



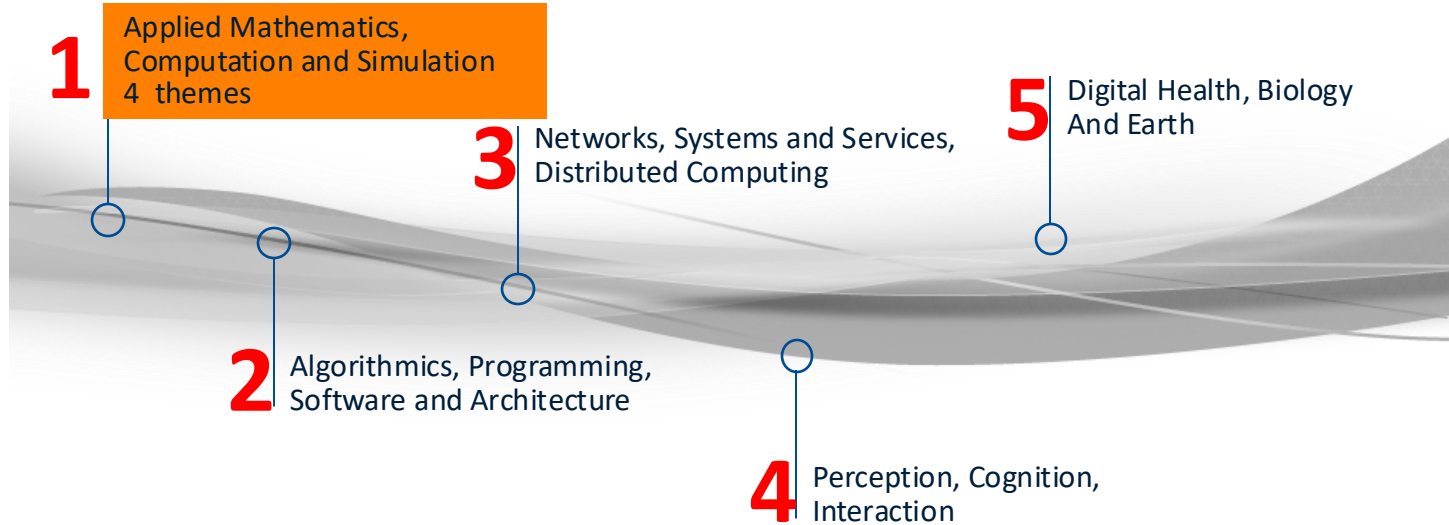
Inria-ECDF Partnership
Kick-Off Workshop
June 5-7, 2024

Applied_Mathematics@Inria

Applied Mathematics, Computation and Simulation

Christophe Biernacki, *deputy scientific director*

Global view of research at Inria



T1. Numerical Schemes and Simulations

Topics: Numerical analysis of PDE and ODE, Multiphysics, Meshes, MOR, Fluid/solid mechanics, Waves, UQ

Applications: Materials, Aerospace, Nanotechnology, Quantum syst., Nuclear/hydro energy, Water (sea, nearshore), Optic, Traffic...

T2. Stochastic Approaches

Topics: Stochastic analysis and modeling, Numerical probability, Deterministic/stochastic/optimal control, Statistical methods

Applications: Energy & physics, Life science, Defense, Financial risks, Geophysics & natural risks...



T3. Optimization, Machine Learning and Statistical Methods

Topics: Machine Learning & statistics, Deterministic & stochastic optimization, Exascale, Networks, Signal/image/audio processing

Applications: Energy, Health, Physics, Logistics, Fairness & privacy, Natural and industrial risks, Sciences of universe...

T4. Optimization and Control of Dynamic Systems

Topics: Automatic control, Multiphysics, Numerical linear algebra, Sensor/social networks, Robot control, Formal methods

Applications: Industry of the future, Transport & logistics, Health, IT & telecom, Environment & planet, Physics & mechanics...

