Validation des modèles de simulation en géographie: nouvelles pratiques et perspectives

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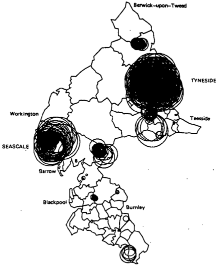
Séminaire EpisteMod

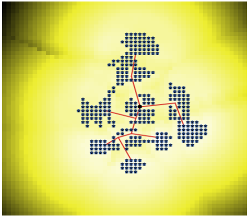
IHPhST

October 9th 2018

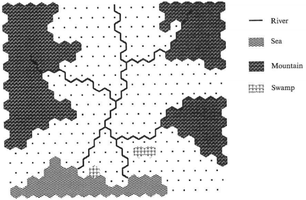
Une longue histoire de modélisation et simulation en TQG



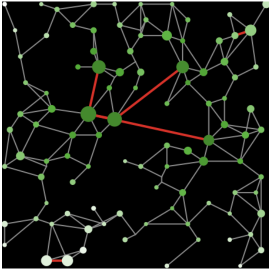
Machine d'analyse géographique [Openshaw et al., 1987]



Morphogenèse urbaine hybride [Raimbault et al., 2014]



Modèle Simpop 1 [Sanders et al., 1997]



Modèle SimpopNet [Schmitt, 2014]

Système géographique et complexité

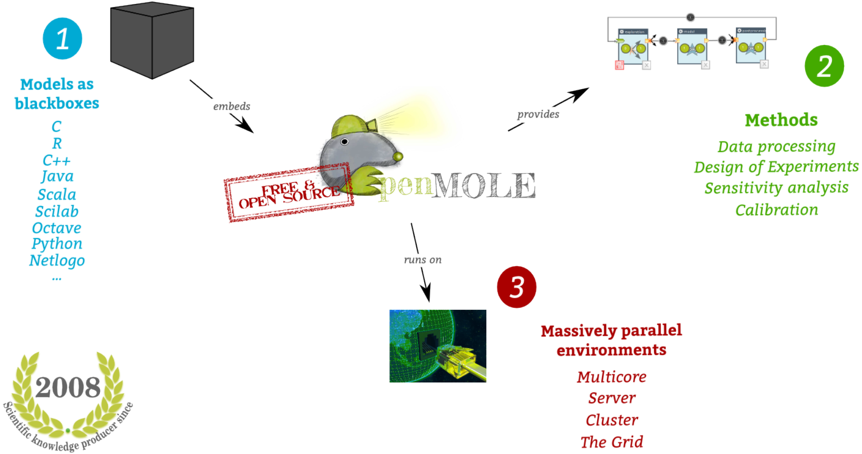
Validation des modèles de simulation

Vers de nouvelles pratiques: ERC Geodivercity

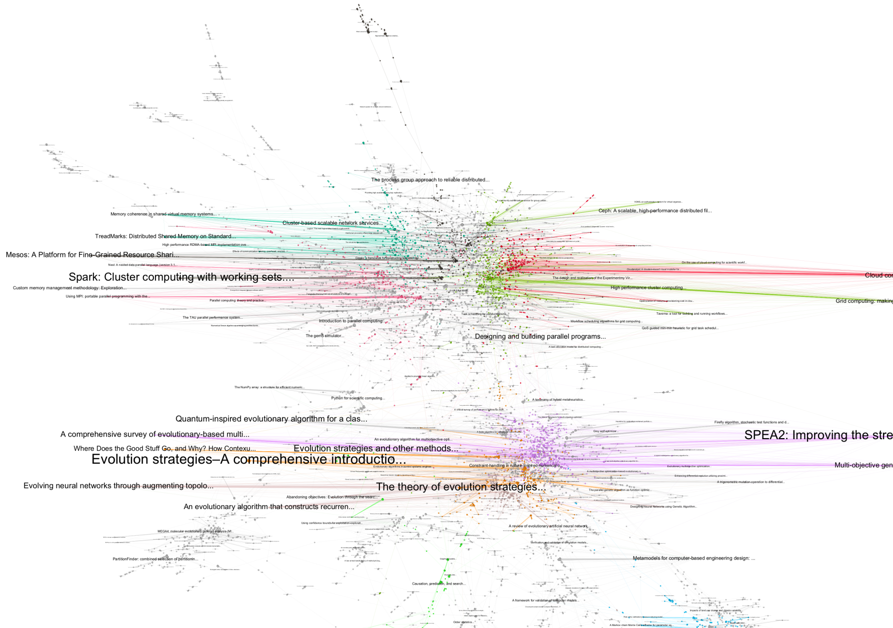
Méthodes et outils: OpenMOLE

Manifeste d'OpenMOLE

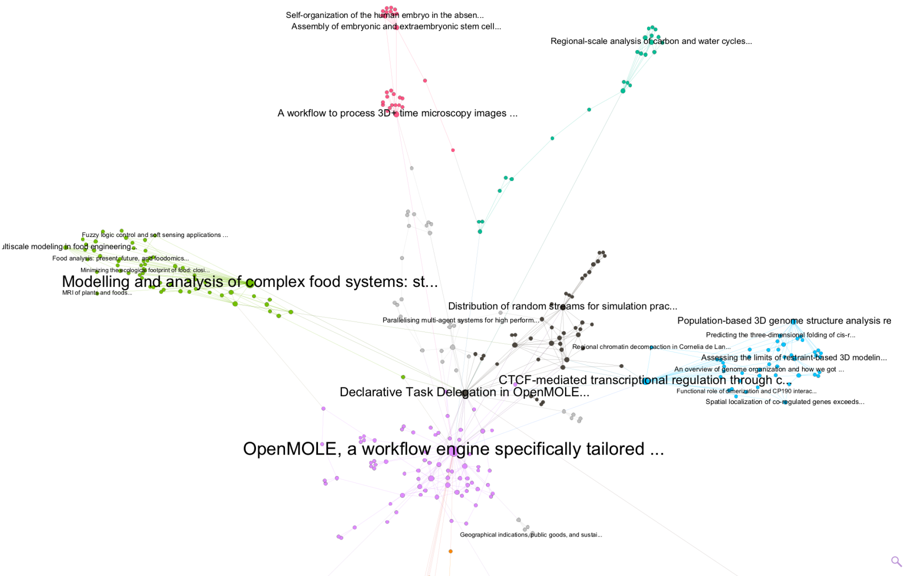
(i) Méthodes d'exploration innovantes; (ii) Passage à l'échelle par calcul distribué; (iii) Pas d'interférence avec le modèle.



