How MDO can help to address the energy transition as an optimal decision problem, with concrete illustrations of the GEMSEO framework features

François Gallard

Some results are from Ian Costa Alvez’s PhD, co adivsed with Anne Gazaix (IRT&Airbus) & Nicolas Gourdain (ISAE, Director)
Others from a collaboration with the SOS trades Team from Capgemini
And a collaboration with the AeroMAPS team
And of course GEMSEO contributors

Introduction

Achieving the **1.5°C global warming target** in 2100 while ensuring a viable economy will require to take many **decisions**.

Models can help to ensure that these decisions, (ex: SAF / H2/ Synthetic fuel to power aircraft ?) are **compatible with what we know of the physical world** (energy conservation, available resources, land use, aircraft design constraints).

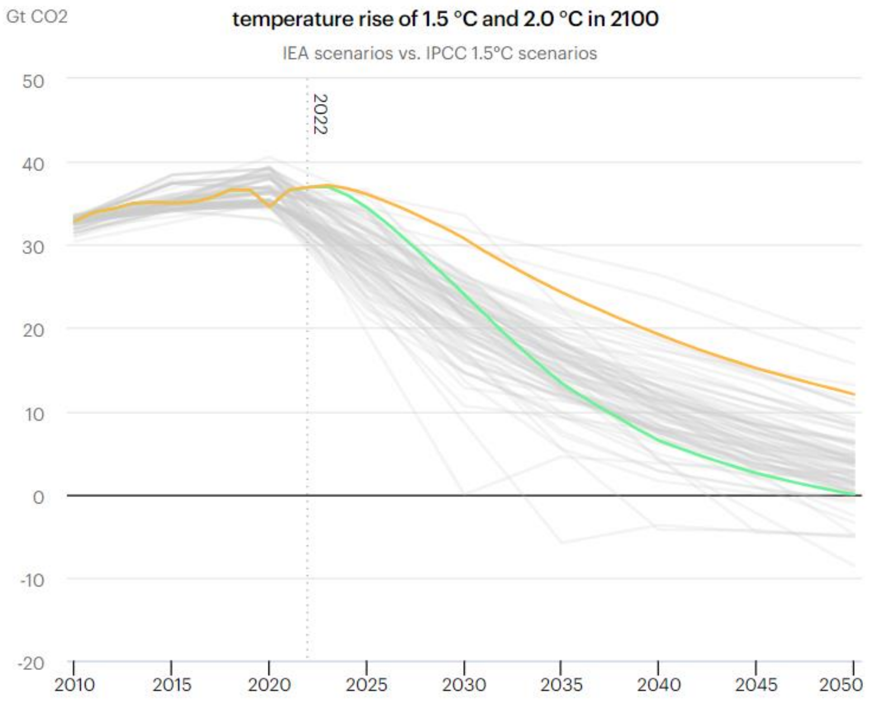
The **IAM** (Integrated Assessment Model) approach is widespread:

- **International Energy Agency scenarios**
- **IPCC**
- **DICE** (1992, W. Nordhaus, lead to Nobel price, still used by US environment agency)

⇒ In Toulouse :

- **AeroMAPS (ISAE)**
- **Witness (Capgemini / OS Climate)**

These two use a MDO framework, why?



Global Energy and Climate Model Scenario analysis of future energy trends
https://www.iea.org/reports/global-energy-and-climate-model
https://aeromaps.isae-supaero.fr/
https://www.witness4climate.org/sostrades-3/

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Introduction: why MDO?

“IAMs (Integrated Assessment Models) lie at the basis of the assessment of mitigation pathways in this chapter, as much of the quantitative global scenario literature is derived with such models. IAMs combine insights from various disciplines in a single framework, resulting in a dynamic description of the coupled energy–economy–land-climate system that cover the largest sources of anthropogenic greenhouse gas (GHG) emissions from different sectors”.

“Mitigation Pathways Compatible with 1.5°C in the Context of Sustainable Development”, IPCC report 2019, S15 Ch2.

“Multi-disciplinary design optimization (**MDO**) is a field of engineering that uses optimization methods to solve design problems incorporating all relevant disciplines simultaneously. The optimum of the simultaneous problem is superior to the design found by optimizing each discipline sequentially, since it can exploit the interactions (couplings) between the disciplines. However, including all disciplines simultaneously significantly increases the complexity of the problem.”
https://en.wikipedia.org/wiki/Multidisciplinary_design_optimization

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Introduction: why MDO frameworks can be useful for IAMs?

IPCC *“**Variations in scenario assumptions** and design define to a large degree which questions can be addressed with a specific scenario set, for example, the **exploration of implications of delayed climate mitigation** action.”*

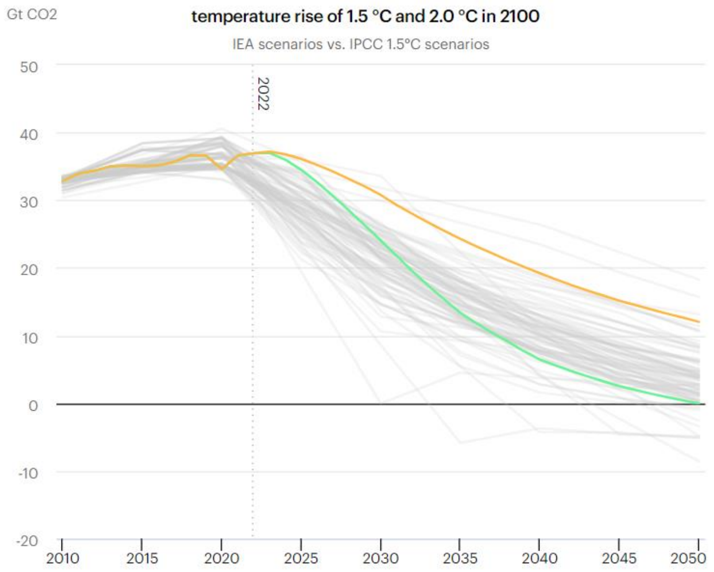
IEA : *“The GEC Model is used to **explore various scenarios, each** of which is built on a **different set of underlying assumptions** about how the energy system might evolve over time.”*

The problem with scenarios :

- *They **hide many parameters** that are changed consistently together (hidden hypothesis)*
- *How many scenarios can we compare through human analysis?*

Possible strategy : use an optimization (MDO) approach instead:

- Enables to **formalize** the problem underlying the exploration scenario in a comprehensive manner
- The **hidden** parameters are **optimized**
- Enables to solve this problem with **validated trade-off or optimization techniques**



- *On which **technology to invest** at which optimal moment ?*
- ***What aircraft type** should be on the market at what moment?*
- ***Can the constraints be satisfied** with the limited resources and available technology?*
- *Given the past data, **what are the parameters** of the model?*

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IPCC report “Mitigation Pathways Compatible with 1.5°C in the Context of Sustainable Development" , 2018

GEMSEO FEATURES

Study analysis
An intuitive tool to discover MDO without writing any code, and define the right MDO problem and process. From an Excel workbook, "specify your disciplines, design space, objective and constraints, "select an MDO formulation and plot both coupling structure (N2 chart) "and MDO process (XDSM), even before wrapping any software.