The Inria research team concept (~220):

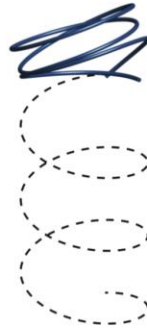
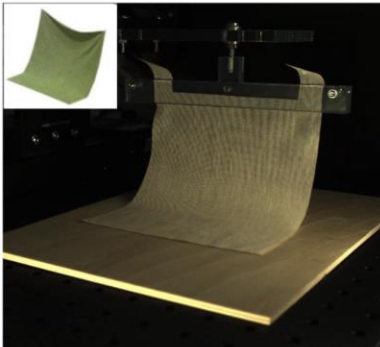
focus topic, 4-10 permanent members, max 12 years, financial support

16 project-teams - included 1 joint team with industry

ACUMES	Analysis and Control of Unsteady Models for Engineering Sciences
ATLANTIS	modeling and numerical methods for computATIonal wave-mAtter iNteracTIons at the nanoScale
CAGIRE	Computational AGility for internal flows simulations and compaRisons with Experiments
CARDAMOM	Certified Adaptive discReTe moDels for robust simulATIons of CoMplex fLOws with Moving fronts
DEFI	Shape reconstruction and identification
ECUADOR	Program transformations for scientific computing
ELAN	modELing the Appearance of Nonlinear phenomena
GAMMAO	Adaptive Mesh Generation and Advanced numerical Methods - joint team with ONERA
MATHERIALS	MATHeMatics for MatERIALS
MEMPHIS	Modeling Enablers for Multi-Physics and InteractionS
MINGUS	Multi-scale Numerical Geometric Schemes
MOKAPLAN	Advances in Numerical Calculus of Variations
PARADYSE	PARTicles And DYnamic al SystEmS
PLATON	Uncertainty Quantification in Scientific Computing and Engineering
POEMS	Wave propagation: mathematical analysis and simulation
RAPSODI	Reliable numerical approximations of dissipative systems

Focus on “ERC STG GEM (Geometry for Motion)”

- **Leader:** Florence Bertails-Descoubes (**ELAN**) – 2015-2022 – (1.49M€)
- **Aim:** investigate the tight links between the geometry of slender elastic structures (rods, plates, shells), and their mechanical properties (natural shape, material properties, friction coefficients)
- **Method:** an original inverse modeling strategy based upon **non-invasive** method for inferring the mechanical properties of complex objects from a minimal set of geometrical poses, in order to predict their dynamics
- **Motivation:** motivated by automatic image-based capture in Computer Vision and Computer Graphics
- **Some selected results:**
 1. **Application:** a new non-invasive protocol for estimating material properties of cloth and friction during dynamic interaction. The method relies on a neural network fed only with simulated data.
 2. **Theory:** a theorem of existence and uniqueness for the natural shape of a rod sagged under gravity
 3. **Community leadership:** creation of the first graphics-physics workshop (GRAPHYZ).

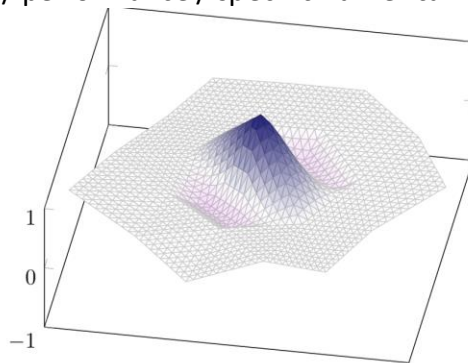


New!

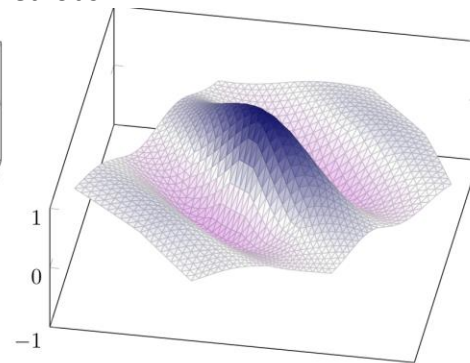
Focus on "Exploratory Action POPEG"

