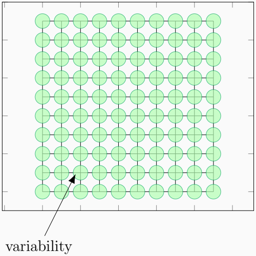

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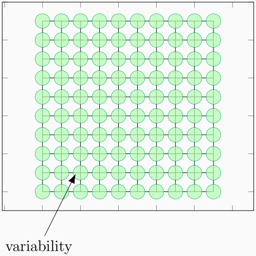

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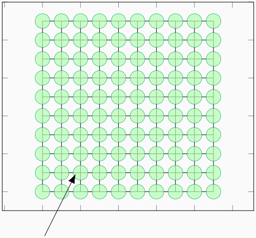

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Lemma

For any arbitrary $\varepsilon > 0$, there exists an integration step h such that

$$0 < \varepsilon_h < \varepsilon, \quad \forall \lambda.$$

POC: Duffing's oscillator[3]

Non-linear second order equation used to model damped and driven oscillators.

- $\begin{cases} \frac{\mathrm{d}x_1(t)}{\mathrm{d}t} = x_2(t), \\ \frac{\mathrm{d}x_2(t)}{\mathrm{d}t} = -bx_1(t) - ax_2(t) - dx_1(t)^3 cx_1(t)^2 x_2(t). \end{cases}$
- $\varphi =$ "Stability around x_e."

Stability

Lyapunov: For every $\delta > 0$, there exists $\rho > 0$ such that $\| x(0) - x_e \| < \rho \Rightarrow \| x(t) - x_e \| < \delta$, for all $t > 0$.

[3][Holmes et al. 1980] Phase portraits and bifurcation of the non-linear oscillator $\ddot{x} + \alpha\dot{x} + \gamma x^2 \dot{x} + \beta x + \delta x^3 = 0$. *International Journal of Non-Linear Mechanics.*

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- $\begin{cases} \frac{\mathrm{d}x_1(t)}{\mathrm{d}t} = x_2(t), \\ \frac{\mathrm{d}x_2(t)}{\mathrm{d}t} = -bx_1(t) - ax_2(t) - dx_1(t)^3 cx_1(t)^2 x_2(t). \end{cases}$
- $\varphi =$ "**(ρ, δ)-stability around x_e.**"

Relaxed stability

(ρ, δ)-stability: $\| x(0) - x_e \| < \rho \Rightarrow \| x(t) - x_e \| < \delta$, for all $t \in [T_1, T_2]$.

[3] [Holmes et al. 1980] Phase portraits and bifurcation of the non-linear oscillator $\ddot{x} + \alpha\dot{x} + \gamma x^2 \dot{x} + \beta x + \delta x^3 = 0$. *International Journal of Non-Linear Mechanics.*

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- $\varphi_- =$ "$\varphi - \varepsilon$"
- $\varphi_+ =$ "$\varphi + \varepsilon$"

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Stability analysis

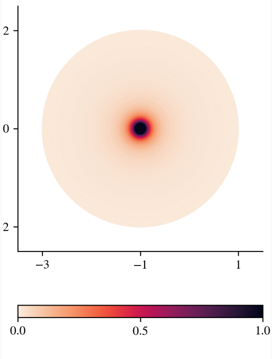

Fig. 3: Stability of $x_e = (-1, 0)$, $\delta = 0.5$.

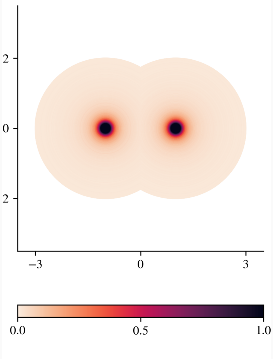

Fig. 4: Stability of $x_{e,1} = (-1, 0)$ and $x_{e,2} = (1, 0)$.

Basins of attraction

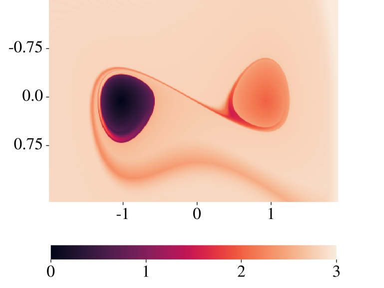

Fig. 5: Basin of attraction of $x_{e,1}$.