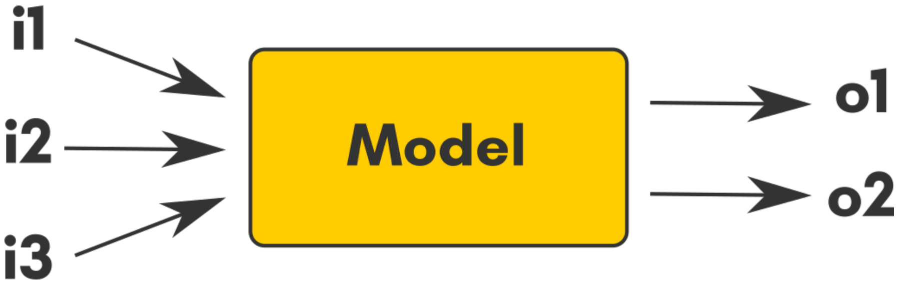
Citation network analysis (full)



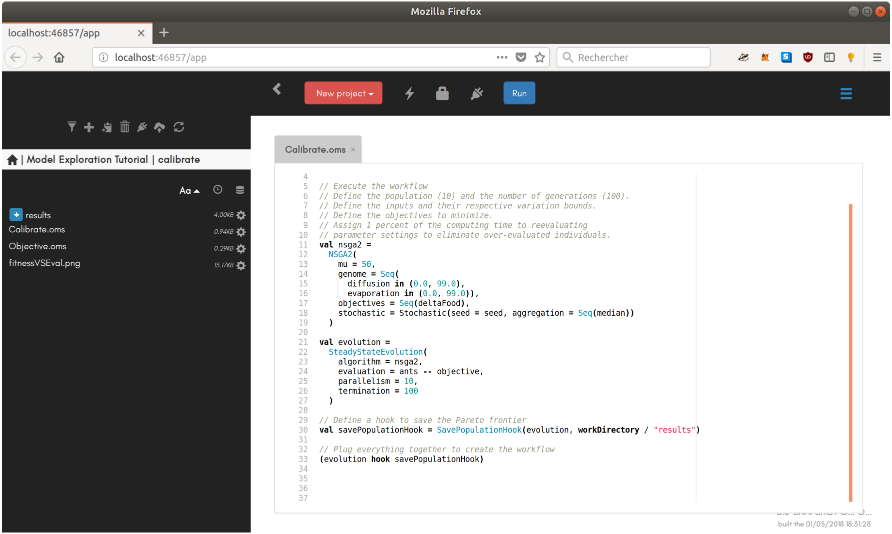
Citation network analysis (OpenMOLE)



Modèles de simulation



Une interface web ergonomique



Agnostique aux langages

Modèle NetLogo

```
val model =
  NetLogo6Task(
    workDirectory / "Fire.nlogo",
    List("setup", "while [any? turtles] [go]")) set (
    inputs += seed,
    outputs += (seed, density),
    inputs += density mapped "density",
    outputs += burned mapped "burned-trees"
  )
```

Code R

```
val i = Val[Int]

val rTask =
  RTask("""
    source("function.R")
    function(i)""") set (
    resources += workDirectory / "function.R",
    inputs += i
  )
```

Code Python en package

Package

```
care -o python.tgz.bin python matrix.py data.csv 1 out.csv
```

Run

```
val pyTask =
  CARETask(
    workDirectory / "../python.tgz.bin",
    "python matrix.py data.csv 2 out.csv"
  )
```

Méthodes

- Reconstruction de données
- Estimation de paramètres
- Analyse de sensibilité
- Étude de robustesse
- Optimisation

Conçues pour passer à l'échelle, prendre en compte la stochasticité, être utilisable sur n'importe quel modèle et environnement de calcul.

Méthodes: scripting

```
DirectSampling(
  evaluation = myModel,
  sampling =
    LHS(
      500,
      diffusion in (10.0, 100.0),
      evaporation in (10.0, 100.0)
    )
)
```

Environnements de calcul

Passage à l'échelle

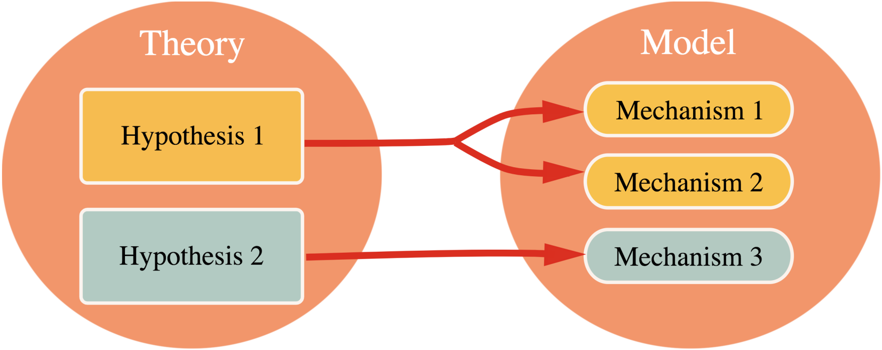
```
val cluster = SLURMEnvironment("login", "cluster.domain.org")

DirectSampling(
  evaluation = myModel on cluster,
  sampling =
    LHS(
      500,
      diffusion in (10.0, 100.0),
      evaporation in (10.0, 100.0)
    )
)
```

Environnements supportés

Supported environments today Multi-thread Delegation through SSH PBS SLURM Condor SGE OAR EGI Grid

Computer assisted modeling Build a general framework and algorithms to guide the modeling process.
Make the modeling process:
traceable: understand what choices were made, reproducible: recompute the reason why they were made, reusable: study alternative choices.