- **Name:** Galerkin's methods allow to numerically approximate a harmonic wave by assembling basis functions
- **Leader:** Théophile Chaumont-Frelet, young Inria researcher (2018) in **ATLANTIS**
- **Period:** start in 2nd semester 2021 (3 years)
- **Motivation:** High-frequency wave propagation problems play a major role in many physical and industrial applications (sismic, aeracoustic). However, the « standard » methods of finite elements use polynomials, which necessite many elements/calculus in the case of high frequency waves
- **Idea:** more physics in modeling!
- **Method:** replace the polynomials of finite element methods with specifically adapted functions to the wave character of the solution → use "Gaussian states" as new basis functions
- **Lock:** theoretical complexity for convergence / performance / specific numerical methods

$$\phi_k(\mathbf{x}) = \exp\left(-\frac{\omega}{2}|\mathbf{x} - \mathbf{x}_k|^2\right) \exp(i\omega \mathbf{d}_k \cdot \mathbf{x})$$



(c) Onde plane



(d) État gaussien

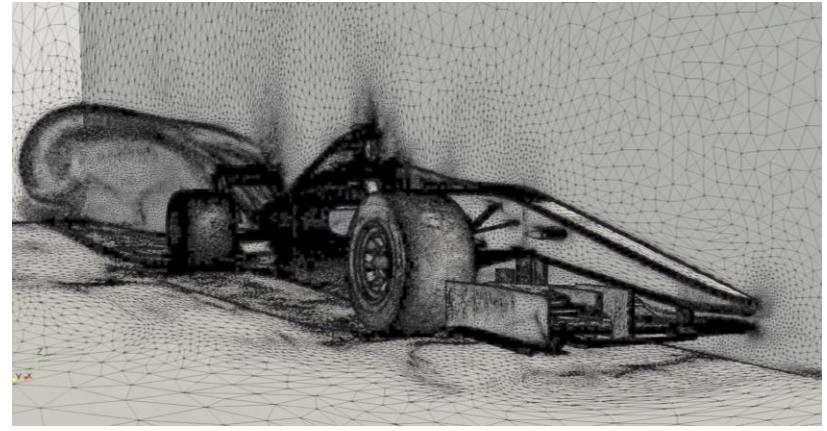
The Inria exploratory action concept (~50):

risky topics, 1-2 researchers, 2-4 years, financial support

Focus on “Software of GAMMAO team”

- **Leader:** Frédéric Alauzet (**GAMMAO**)
- **Mesh generation methods:** time saving factor 1000
- **Hint:** develop a suite of software to control the entire CFD/EDP calculation chain with innovative high-fidelity methods that certify digital solutions
- **Pipeline:** Feflo.a/AMG-Lib - GHS3D - Hexotic - Wlf-Bloom (meshers & adaptive remeshers), ViZiR (visualization), Wolf (Navier-Stokes flow solver)...
- **Industrial and academic users:** Safran, Ariane Group, Dassault-Aviation, ONERA, Boeing, NASA, ...
- **Industrial example** of automatic / dynamic meshing

Common team with ONERA



RAPSODI: corrosion of iron for nuclear waste repository in deep underground



Overall goal of our project within EURAD (2019-2023)

Derivation of a thermodynamically consistent model

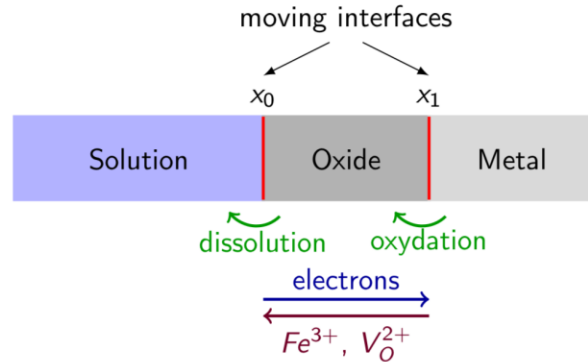
- ▶ Same physical ingredients as in [Bataillon *et al.* '10, '12]
- ▶ Compatibility with thermodynamics (2nd principle)