Read more | Examples

Optimization
Define, solve and post-process an optimization problem from an optimization algorithm.

Based on *GCMMA-MMA, NLopt, PDFO, pSeven, pymoo, SciPy.*

Read more | Examples | Algorithms

DOE & trade-off
Define, solve and post-process a trade-off problem from a DOE (design of experiments) algorithm.

Based on *OpenTURNS, pyDOE.*

Read more | Examples | Algorithms

MDO formulations
Define the way as the disciplinary coupling is formulated and managed by the optimization or DOE algorithm.

Read more | Examples | Algorithms

MDA
Find the coupled state of a multidisciplinary system using a Multi-Disciplinary Analysis.

Read more | Examples | Algorithms

Linear solvers
Define and solve a linear problem, typically in the context of an MDA.

Based on *PETSc, SciPy.*

Algorithms

Visualization
Generate graphical post-processings of optimization histories.

Read more | Examples | Algorithms

Surrogate models
Replace a discipline by a surrogate one relying on a machine learning regression model.

Based on *OpenTURNS, scikit-learn.*

Read more | Examples | Algorithms

Scalable models
Use scalable data-driven models to compare MDO formulations and algorithms for different problem dimensions.

Features: scalability study, scalable problem, scalable discipline, diagonal-based.

Read more | Examples

Machine learning
Apply clustering, classification and regression methods from the machine learning community.

Features: clustering, classification, regression, quality measures, data transformation.

Based on *OpenTURNS, scikit-learn.*

Read more | Examples | Algorithms

Uncertainty
Define, propagate, analyze and manage uncertainties.

Features: distribution, uncertain space, empirical and parametric statistics, distribution fitting, sensitivity analysis.

Based on *OpenTURNS.*

Read more | Examples | Algorithms

Ordinary differential equation
Define and solve an ordinary differential equation.

Based on *SciPy.*

Read more | Examples | Algorithms

IRT SAINT EXUPÉRY

MDO frameworks can provide **easy access to numerical methods** and assemble large scale MDO problems **automatically**.

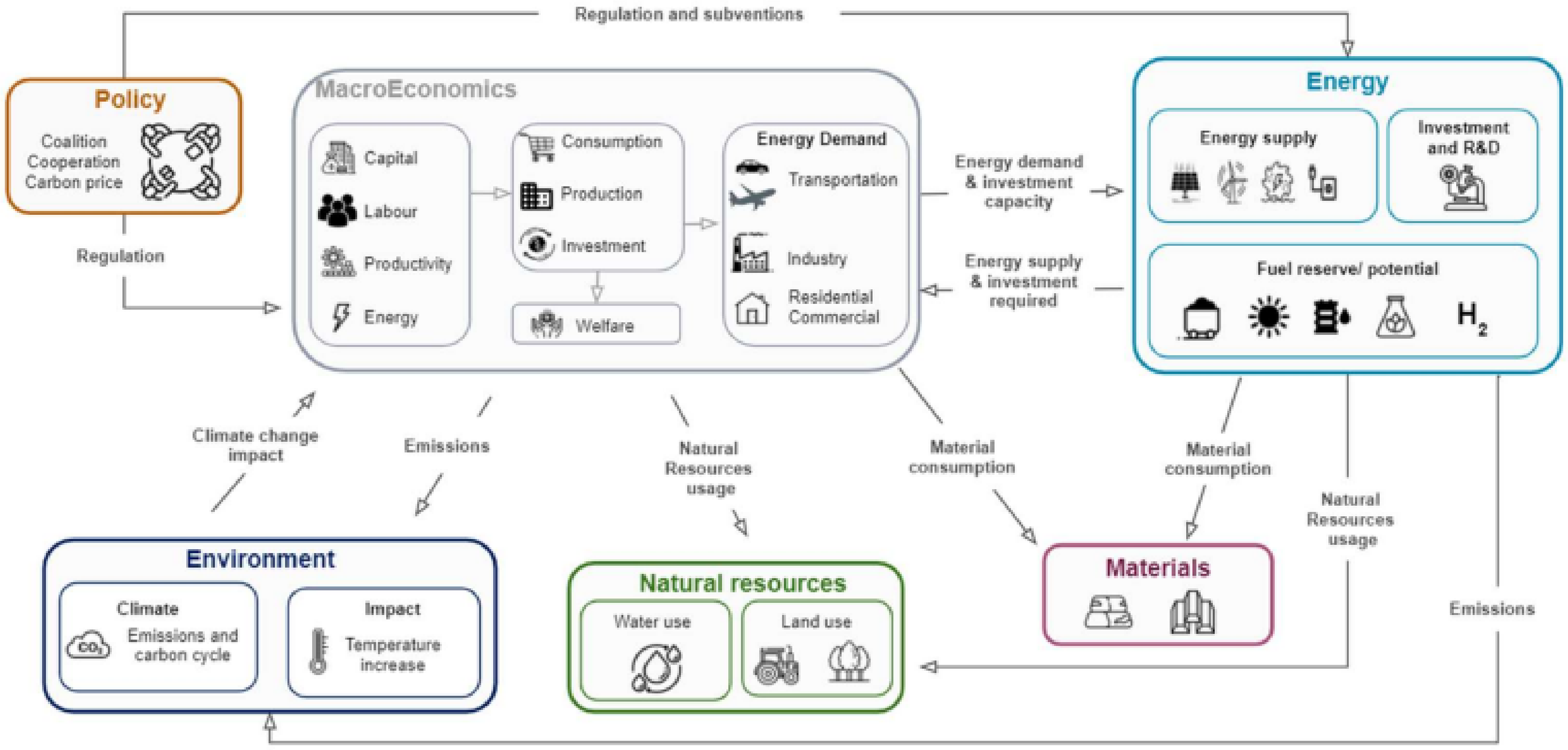
- Integration of state of the art methods and algorithms
- Full interoperability of the features
- Standardized interfaces
- Standardized documentation

Several IAMs using GEMSEO

The Witness IAM

For example, you can use WITNESS to answer such questions as :

- What would be the influence of carbon tax rate on transition evolution ?
- What would be the right parameters to link such tax evolution to, in order to get a good "autopilot" mode limiting need for new agreements to update it according to transition trajectory ?
- What is the potential of a new energy production technology ?