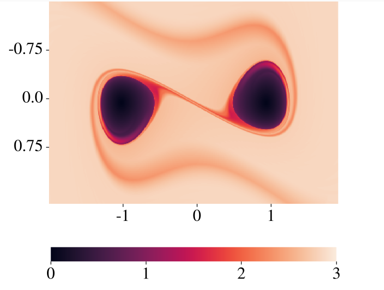

Fig. 6: Basin of attraction of $x_{e,1}$ and $x_{e,2}$.

Abstraction of ODE systems

Context

Formal verification for hybrid systems

- Existing formalisms not adapted for real life systems
- Need for discrete control of ODE models
- Need for formal verification of such models

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Objective

New discrete abstraction for ODE models, that can be combined with discrete control

▶ The hybrid model $(\mathcal{H})$ determines a piecewise deterministic dynamical system, with random jumps:

$$(\mathcal{H})\begin{cases}\dfrac{dU}{dt}=f(U,\lambda_k), k\tau\leq t\leq (k+1)\tau, k\geq 0, \lambda_k\in\Lambda, U\in\Phi,\\ U\big((k+1)\tau^-\big)\mapsto U\big((k+1)\tau\big),\\ \lambda_k\mapsto\lambda_{k+1},\\ (U_0,\lambda_0)\in\Phi\times\Lambda.\end{cases}$$

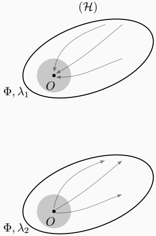

Fig. 7: Trajectories of the hybrid model.

Trajectories of a hybrid model

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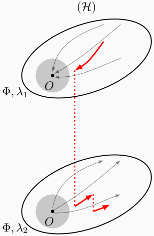

Fig. 7: Trajectories of the hybrid model.

Verification of dynamical properties

▶ Our aim is to verify, using (statistical) Model Checking, several dynamical properties of the hybrid model $(\mathcal{H})$:

- invariance of a neighborhood of the persistence equilibrium,
- reachability of a neighborhood of the persistence equilibrium,
- oscillations between persistence and extinction,
- emergent and chaotic behaviors.

▶ We construct an abstraction of the hybrid model as a discrete Markov decision process.

Design and properties of the abstraction

▶ Abstraction ($\mathcal{M}_{\psi,\tau,\Lambda}$) of the hybrid model as a Markov decision process
Depends on property ψ, time step τ, parameter space Λ.

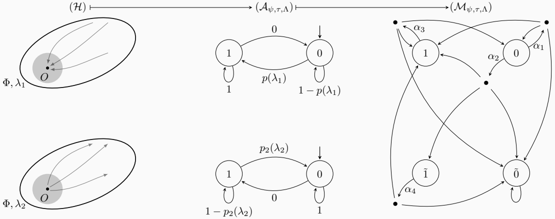

Fig. 8: Abstraction of the hybrid model.

▶ We can use (S)MC on ($\mathcal{M}_{\psi,\tau,\Lambda}$).

▶ Questions on the abstraction $\mathcal{H} \mapsto \mathcal{M}_{\psi,\tau,\Lambda}$: well-defined? computable? complexity? one-to-one? bisimulation? image of a property? invertible?

Example: avoid the extinction

- We consider the property "Avoid **O** after time **T**"

$$\psi_O(\rho, T) = \{\mathbb{U}(t, U_0, \lambda_0) \notin B(O, \rho), t \geq T\}.$$

$\rightsquigarrow$ Its image becomes $\tilde{\psi}_O(\rho, T) = \{\pi(t_s) \notin (1) \cup (\tilde{1}), t_s \geq T\}$.