Mathematical analysis of the model

- ▶ Generalized gradient flow structure [Mielke '11]
- ▶ Existence, uniqueness
- ▶ Long-time behaviour

Design, analysis and implementation of relevant schemes

- ▶ Entropy production at the discrete level
- ▶ Convergence
- ▶ Long-time behaviour



Physical driven applications

- Pursue/reinforce **collaborations with physicists**
- Innovative numerical methods for differential models of **nanoscale light-matter interactions**
- **Applications:** wing ice modeling, aquifers, wave energy, natural hazards, Geo-/astro-physics, wave energy converters, wind turbine
- Challenges in extreme numerical mechanics relevant for both the **physics and graphics communities**
- Physical and numerical validation

Model-data coupling

- Focus on the development of new hybrid modeling and optimization strategies with **modern ML techniques**
- Combine the **advantages of model-driven and data-driven** approaches, while overcoming their weaknesses
- Data science for the development of efficient sampling techniques, the derivation of model order reduction
- Develop and analyze **hybrid approaches** that combine and merge first-principle models with data-fit models
- Ex: numerical schemes for Hamiltonian systems (discrete pseudo-differential operators and neural networks)

Need for HPC techniques (in particular GPU, but maths also)

For PDE reduction techniques, sparse regularization methods and domain decomposition methods

Industrial dissemination of software targeted by many teams

AEROSOL software, DIOGENeS, UHAINA, MMG, GeoFun, Tapenade, MM propagation...

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T2 - 6 project-teams - included 1 joint team with industry

ASCII	Analysis of Stochastic Cooperative Intelligent Interactions
ASTRAL	Advanced Statistical inference And control - joint team with Naval Group
CALISTO	Stochastic Approaches for Complex Flows and Environment
MATHRISK	Mathematical Risk handling
PASTA	Space-time random processes and applications
SIMSMART	SIMulating Stochastic Models with pARTicles

PREMIA - A numerical platform for computational finance



www.premia.fr

A software designed for option pricing, hedging and financial model calibration

- Efficient computations of prices and hedges for derivative products on equities, interest rates, credit, energy, and insurance, using advanced stochastic and numerical analysis.
- Deep learning techniques using neural network approximations, and Machine Learning algorithms for high-dimensional problems. Exploration of Quantum computing methods.
- C/C++/Python source code - 385000 lines - with extensive scientific documentation.
24 releases registered at APP, next release June 2023.

Coming event

International Conference

14-16 Jun 2023 @Udine

<https://mathrisk2023.sciencesconf.org>

Finance industry perennial partnership

Premia Bank consortium since 2000

Financial institutions

Long term development

Aex Apollon (2023—2025)

- Projet interdisciplinaire maths-SHS-info dans le but d'aider des experts à créer un *lexique des idées*.
- Équipe-projet Inria PASTA, UMR Archimède (histoire antique; Strasbourg & Mulouse), Institut Élie Cartan de Lorraine (mathématiques, Nancy), collaborateurs à l'Université de Pavie & MISHA.
- Soutiens financiers : AEX, CNRS Innovation, INSHS & Insmi.
- Projet scientifique et développement :
 - Explorer les relations entre mots/concepts par le biais d'hypergraphes et leur validité logique, puis ajout de d'apprentissage par renforcement avec feedback d'un expert.
 - S'approcher le plus possible de la logique d'un expert (test d'hypothèses historiques, quantifications de leurs plausibilités, ...), et limiter au maximum les biais d'interprétation liées à la sémantique.
 - Création d'une plateforme d'expérimentation : visualisation du texte et des hypergraphes.
 - Valider notre approche sur *la Politique* d'Aristote, ouvrage fondateur des sciences politiques.
- <https://project.inria.fr/aexapollon/>
- Workshop **Réflexion sur les modèles d'apprentissage dans les humanités**, 27 juin à Strasbourg

Selection of good descriptors in the text (core of text mining)

A mix between text/data (with RL) and expert knowledge (historians)