Modèles descriptifs



Descriptive models Design/evaluate a theory involving causal effects through its capacity to (re-)produce some patterns/data.

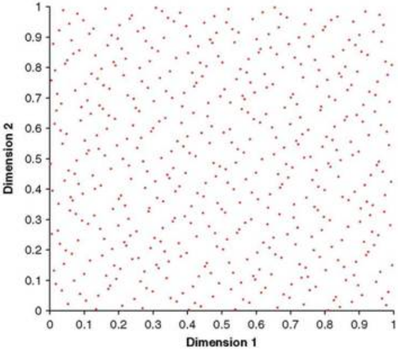
Model evaluation How to assess:

the sufficiency of the mechanisms ? the necessity of the mechanisms ?

the uniqueness of the mechanisms ?

Sufficiency

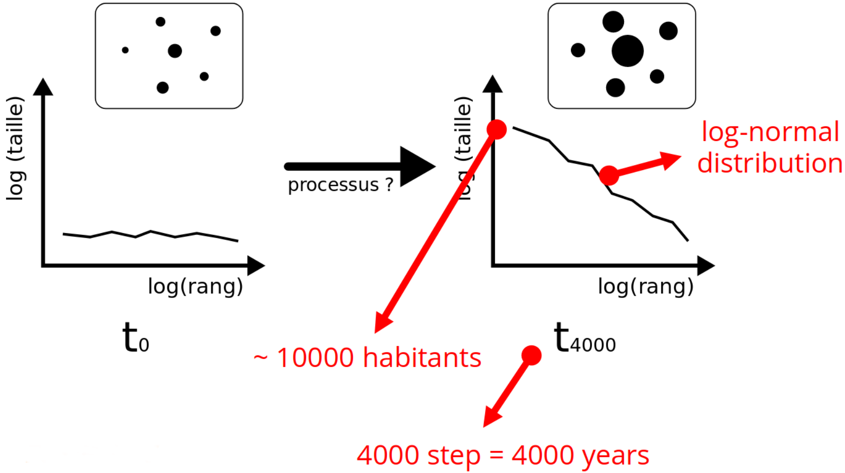
The usual approach Use a classical design of experiment.



Limits It produces a huge quantity of data. It transform a problem into a data-mining problem. The parameter space is mostly left unexplored due to the curse of dimensionality.

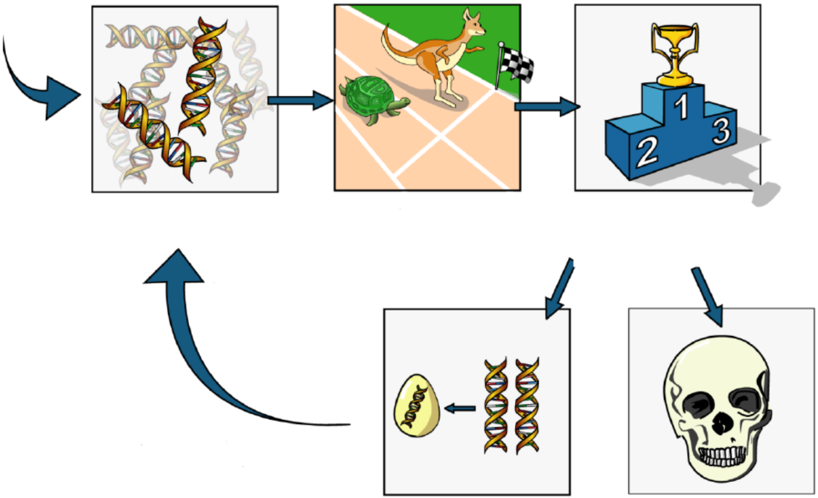
Proposed method

Reverse approach: From output values to parameter values.
Formalising the expectations



Calibration algorithm

Genetic algorithm as a calibration algorithm

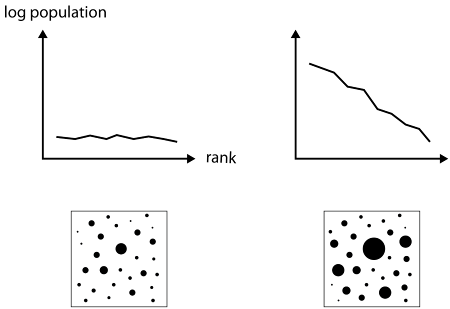


Calibration method Genome: 6 parameters of the model
Fitness: 3 descriptors of the quality of the simulated dynamic

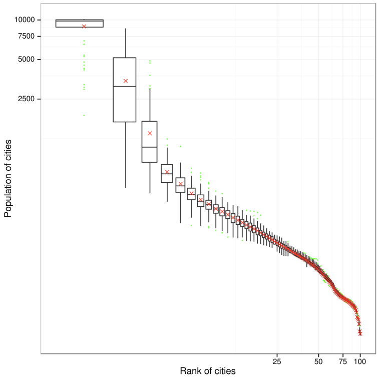
Calibration results

No compromise between the 3 objectives.