WITNESS : World environmental ImpacT aNd Economics ScenarioS

Complex system of systems simulation for energy transition OS-C Transition tool NAFEMS NRC France 2022
B Gauthier, M Morere, M Meaux, PJ Barjhoux, T Chevalier …and all the SoSTrades project team

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Witness

Objective	*maximize* **welfare** for a defined **CO_2 policy**
Design Variables	technology investment mixes *(from 2020 to 2100)*
Constraints	*(from 2020 to 2100):* – total energy production > energy lower bound – net energies production > energies demand – liquid fuel + H2 prod + H2 liquid production > % total production – solid fuel + electricity + biomass production > % total production – hydropower production < hydropower production in 2020 – H2 liquid production > %H2 total production – available land > land demand (for forest, agriculture....)

MDO GEMSEO

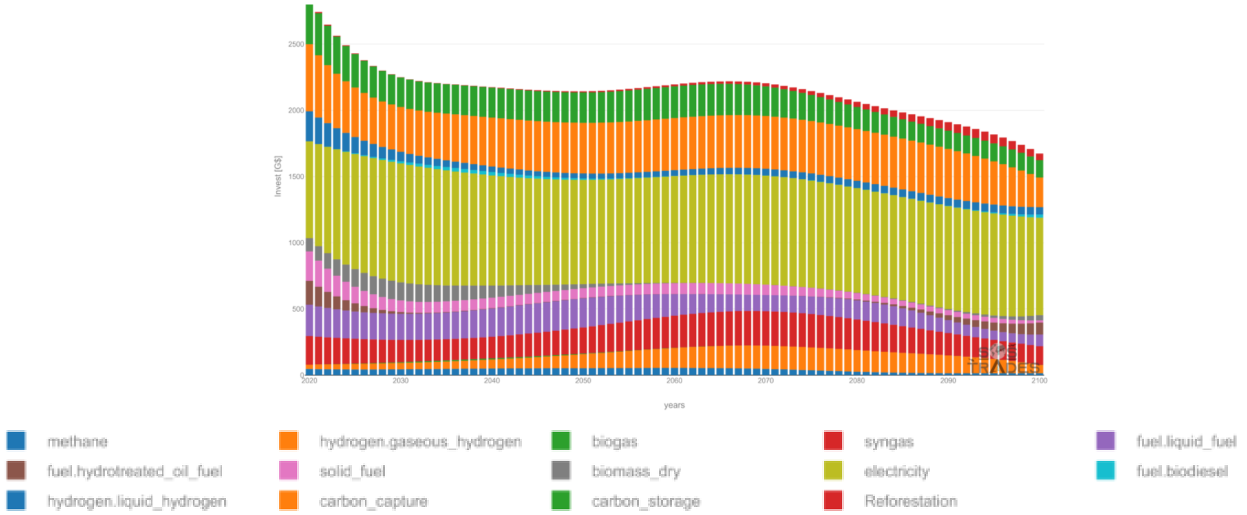
65 disciplines
424 design variables
261567 variables

MDA

63 disciplines
25064 coupling variables
262715 variables

solved in ~10 hours

Distribution of investiment on each energy vs time

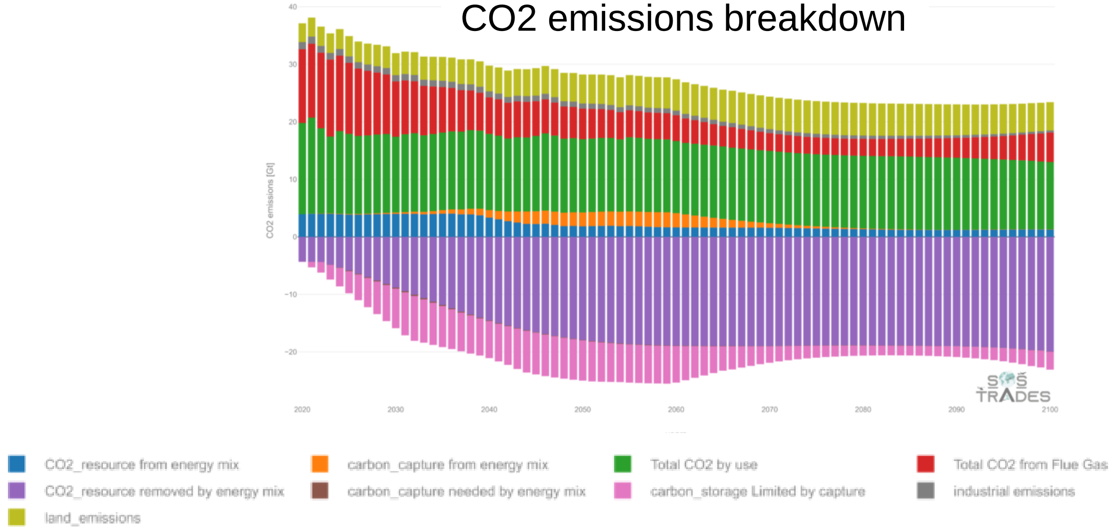


Witness is **based on GEMSEO**
They improved it by proposing new concepts: namespaces, data types extensions, and more.

And allowed to **improve the performance by providing a challenging test case** for:

- coupled adjoint (gradient based optimization)
- graph algorithms (« smart MDA »)
- coupling algorithms

CO2 emissions breakdown



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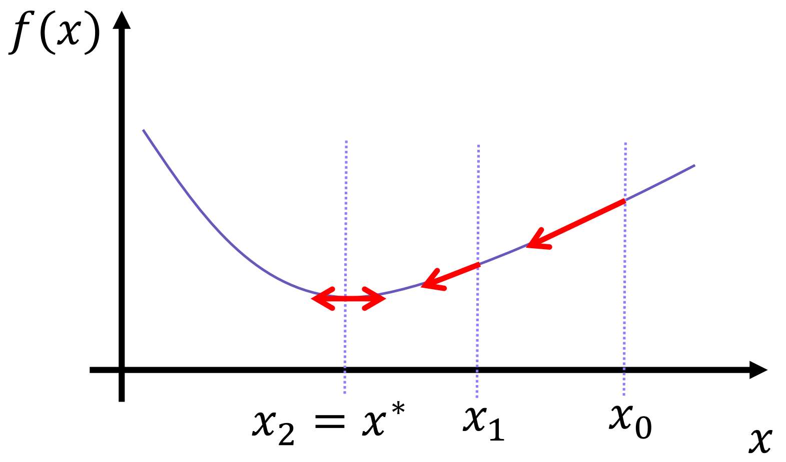
https://www.witness4climate.org/optimizing-investments-in-energy-production-technology/

Gradient Optimization



Gradient

- For a high-dimensional x, knowing the derivative of f is necessary in order to use efficient algorithms.