Develop the collaboration intensity between communities

Interaction with challenging applications fields

- **Natural phenomena:** climate, molecular simulation, geophysical phenomena (e.g. avalanches)
- **Energy:** neutron transport for nuclear safety, renewable energies, in particular wind power, demand response, electric car charging station management
- **Industry:** complex industrial systems
- **Finance:** risk indicators (e.g. detection of financial crises)
- **Crossing fields:** energy market and insurance (risk understanding between energy market and temperature)
- **sustainable development & agro-ecology**

Model-data coupling, knowledge-data coupling

- Development of **AI/ML techniques for model** development or intricate **optimization** problems, in particular in the context of fluid dynamics
- **Deep learning for high-dimensional problems** in finance and insurance
- Combining **stochastic** analysis, **PDEs'** analysis and **data** interpretation for complex geophysical problems
- **Digital humanities**, in particular using RL for coupling with human expertise

Other questions within the stochastic domain

- **Uncertainty** quantification
- Modeling in **turbulence** and uncertainty
- **Rare Event** Simulation
- Study of **quantum computing and its application** to option pricing and hedging
- **Data:** massive & stream data analysis, mixed data

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T3. Optimization, Machine Learning and Statistical Methods

Strong IA component

Topics: **Machine Learning & statistics**, **Deterministic & stochastic optimization**, Exascale, Networks, Signal/image/audio processing

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T3 - 12 project-teams + 3 new - included 1 joint team with industry

BONUS
CELESTE
GEOSTAT
INOCS
MAASAI
MODAL
RANDOPT
REALOPT
SCOOOL
SIERRA
STATIFY
TAU

Big Optimization and Ultra-Scale Computing
 Mathematical **statistics** and **learning**
Geometry and **Statistics** in acquisition data
INtegrated Optimization with **Complex Structure**
 Models and Algorithms for **Artificial Intelligence**
MOdel for Data Analysis and **Learning**
Randomized Optimization
 Reformulations based algorithms for **Combinatorial Optimization**
Sequential decision making under uncertainty problem
 Statistical **Machine Learning** and Parsimony
Bayesian and **extreme value** statistical models for structured and high dimensional data
TAckling the Underspecified

FAIRPLAY

MALICE

OCKHAM

Coopetitive AI: Fairness, Privacy, Incentives
joint team with Criteo
MAchine Learning with Integration of
 surfaCe **Engineering knowledge:** Theory
 and Algorithms
Optimization, pHysical Knowledge,
 Algorithms and Models

History

Computing power (1)

mid-1950s: workshop at Dartmouth (1956), symbolic AI

1973: Lighthill report, 1st AI Winter



(1') + new languages (2)

198x: Prolog, List, expert systems

1997: collapse of the Lisp Machine market, 2nd AI Winter



(1'') + (2') + data deluge (3)

20xx: data from the web, deep learning (triumph of CNN)

202x: towards a 3rd AI Winter?



Need fundamental research in AI
Inria leader at the national level

Success

- **2012:** human outperformed by **CNN** on image recognition (ImageNet)
- **2015:** human European Champion outperformed by **AlphaGo** (score 5-0)
- **2022:** **ChatGPT** is a disruptive chatbot based on Generative Pre-trained Transformers (GPT)

Risk

- No formal **certification** (only experimental)
- Black boxes (**interpretability**, explainability)
- Reproduce the past, **poor innovation**
- Reproduce bias conveyed by data (**fairness**)
- Huge **computational cost** (ecological disaster, irreproducible science)

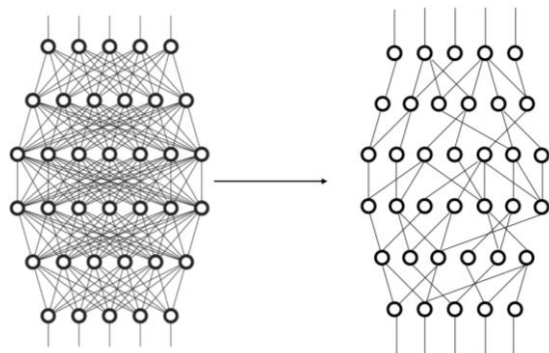
Focus on project-teams OCKHAM & SIERRA

What we have learnt with the algorithm (known)