Searched pattern



Produced pattern

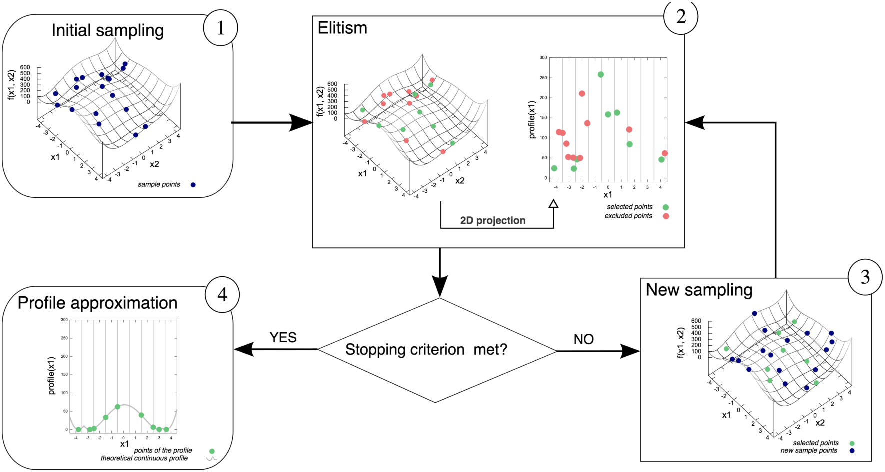


Evaluation approach Would not have been found using a direct method.
The method is tractable (even for ABMs):
Handles stochasticity: 100x gain. Support for distributed computing: 1000x gain.

Necessity

A new algorithm To detect if a parameter is useful: it impacts the capacity of the model to produce plausible outcomes.
To better constrain the parameter ranges.
As an indirect way to detect if some of the mechanisms are expandable
Objective Hundreds of calibrations

Algorithme des profils

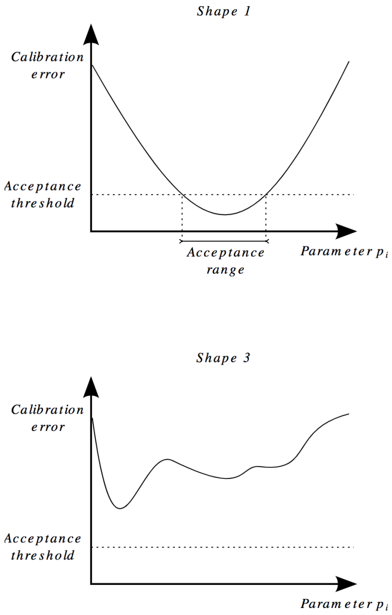


The profile algorithm Compute the best of calibration for hundreds of values along the definition domain of a parameter.

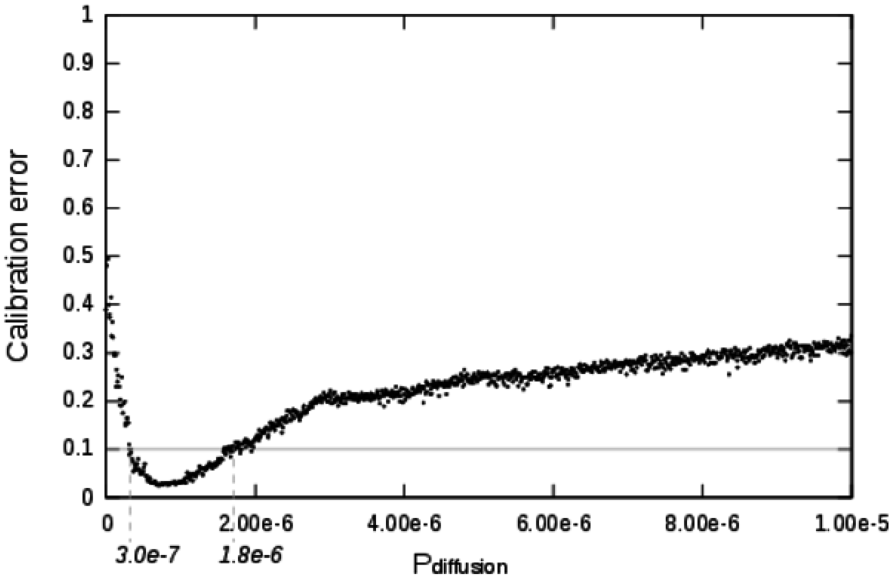
The method is tractable (even for ABMs):

Converges almost as fast a single calibration. Handles stochasticity: 100x gain. Support for distributed computing: 1000x gain.

Algorithme des profils

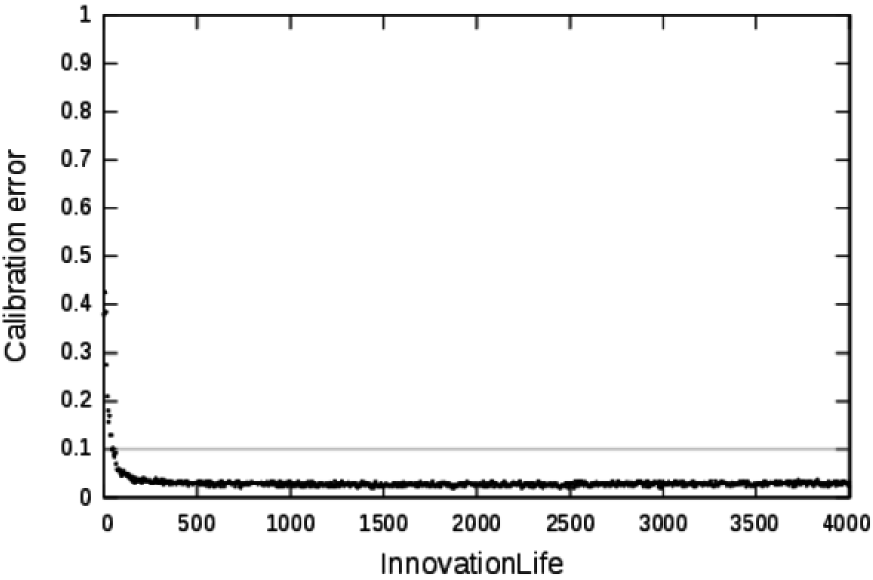


Results



Calibration error
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2.00e-6
4.00e-6
6.00e-6
8.00e-6
1.00e-5
3.0e-7
1.8e-6
Pdiffusion