⇒ Requirement: computing the "gradient" of the calculation process, including the coupling phases (MDA)

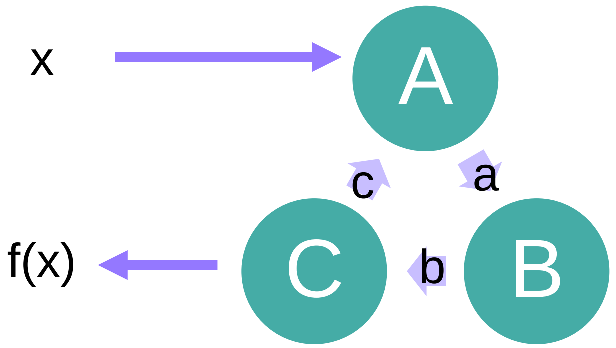
Sequential process

Direct mode

$$\frac{df}{dx} = \frac{da}{dx}\frac{db}{da}\frac{df}{db}$$

Reverse mode

Looped process (MDA)

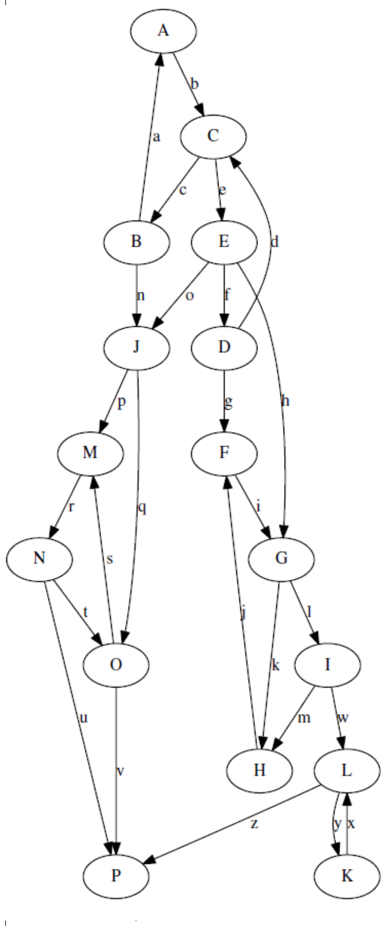


Adjoint mode

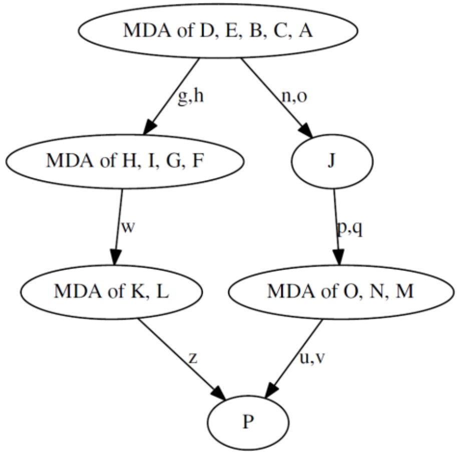
$$\frac{df}{dx} = \left[\frac{\partial R}{\partial x}\right]\left[\frac{\partial R}{\partial abc}\right]^{-1}\frac{\partial f}{\partial abc} + \frac{\partial f}{\partial x}$$

Smart MDAs in GEMSEO

Disciplines dependency analysis →



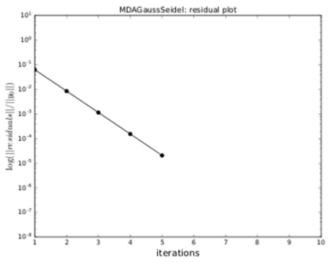
Automated generation of the MDA process →



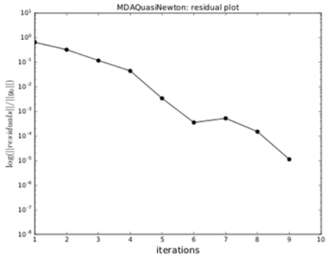
State-of-the art resolution methods

&

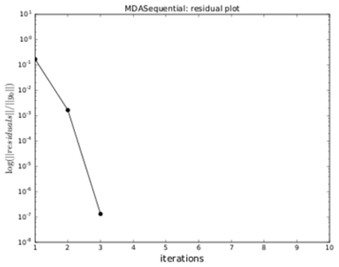
automated hybridization →



(a) Gauss-Seidel MDA



(c) Quasi-Newton MDA



(d) Hybrid MDA

Automated coupled adjoint resolution

$$\begin{pmatrix} \partial A/\partial a & \partial A/\partial b & \partial A/\partial c \\ \partial B/\partial a & \partial B/\partial b & \partial B/\partial c \\ \partial C/\partial a & \partial C/\partial b & \partial C/\partial c \end{pmatrix}^{T} \begin{pmatrix} \lambda a \\ \lambda b \\ \lambda c \end{pmatrix} = \begin{pmatrix} \partial F/\partial a \\ /\partial \\ \partial F/\partial c \end{pmatrix}^{T}$$

Partial derivatives come:

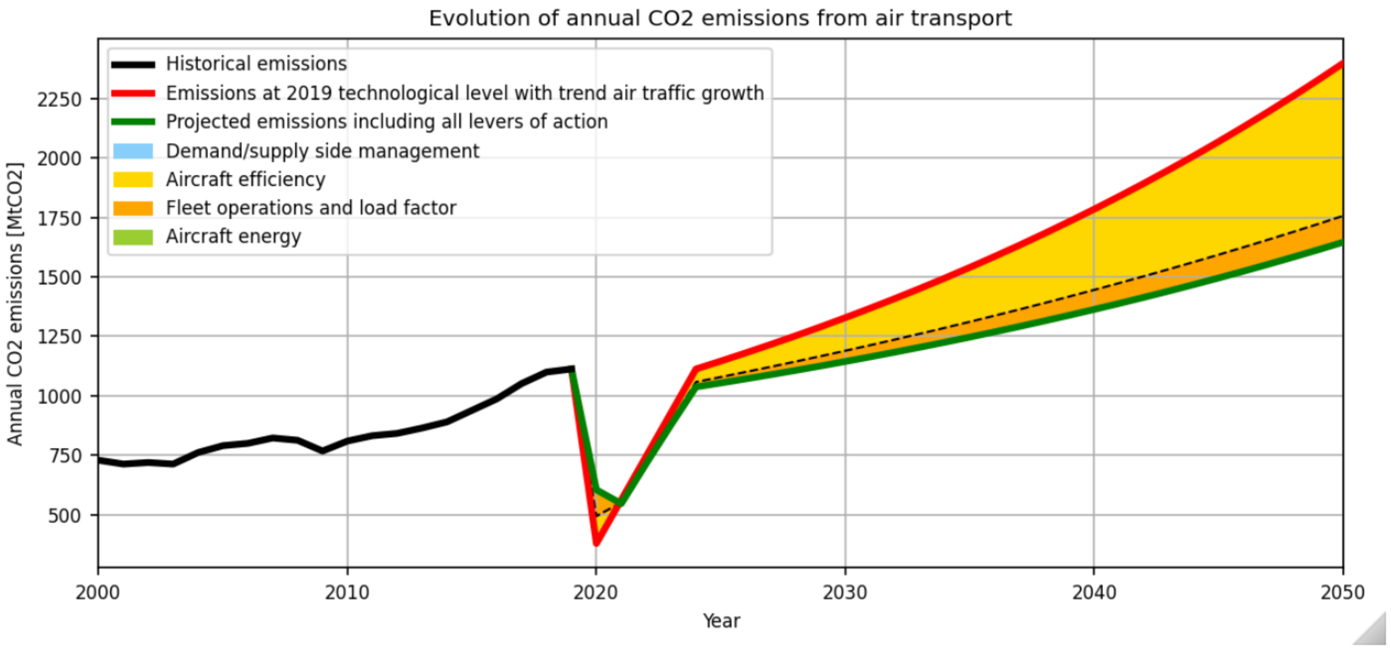
- from the disciplines if provided
- or generated by GEMS using complex step or finite differences
- A mix of the three

ISAE's AeroMAPS IAM

- Open source tool for modelling **transition scenarios** for the **aviation sector**
- Enables the effectiveness of different **impact reduction strategies** to be finely assessed in the light of international commitments to combat climate change.

Uses GEMSEO as execution engine:

- The **« smart MDA »** that automatically generates the execution process from the computational graph.
- To enable **multiple data types exchange between disciplines** (float, numpy array, pandas Series…).
- Soon **optimization** and **uncertainty analysis**



https://aeromaps.isae-supaero.fr/

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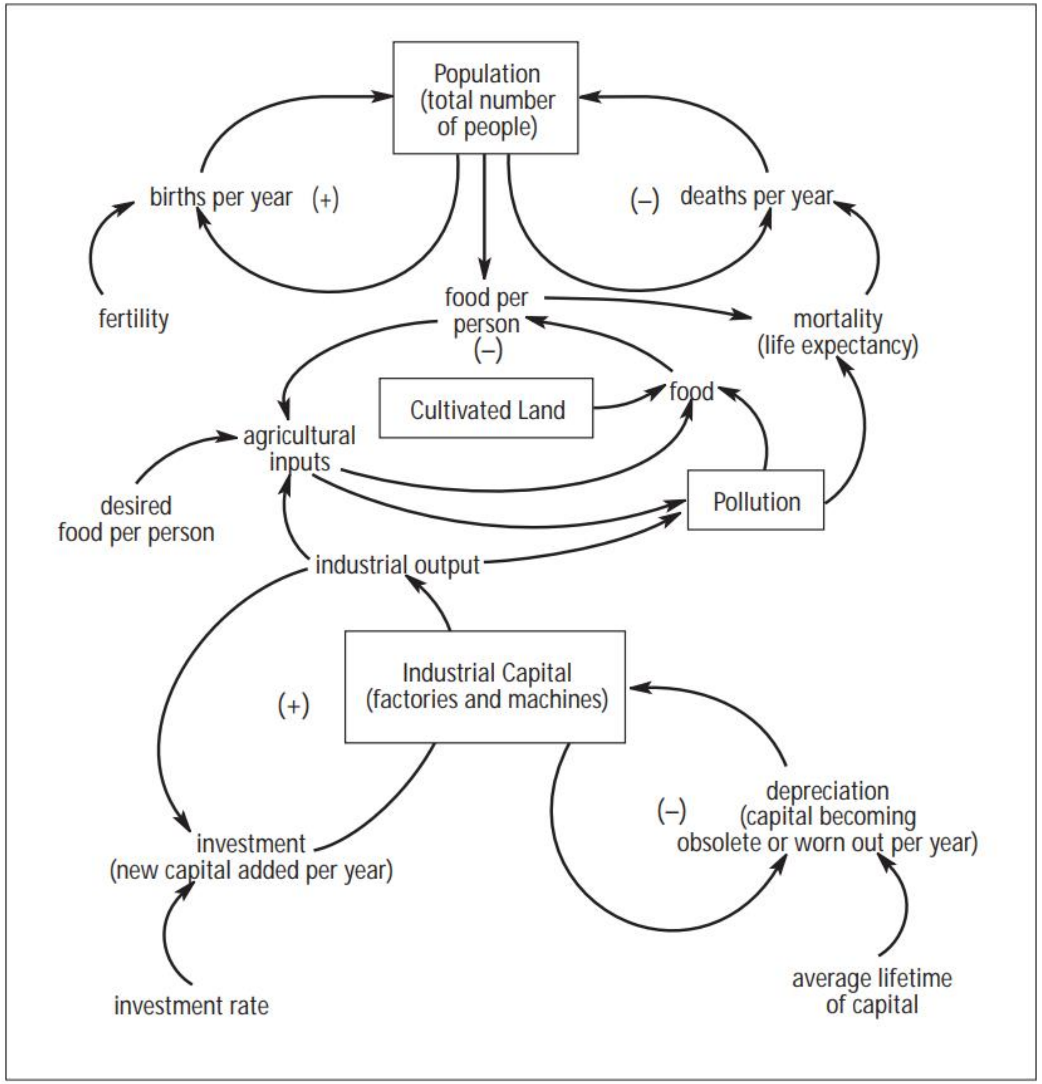
World3
I. Costa Alvez PhD, co advised with A. Gazaix, N. Gourdain

Story

Model developed in the 70s by a team at the MIT, commissioned by the Club of Rome and used in the best seller *The Limits to Growth* and in its 30-year update.

It is said to be the first application of system dynamics for modeling social systems.

The model is built upon the feedback loops that rule population and capital growth. These loops are coupled with Agriculture, Resources & Pollution.