Truth (unknown)

Guarantees needed

- Algorithms with **provable** guarantees
- **Reduced** computational cost (**minimal** if possible)
- Practicable on **existing/classical architectures**



Theoretical limits in learning

- Minimax lower bounds (example of multivariate regression):
- Given n examples in the dataset.
- f^* is s -times differentiable, $X = \mathbb{R}^d$ and $L(y, y') = (y - y')^2$

Theorem: For any algorithm there exists a learning problem for which

$$\mathbb{E}L(\hat{f}(x), y) - \mathbb{E}L(f^*(x), y) \geq cn^{-\frac{2s}{2s+d}}$$

A Distribution-Free Theory of Nonparametric Regression, Györfi et al. 2002

Can we build an algorithm which reaches this kind of optimal bound (memory, compute)?



Trade-off learning/unlearning

A new Bayes-Duality principle for adaptive, robust, and lifelong learning of AI

Collect new knowledge (data)

BUT robustly preserving the old knowledge

Summarizes relationships between the data and the model, by connecting model parameters and its effect on training data through a loss function.

One fundamental equation to measure perturbation in “generic” machine-learning problems

$$\nabla H(q_*) = \sum_{i=1}^N \nabla \mathbb{E}_{q_*}[\ell_i(w)]$$

Diagram annotations: An arrow points from the text 'Summarizes relationships...' to the equation. Labels include: 'Posterior' pointing to $H(q_*)$, 'Entropy' pointing to $H(q_*)$, 'Model parameters' pointing to w , and 'Training data' pointing to the index i in the summation.