Proposition / Intuition

Let $\rho^* > \rho$. Assume that $\mathbb{P}\big(\{\mathcal{M}_{\psi,\tau,\Lambda} \models \tilde{\psi}_O(\rho^*, T)\}\big) = 1$. Assume moreover the interpolation condition:

$$\forall k \geq 0, \quad U(t_k) \notin B(O, \rho^*) \wedge U(t_{k+1}) \notin B(O, \rho^*)$$
$$\Rightarrow U(t) \notin B(O, \rho), t_k \leq t \leq t_{k+1}.$$

Then we have

$$\mathbb{P}\big(\{\mathcal{H} \models \psi_O(\rho, T)\}\big) = 1.$$

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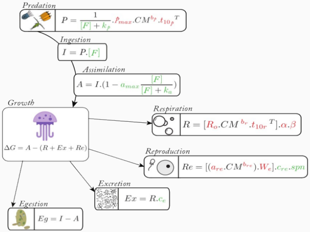
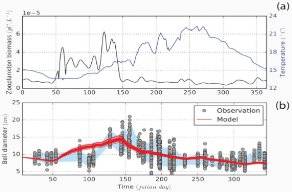
Applications

Goal : Parameterize a growth model of *Pelagia Noctiluca* that fits experimental data

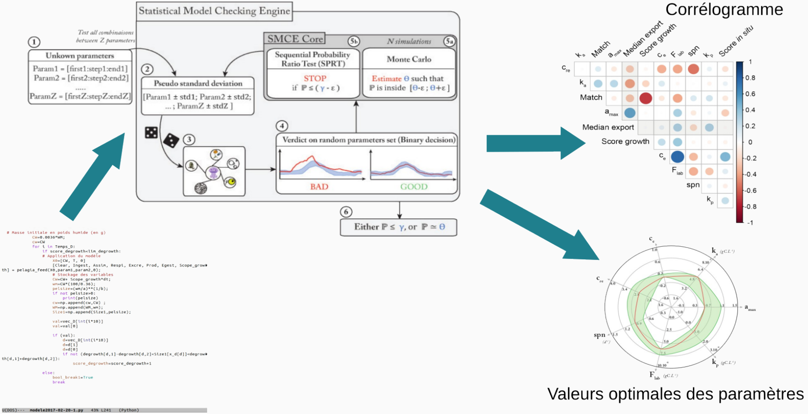


+ Données expérimentales

```
# Masse initiale en poids humide (en g)
            CW=0.0036*WM;
            cw=CW
            for i in Temps_D:
                if score_degrowth<lim_degrowth:
                # Application du modèle
                    X0=[CW, T, 0]
                    [Clear, Ingest, Assim, Respi, Excre, Prod, Egest, Scope_grow
th] = pelagia_feed(X0,param1,param2,0);
                    # Stockage des variables
                    CW=CW+ Scope_growth*dt;
                    wm=CW*(100/0.36);
                    pelsize=(wm/a)**(1/b);
                    if not pelsize>0:
                        print(pelsize)
                    cw=np.append(cw,CW) ;
                    WM=np.append(WM,wm);
                    Size1=np.append(Size1,pelsize);

                    val=vec_D[int(i*10)]
                    val=val[0]

                    if (val):
                        d=vec_D[int(i*10)]
                        d=d[1]
                        d=d[0]
                        if not (degrowth[d,1]-degrowth[d,2]<Size1[x_d[d]]<degrow
th[d,1]+degrowth[d,2]):
                            score_degrowth=score_degrowth+1

                else:
                    bool_break1=True
                    break

U(DOS)---  modele2017-02-20-1.py   43% L241   (Python)
```



Pelagia Noctiluca 2/2

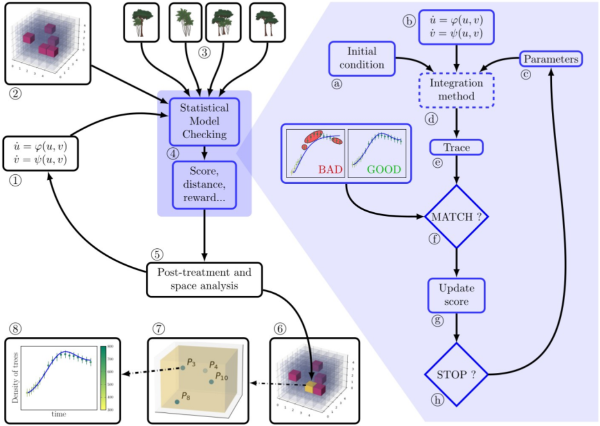


▶ S. Ramondenc, D. Eveillard, L. Guidi, F. Lombard, B. Delahaye. *Probabilistic modeling to estimate jellyfish ecophysiological properties and size distributions.* In Scientific Reports, Vol 10-1, pp 1-13, 2020.