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World3 overview (I. Costa Alvez PhD)

Scenarios and outcomes

1. BAU: Business as usual

   The world proceeds **without any major changes from the policies** pursued during most of the century.

2. BAU2: Business as usual 2

   Hypothesis similar to those made in BAU, except with **doubled reserves of nonrenewable resources**.

3. CT: Comprehensive Technology

   Same stock of resources as in BAU2, strong hypothesis are made counting on the **fast development of technologies** for pollution abatement, land yield enhancement, land protection, and conservation of nonrenewable resources.

4. SW: Stabilized World

   Similar hypothesis to CT regarding technology development and resource reserves, two extra hypothesis are added to **stabilize growth of population and industrial output**.

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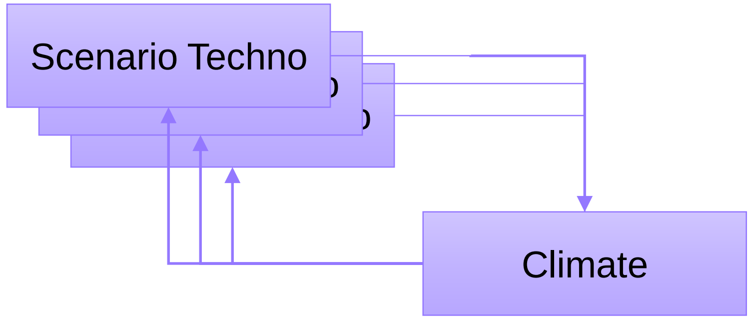
Use cases (I. Costa Alvez PhD)

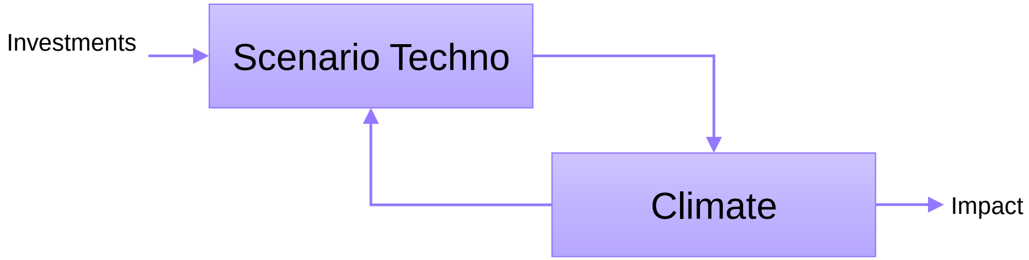
Scenario regionalization

Disaggregation of global scenarios into world regions: how to take into account interactions between regions: international exchange of goods, resources, etc.



Scenario optimization

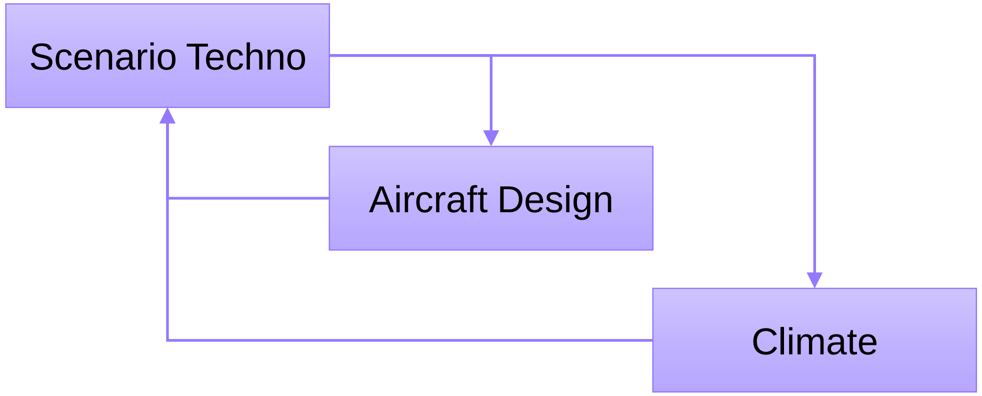
Scenario formulation based on optimization: how to distribute investment over time between different technologies?



$$minimize\ f(x) : impact\,,$$
$$w.r.t.\ x : investments\ per\ techno$$

Trade-off aircraft design

Comparison of aircraft architectures and fuels, taking account of changes in the energy sector.



IAM Calibration problem (I. Costa Alvez PhD)

One of the main **obvious weakness** is the **validation of the models.**

MDO can contribute by providing efficient **model calibration techniques** by **minimizing the error between the model prediction and past data**. This is similar to a **data assimilation** method (in meteorology).

- The IAM ODE depends on parameters to be calibrated (θ):

$$\frac{dy}{dt}(t) = f(t, y(t), \theta)$$

- The calibration optimization problem:

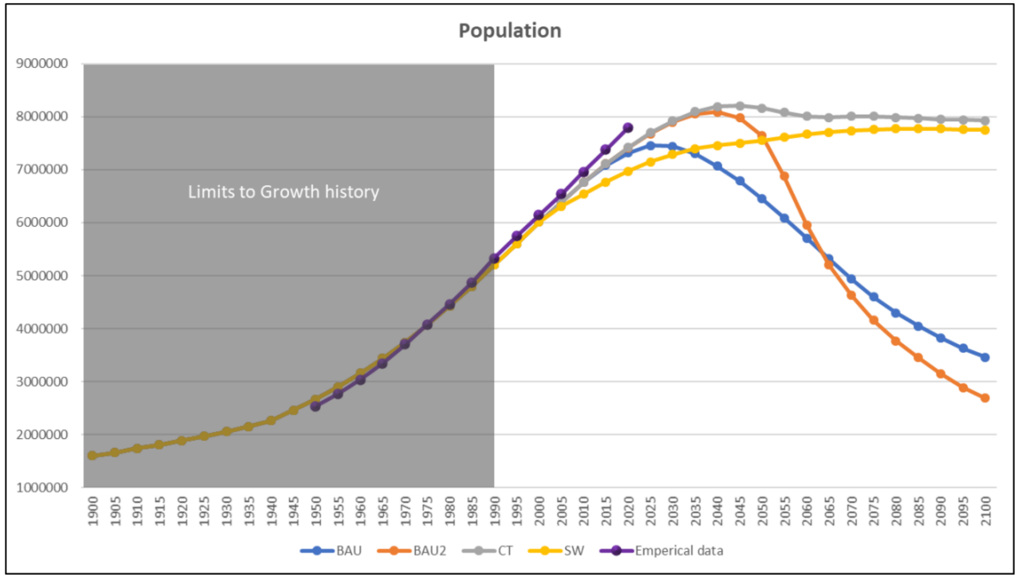
$$minimize \; \|Y_{data}(T_{data}) - Y_{model}(\theta, T_{data})\|$$
$$with\ respect\ to \quad \theta$$