Approx-Bayes team

Stat-Theory team

Math-Science team

HPC team



Emteyaz Khan



Julyan Arbel



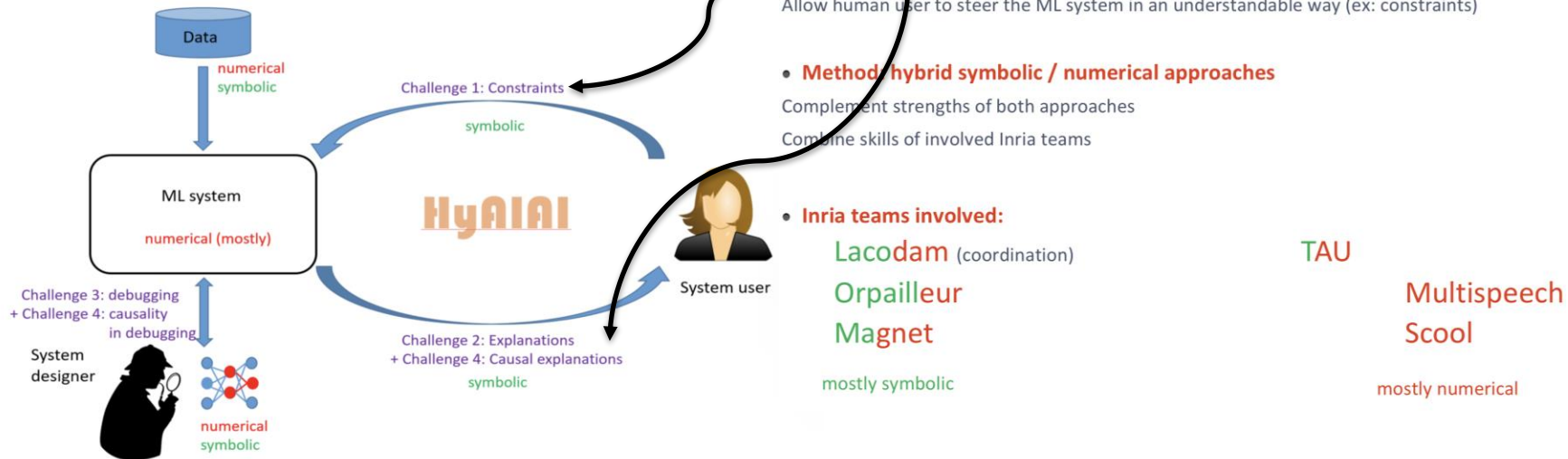
Kenichi Bannai



Rio Yokota

Challenge HyAIAI

Hybrid Approaches for Interpretable AI



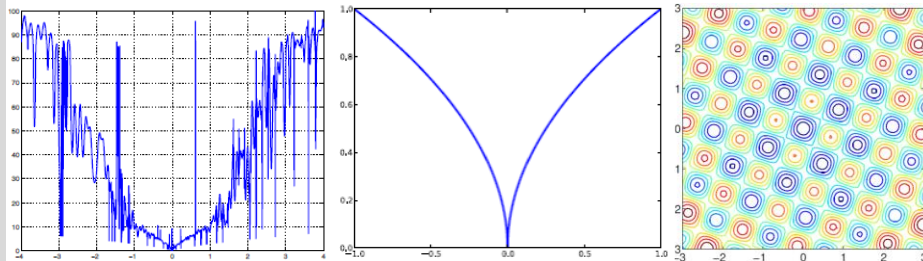
CMA-ES optimization solver

State-of-the-art algorithm to address **difficult** numerical optimization problems

$$\min_{x \in \mathbb{R}^n} f(x)$$

without derivatives (blackbox optimization)

f can be non-convex, non-separable, noisy, ill-conditioned, $3 \leq n \leq 100$



A generic and standard software!



Main features: adaptive, stochastic, affine-invariant

Used to **solve applications** in various domains (medicine, biology, engineering, ...)

Impact: more than **41 million downloads*** for two main Python implementations

- pycma [developed and maintained at **Inria** within **RandOpt** team]
- cmaes [based on pycma, lighter implementation, maintained in Japan]

*as of May 2023

Optimization

- **Types of problem:** complex structures, mixed integer, multiobjective, bilevel optimization problems
- **Methods:** ultra-scale, robust, stochastic

Learning

- **Interpretability:** understanding (deep) learning models, combining symbolic and numerical AI, causality
- **Acceptability:** fairness, adaptability to the end-user, responsible decision making, statistical reproducibility
- **Environmental sustainability:** frugal learning for massive data, learning with few training data (scarcity)
- **Data complexity:** streaming data, time-space dependent data, high-dimensional data, real-world “dirty” data (missing values, outliers, label noise, adversarial examples, ...), distributed databases, massive data
- **Fundamental ML:** shrinking the gap between theory and applications, trade-offs between accuracy / reliability / computations, average-cases or smoothed analysis instead pure worst case, local-global optimization methods with guarantees, control theory and reinforcement learning
- **Types of learning:** unsupervised learning, deep generative models, adaptive and robust learning

Crossing domains

- **ML/optimization:** ML-assisted optimization, interplay between optimization algorithms and statistical properties, bilevel optimization and game theory (domain of equilibrium learning), optimization methods and Bayesian approximation techniques for scalable inference
- **ML/other:** multiscale statistical signal processing coupled with ML, ML with/for statistical physics, ML for numerical simulations

Applications

Medicine, biology, industry, image analysis (e.g. satellite or medical images), health data, ecology (e.g. dispersion and invasion of species), epidemiology (e.g. disease and risk mapping), climate, energy, sustainable development, transportation and logistics (last mile delivery problems, integrated urban transportation systems)

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12 project-teams

CAGE	Control and Geometry
COMMANDS	Control, Optimization, Models, Methods and Applications for Nonlinear Dynamical Systems
DANCE	Dynamics and Control of Networks
DISCO	Dynamical Interconnected Systems in COmplex Environments
FACTAS	Functional Analysis for ConcepTion and Assessment of Systems
I4S	Statistical Inference for Structural Health Monitoring
MCTAO	Mathematics for Control , Transport and Applications
QUANTIC	QUANTum Information Circuits
SPHINX	Heterogeneous Systems : Inverse Problems, Control and Stabilization, Simulation
TRIPOP	Modeling, Simulation and Control of Nonsmooth Dynamical Systems
TROPICAL	Tropical methods : structures, algorithms and interactions
VALSE	Finite-time control and estimation for distributed systems