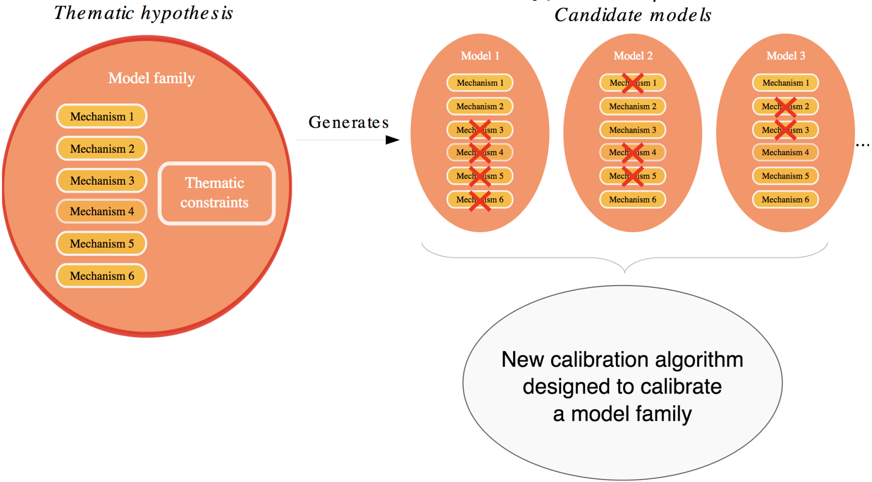
Results



Calibration error
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
500
1000
1500
2000
2500
3000
3500
4000
InnovationLife

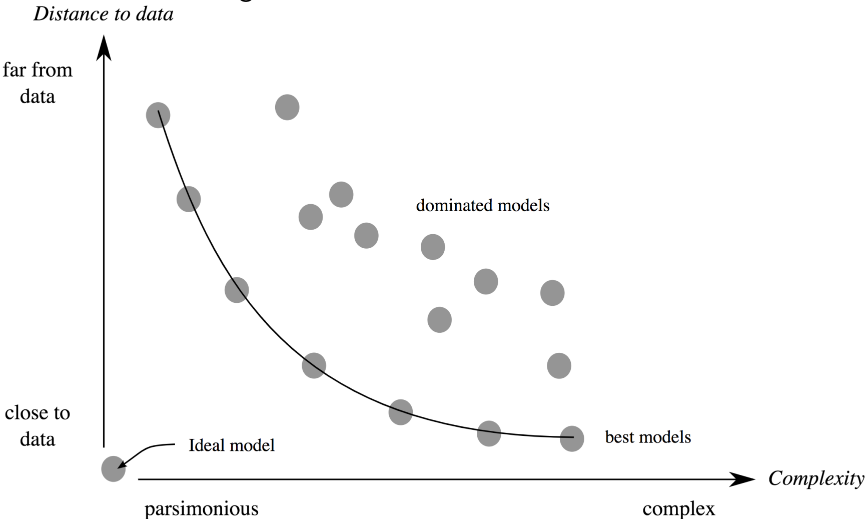
Uniqueness

Automate the confrontation of alternative hypothesis / mechanisms.



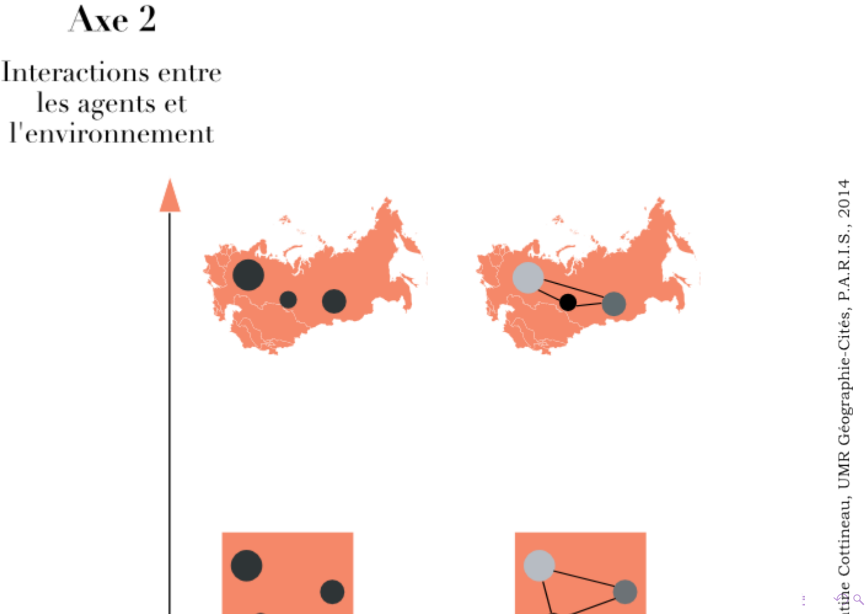
Objective

What we are running after?