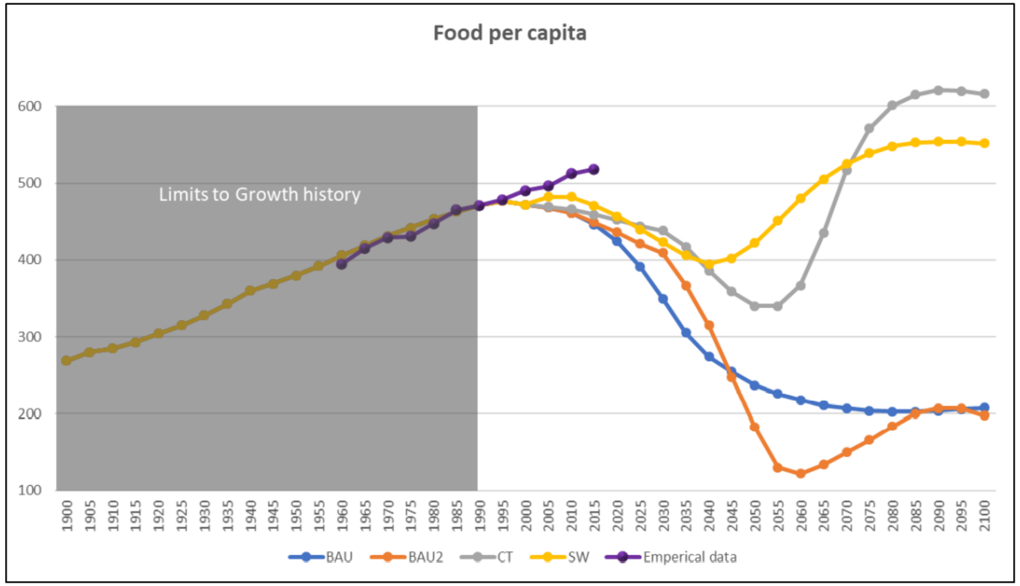
- Usually a **large scale problem** (lots of θs)

=> Costly

=> **Gradient based optimization**

=> Requires **adjoint of the ODE**





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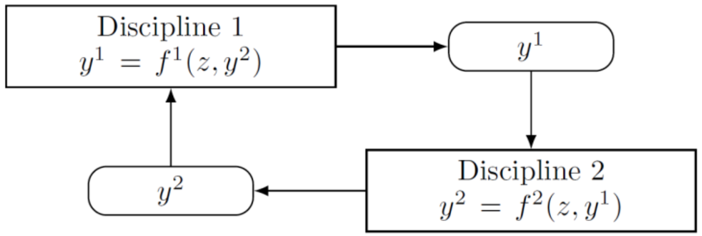
Numerical methods to make these problem affordable (I. Costa Alvez PhD)

Time integration and coupling

Extension of classical coupling



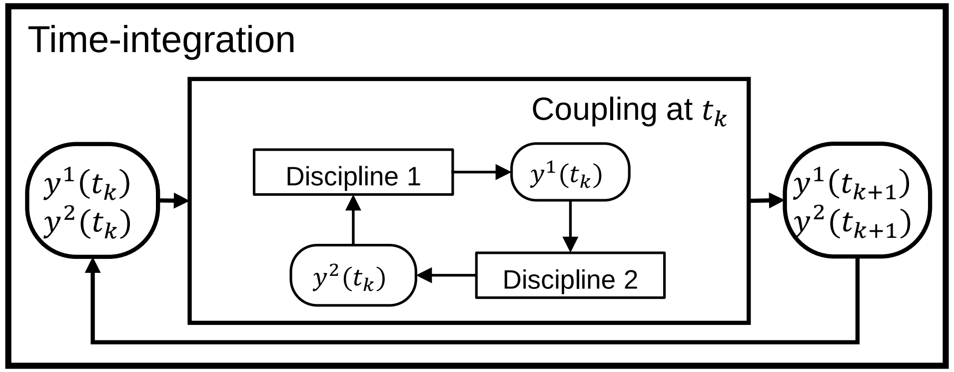
To ODE-based (time integration) disciplines

Automatic differenciation and Just in time compilation

JAX: HPC library https://jax.readthedocs.io

- *AutoDiff*: Automatic differenciation
- XLA: accelerated linear algebra
- JIT: *just-in-time python code compilation*
- *SPMD parallelism*
- *GPU or CPU execution*
- *Adjoint for ODEs*

⇒ New GEMSEO-JAX plugin that combines these features



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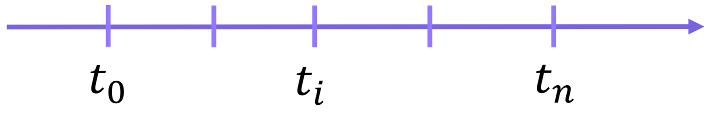
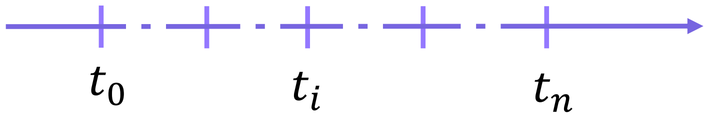
Efficient ODE solvers