Paracou forest regrowth 1/2

Computational assessment of Amazon forest patches regrowth capacity under strong spatial variability

Authors (by alphabetical order): Gilles Ardourel[1], Guillaume Cantin[1,2] Benoît Delahaye[1], Géraldine Derroire[3], Beatriz M.Funatsu[4], David Julien[1].



Paracou forest regrowth 2/2

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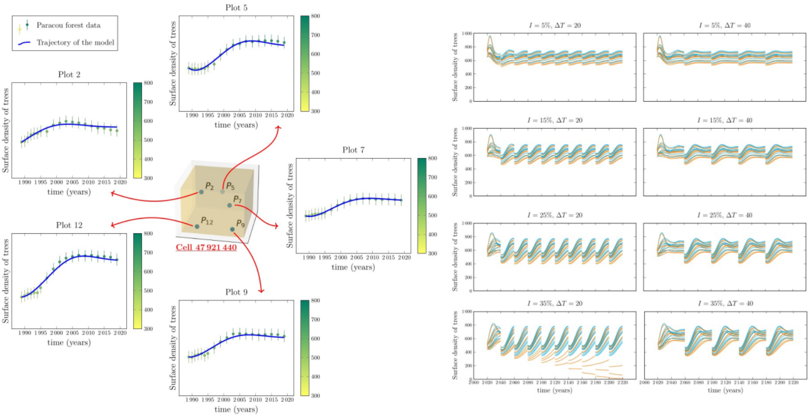

Perspectives and future work

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Lots of things to do...

- Dynamic discretization of the parameter grids
- Choice of the integration step
- Guarantees w.r.t. abstraction + coupling with discrete control
- Application to genomic synthesis / epidemiology
- ...

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- Dynamic discretization of the parameter grids
- Choice of the integration step
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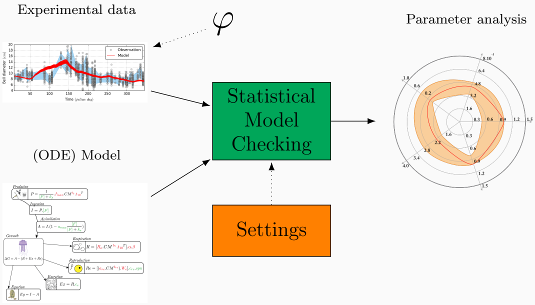
Going further...

- Link/Combination with NN to speed up sampling
- Formal guarantees?
- Link/Combination with agent models
- ...

End

Thanks!



Experimental data
φ
Statistical Model Checking
(ODE) Model
Settings
Parameter analysis

Supplementary materials

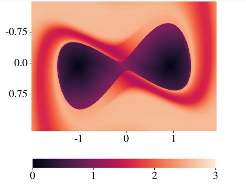


Fig. 9:
$\lambda = (-0.8, -1, 1, 1)$.

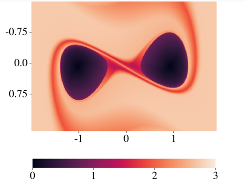


Fig. 10:
$\lambda = (-0.9, -1, 1, 1)$.

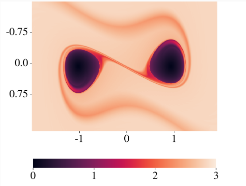


Fig. 11:
$\lambda = (-1, -1, 1, 1)$.

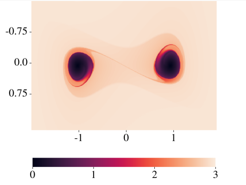


Fig. 12:
$\lambda = (-1.1, -1, 1, 1)$.

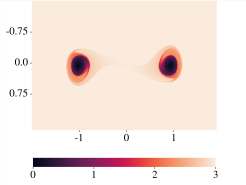


Fig. 13:
$\lambda = (-1.2, -1, 1, 1)$.