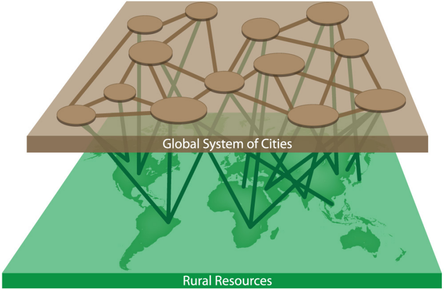
Multi-modeling

64 models



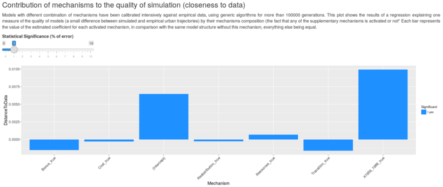
Example of concurrent hypotheses

Exchange mechanism:
Market based Centrally planned
City growth mechanism:
Purely inter-urban interactions Influenced by environmental situation



Model family calibration

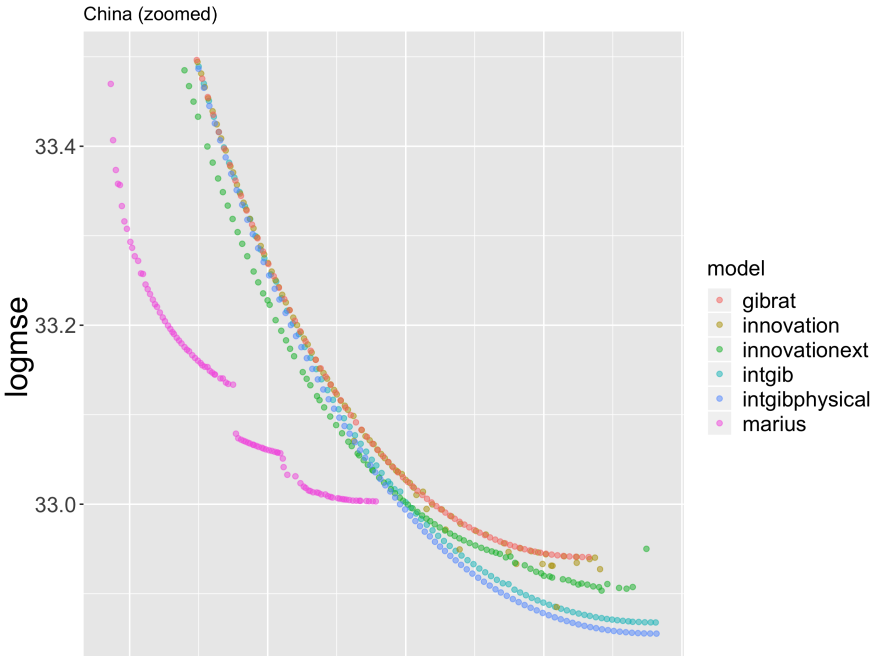
Compute the best set of parameters for all 64 models.



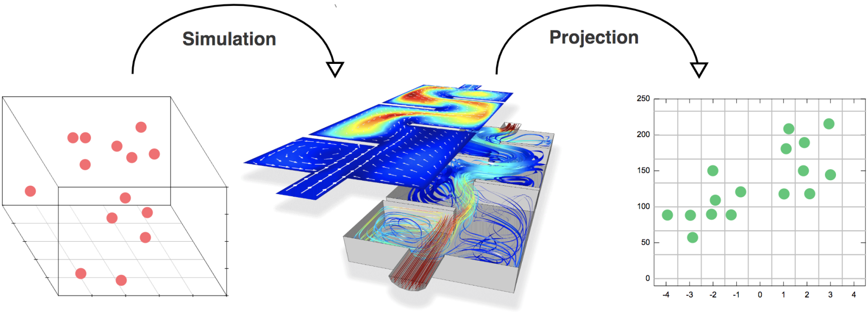
Calibration

Calibration method Algorithm principle: reuse the good parameters found on one model to calibrate on the others.
The method is tractable (even for ABMs):
as fast (faster ??) as calibrating a single model. Handles stochasticity: 100x gain. Support for distributed computing: 1000x gain.
Alternative approach All these methods are based on an a priori mesurement of the quality.
Can we propose an alternative approach to evaluation?