Focus on “AEX StellaCage”

- **Name:** stellarator to confine ionized gas (plasma) during the fusion reactions
- **Leader:** Mario Sigalotti in **CAGE**
- **Period:** start in 1st semester 2020 (2 years)
- **Motivation:** The stellarator is another magnetic confinement approach, alternative to the tokamak (tokamak is simpler). It is naturally steady-state and immune from disruptions because it does not require a plasma current to confine the plasma: it obtains the same effect (helical fields) by means of specially deformed magnetic coils.
- **Lock:** the complexity of the coils’ shape
- **Method:** From a mathematical point of view, the first step consists in understanding the topological properties of phase portraits of magnetic fields in toroidal domains. Then, a strategy is needed to optimize the magnetic field “bottle” or “cage” as to better confine the plasma and make it more stable.

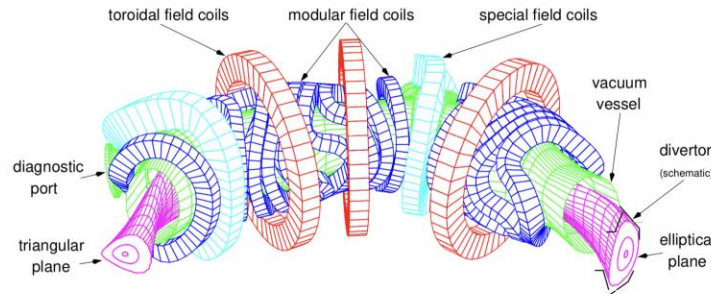


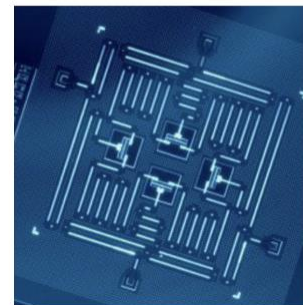
Figure 1: Cut view of portions of the W7-AS stellarator plasma (magenta), vacuum-vessel (green) and coils (blue, cyan and red) [1].

Focus on “Inria Challenge EQIP”

- **Name:** Engineering for Quantum Information Processors
- **Leader:** Anthony Leverrier (**COSMIQ**)
- **Partners:** **CAGE**, **QUANTIC**, (**MCTAO**) + **8 other teams** + Atos Quantum
- **Period:** October 2020 - September 2024 (4 years)
- **Challenge:** bring together all the competences already present in the institute, and to turn Inria into a major international actor in quantum engineering, including both the software and hardware aspects of quantum computing
- **Scientific approach:**
 - ▶ *WP1: Building a quantum processor.*
 - ▶ questions at the interface between physics and applied mathematics
 - ▶ goal: to design and understand systems that can process quantum information
 - ▶ *WP2: Operating quantum computers.*
 - ▶ how to encode quantum information so as to process it efficiently?
 - ▶ how to program quantum computers?
 - ▶ *WP3: Overtaking classical computers.*
 - ▶ quantum algorithms, e.g. for cryptanalysis
 - ▶ computing with NISQ devices
 - ▶ integration between HPC and quantum computing

Superconducting circuits

(IBM, Google, QUANTIC, Alice&Bob)



Most of them are driven by applications

- Geometry of confining magnetic fields at equilibrium (**fusion**)
- Mathematical methods for open and many-body **quantum** systems
- Controlability of non-controllable systems perturbed by a small static field (**quantum** control)
- Control for **health** and **biological** systems, for CPSs
- Non-smooth simulation and numerical modeling for **natural gravitational risk in mountains**
- Open networks (multimodal **transportation**)
- Inverse problems (**EEG-MEG, paleomagnetism, gravimetry, acoustic, wave, structural analysis and monitoring...**)
- Homogenization for simulation of **composite materials**
- Optimization and game theory methods applied to **energy**

A generic paradigm

- Control, estimation, filtering and detection in remarkably **uncertain scenarios**
- Improving estimation and control methods by **ML and IA**
- "**data-driven mechanics**" approaches when behavioral models are far from the observed physical phenomena

Thanks!

Visit www.inria.fr