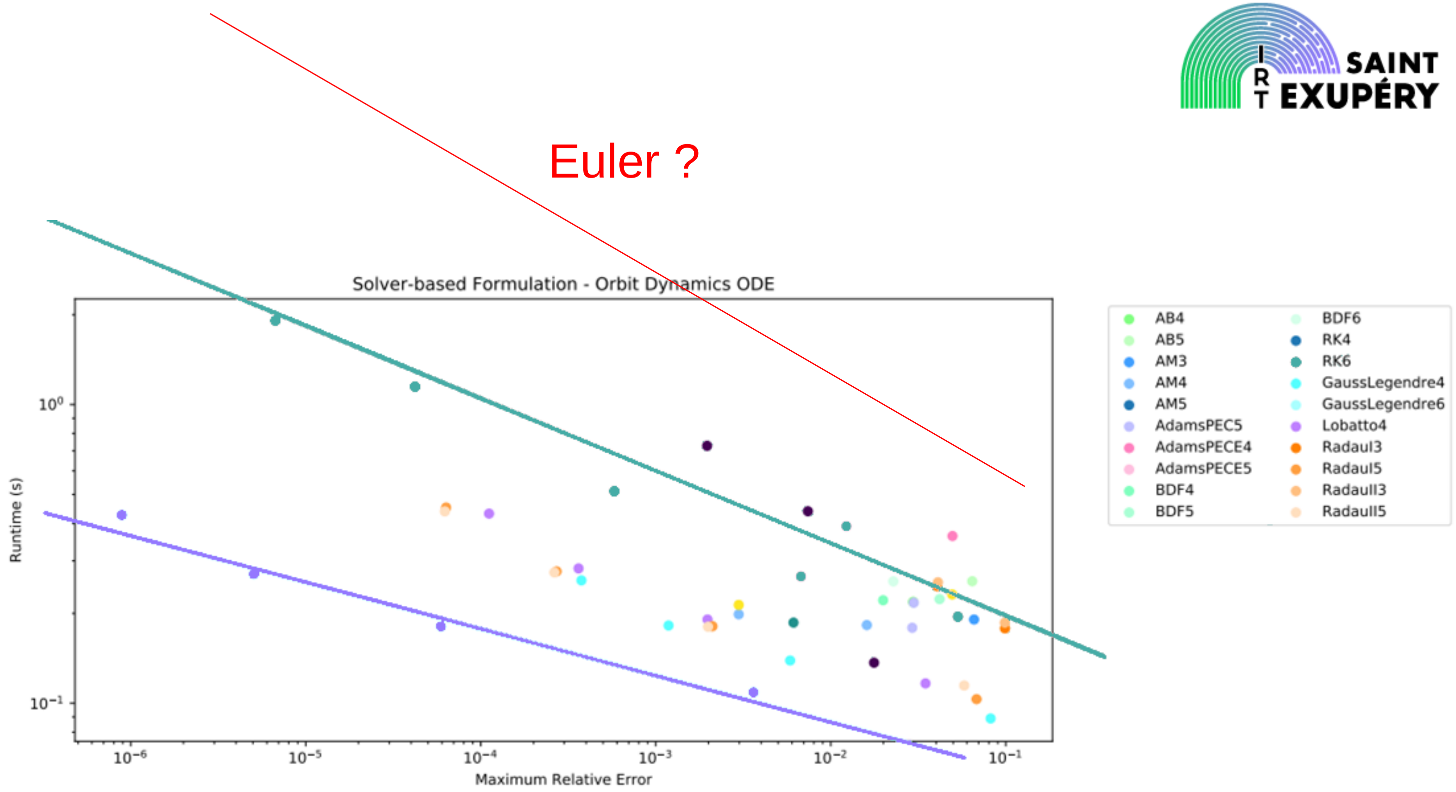
Time integration



Explicit



Parallel



Classical Runge-Kutta 6^{th} order
Best implicit method

Using **efficient time integration solvers** instead of the classical **Euler scheme used in many IAMs**

$$\text{GDP(year n+1)} = \text{GDP(year n)} + \Delta t \, \frac{dGDP}{dt} \text{(year n)} :$$

- Can provide **10 to 100x CPU cost reduction**
- Improves the **solution precision**
- Can reduce restitution time through **parallel in time integration**

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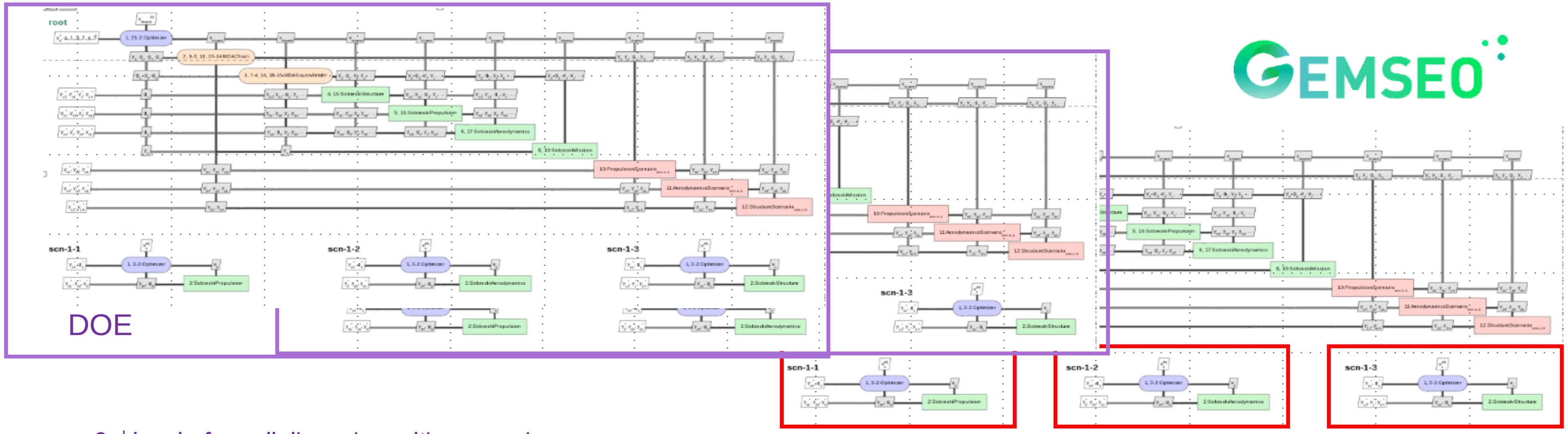
Exploiting parallelism in the MDO process



GEMSEO

2nd level of parallelism via multi-processing (distributed memory via process fork)

1st level of parallelism via Multi- Threading (shared memory)

3rd level of parallelism at the job scheduler level

4th level of parallelism at the Simulation level (MPI…)

Conclusion

- **MDO methods and frameworks can help to develop better IAMs**
  - **Less code** (often much less !)
  - **Faster execution** (parallelism, Graphs, GPUs, Automatic Differentiation)
  - Easily perform **optimization** instead of only comparing scenarios
- 3 examples were given, some with applications in the **aircraft design** field
- The **work is ongoing**, and lots of efforts are put in the world wide community
  - On the **modeling** and **validation** [Turner, 2008]
  - On the **software** => here we can help
  - On the **algorithms**, where there are **open research problems**: such as fast resolution of **mixed integer continuous problems in high dimension**
- The elephant in the room, in addition to, is **Uncertainty Quantification** ! [Vermeulen, 1976; Plessix 2021]
- We are happy to have feedbacks on GEMSEO, and improve it accordingly.

*"A comparison of The **Limits** to **Growth** with **30 years** of reality" GM Turner, 2008*
"Parameter sensitivity of the 'Limits to Growth' world model" Vermeulen, Jongh, 1976
"Analysing the validity and robustness of the iconic World 3 global model: what can sensitivity and feedback loop analysis say?", Plessix, Feynet, 2021