Autre exemple de multimodélisation



Pattern search



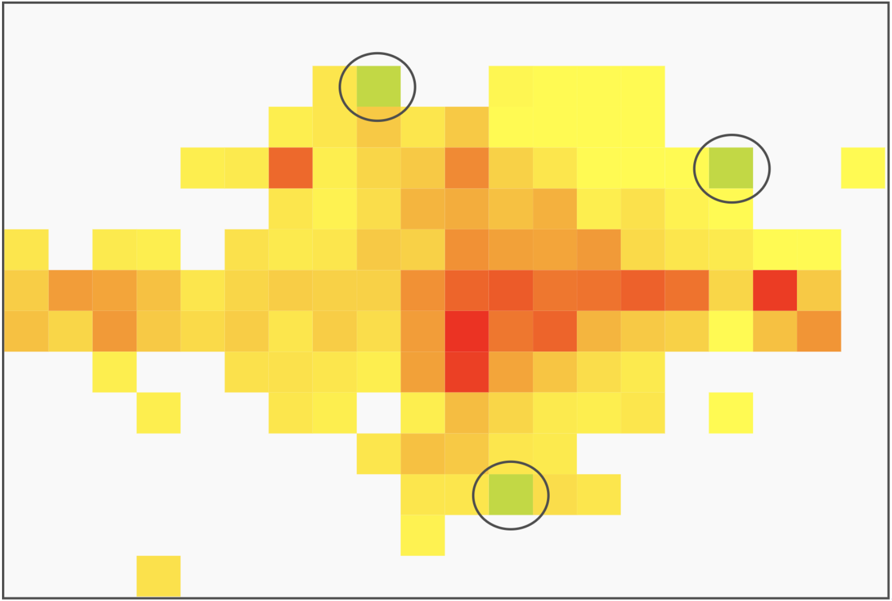
High dimension input space

High dimension space of dynamics

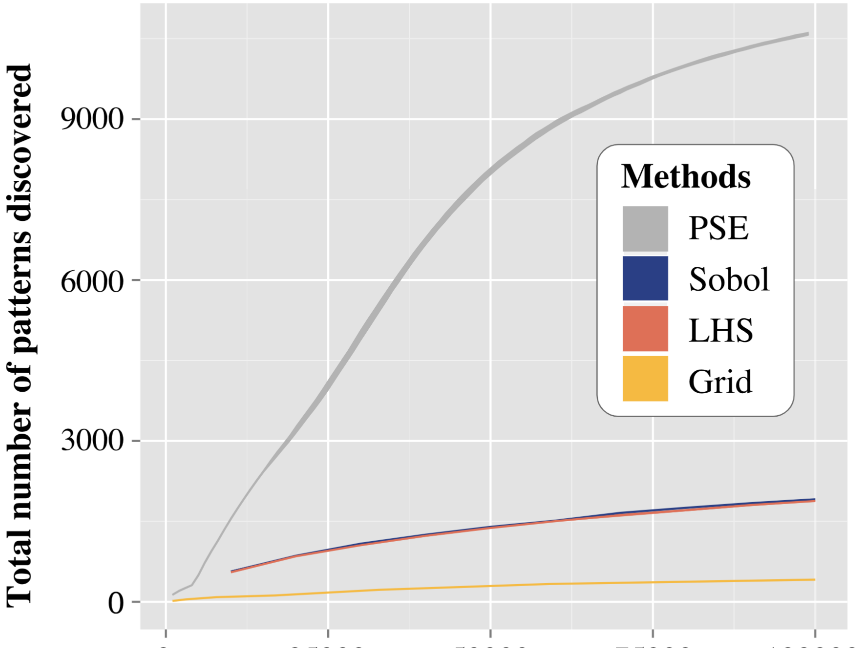
Low dimension space of patterns

Recherche de nouveauté

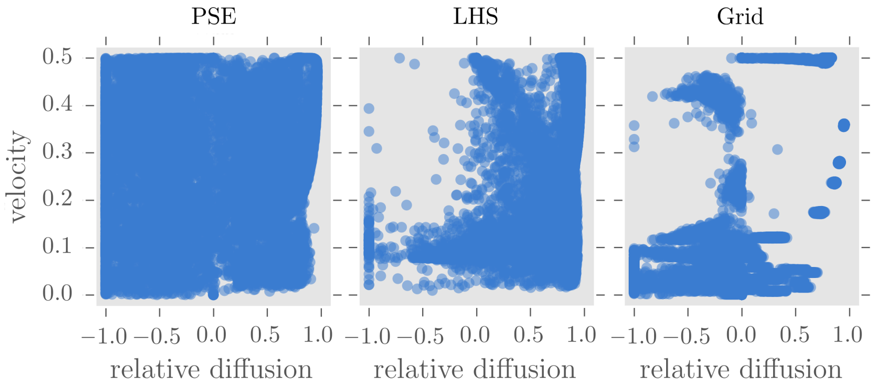
The inputs producing rare patterns have high fitness values.



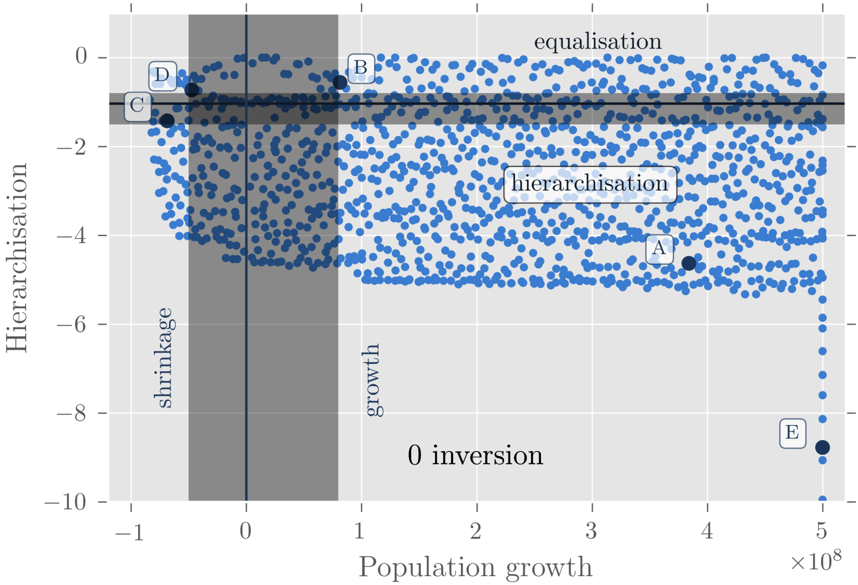
Résultats


Total number of patterns discovered
9000
6000
3000
0
Methods
PSE
Sobol
LHS
Grid

Résultats


PSE
LHS
Grid
velocity
0.5
0.4
0.3
0.2
0.1
0.0
−1.0 −0.5 0.0 0.5 1.0
relative diffusion
−1.0 −0.5 0.0 0.5 1.0
relative diffusion
−1.0 −0.5 0.0 0.5 1.0
relative diffusion

Résultats

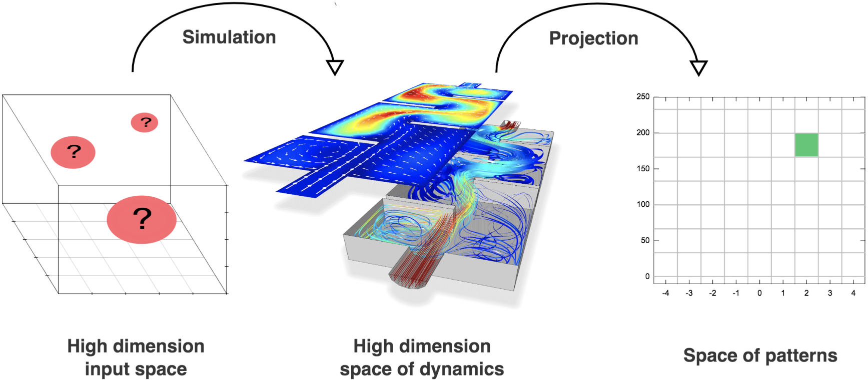


equalisation
hierarchisation
0 inversion
shrinkage
growth
A
B
C
D
E
Hierarchisation
Population growth
$\times 10^8$
0
−2
−4
−6
−8
−10
−1
0
1
2
3
4
5

G

F

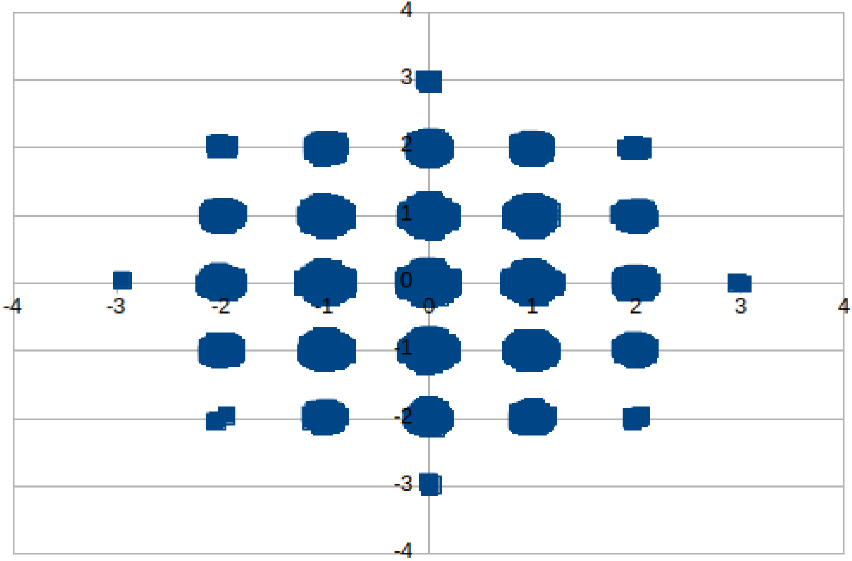
Origin search



First results

Formulation: Δ pattern $< \varepsilon$

f(x1, x2, .., xn) < 10



OpenMole's positioning

A qualitative shift in knowledge that can be extracted from a simulation model with model exploration methods.

Success stories: SimpopLocal [Schmitt et al., 2015], Marius [Chérel et al., 2015], Ecological modeling [Lavallée et al., 2018], epidemiology [Arduin, 2018], etc.

Key features:

- Unique role of complementary axis of computation environment access, methods providing, and model embedding.
- Iterative and integrated construction of models and theories, using all dimensions of knowledge enhanced by simulation and computation (modeling, theory, empirical, data, methods, tools [Raimbault, 2017].
- Coupling models and reproducibility at the core of the workflow approach [Passerat-Palmbach et al., 2017]

Perspectives and questions ouvertes pour la simulation en TQG

Question générales:

- Surajustement des modèles de simulation
- Couplage des modèles
- Direct and inverse mapping
- Stochasticité

Spécifiques aux systèmes spatio-temporels:

- Non-stationnarité spatio-temporelle
- Données synthétiques spatio-temporelles

Surajustement

Un perspectivisme appliqué pour coupler les approches de modélisation

Perspectivisme de Giere [Giere, 2010]: a "third way" beyond constructivism-realism: *Any scientific knowledge construction process as a perspective by an agent to answer a purpose with a media (model).*

Applied knowledge framework proposed by [Raimbault, 2017] to study [complex] systems: *co-evolution* of cognitive agents and knowledge domains, through the intermediate of perspectives.

Applied perspectivism principles:

- Foster consistence of perspectives and their communication (Banos' virtuous spiral between disciplinarity and interdisciplinarity)
- Importance of reflexivity to ease the coupling of perspectives
- New model exploration methods increase the integration between knowledge domains
- Coupling of models as a possible medium to couple perspectives (transfer hypothesis)

Still to be formalized, specified as possible implementations, and experimented.

Conclusion

Significant accomplishments beyond disciplines, construction of new research practices (see the satellite presentations) $\rightarrow$ still much to do ? (e.g. how to put into practice ? how to achieve true integration ? etc.)

Related works on epistemological considerations

Raimbault, J. (2017, December). An Applied Knowledge Framework to Study Complex Systems. In Complex Systems Design & Management (pp. 31-45). arXiv:1706.09244.

Raimbault, J. (2018). Caractérisation et modélisation de la co-évolution des réseaux de transport et des territoires (Doctoral dissertation, Université Paris 7 Denis Diderot). `https://halshs.archives-ouvertes.fr/tel-01857741`

Reserve Slides

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PhD thesis, Université Paris-Saclay.

Chérel, G., Cottineau, C., and Reuillon, R. (2015).
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PLoS ONE, 10(9):e0138212.

Giere, R. N. (2010).
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Openshaw, S., Charlton, M., Wymer, C., and Craft, A. (1987).
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Passerat-Palmbach, J., Reuillon, R., Leclaire, M., Makropoulos, A., Robinson, E. C., Parisot, S., and Rueckert, D. (2017).
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Sanders, L., Pumain, D., Mathian, H., Guérin-Pace, F., and Bura, S. (1997).
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Half a billion simulations: Evolutionary algorithms and distributed computing for calibrating the simpoplocal geographical model.
Environment and Planning B: Planning and Design, 42(2):300–315.