Dr. Quentin Malé

Computational scientist, researcher at ETH Zurich

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The interdisciplinary nature of computational science and engineering enables me to grow in many different domains. I enjoy developing sophisticated simulation methods to address crucial needs in our society, and I intend to continue on this path.

EXPERIENCE

ETH Zurich

Established researcher (Oberassistent), SNSF fellowship

- Established a data-driven machine learning framework to model H₂ reaction rates for high-fidelity Large Eddy Simulation (LES).
- Developed an Adaptive Mesh Refinement (AMR) strategy to simulate nonthermal plasma streamer discharge.
- Supported the group with High-Performance Computing (HPC) applications. Developed GPU-accelerated computing.

ETH Zurich

Postdoctoral researcher, part of the ERC "TORCH" project

- Integrated plasma effects into a massively parallel code to better understand plasma-assisted combustion. Clarified the formation
 of nitrogen oxides (NO_x) and control of thermoacoustic instabilities in real systems, giving design indications.
- Led a joint experimental-numerical (LES) project to characterize the operation of a new LEAF H_2 burner, featuring complex flame topology with mixed combustion regimes. Clarified combustion modes and NO_x formation routes.
- Implemented a nonthermal plasma solver (electron Boltzmann equation) in Cantera (open source) for plasma rate computation.
- Supported the group with HPC applications (\approx 15 people).

European Center in Research and Advanced Training on Scientific Computing (CERFACS)Toulouse, FRPostdoctoral researcher, part of the ERC "CoEC" projectDec 2020–Mar 2021

The University of Melbourne Visiting PhD student

- Developed a Direct Numerical Simulation (DNS) framework to acquire high-fidelity data for subsequent reduced modeling.

European Center in Research and Advanced Training on Scientific Computing (CERFACS)	Toulouse, FR
PhD student, ANRT Cifre fellowship	Sep 2017–Nov 2020

- Built a Reduced Order Model (ROM) of a new engine technology to quickly assess designs, enabling optimization process.
- Conceived a ROM to predict the outcome of a hot, turbulent jet penetrating a flammable mixture for energy and safety scenarios.
- Developed dynamic mesh adaptation techniques to handle moving mesh during LES, enabling simulation of reciprocating engines.

EDUCATION

PhD Computational Reacting Flow		MSc Energy Engineering		MRes Energy and Fluids	
CERFACS	2017-2020	INSA Rouen	2014-2017	University of Rouen	2017
Advisor: Thierry Poinsot		GPA: $17.1/20$ (ranked $1^{st}/60$)		GPA: 18.6/20 (ranked $1^{st}/16$)	

AWARDED RESEARCH GRANTS

0	SNSF/ANR Lead Agency, 516K €: "Joint experimental and numerical study of H ₂ plasma-assisted combustion"	2024-2027
0	$3 \times$ CSCS HPC access, 40MM core-h in total (grant no. s1138, s1220 and s1262)	2022-2024
0	2× PRACE HPC access, 35MM core-h in total (grant no. 2019204881 and 2021250004)	2019 & 2021
0	GENCI HPC early access (Irene at TGCC) 8MM core-h (grant no. gch0301)	2018

Zurich, CH Jan 2024 onward

Zurich, CH

Apr 2021–Dec 2023

Melbourne, AU

Dec 2018-Mar 2019



TEACHING AND SUPERVISION EXPERIENCE

• Exercise sessions at ETH Zurich, MSc level, "Numerical simulation of flame archetypes" <i>Design of the solutions to the exercises and discussion of the results</i>	Spring 2023 & 2024
• Lecture at ETH Zurich, MSc level, "Numerical simulation of turbulent reactive flows" <i>Design and execution of the lecture</i>	Spring 2022 & 2023
• Hands-on at CAPS lab., ETH Zurich, "Large eddy simulation of reactive flows using AVBP" Design of the materials and guidance during the tutorials/exercises	Spring 2022
• Hands-on at CERFACS, "Large eddy simulation of reactive flows using AVBP" <i>Guidance of the tutorials/exercises</i>	2018–2020

I supervised the work of five MSc and two BSc students (thesis and projects) on topics such as: Numerical simulation of nonthermal plasma and turbulent reacting flows; Algorithms for reaction path analysis of plasma, combustion and NO_x chemistry; Reduced order modeling of thermochemical systems. The work of my students has all been successfully carried out as part of their studies. I also actively co-supervised PhD work at ETH Zurich on HPC of complex flows, including thermoacoustics, hydrogen combustion and nonthermal plasma.

ACADEMIC SERVICE

Research project peer review:		Journal peer review:	
German Research Foundation (DFG)	2024	Flow, Turbulence and Combustion	2021-2024
		Combustion and Flame	2019-2024
		Proceedings of the Combustion Institute	2022-2024

JOURNAL PUBLICATIONS

- [1] Q. Malé, C. Lapeyre, N. Noiray, "Hydrogen reaction rate modeling based on convolutional neural network for large eddy simulation", 2024, Submitted to Data-Centric Engineering, arXiv:2408.16709 [cs.CE]. URL.
- [2] M. Impagnatiello, Q. Malé, N. Noiray, "Acoustic scattering of a sequential combustor controlled with non-equilibrium plasma: A numerical study", *Proc. Combust. Inst.*, 2024. URL.
- [3] Q. Malé, K. Pandey, N. Noiray, "The LEAF concept operated with hydrogen: Flame topology and NOx formation", *Proc. Combust. Inst.*, 2024. URL.
- [4] Q. Malé, S. Shcherbanev, M. Impagnatiello, N. Noiray, "Stabilization of a thermoacoustically unstable sequential combustor using non-equilibrium plasma: Large eddy simulation and experiments", *Proc. Combust. Inst.*, 2024. URL.
- [5] M. Impagnatiello, Q. Malé, N. Noiray, "Numerical Study of Ignition and Combustion of Hydrogen-Enriched Methane in a Sequential Combustor", *Flow Turbul. Combust.*, 2024. URL.
- [6] Q. Malé, N. Barléon, S. Shcherbanev, B. Dharmaputra, N. Noiray, "Numerical study of nitrogen oxides chemistry during plasma assisted combustion in a sequential combustor", *Combust. Flame*, 2024. URL.
- [7] Q. Malé, S. Shcherbanev, N. Noiray, "Numerical study of plasma assisted combustion in a sequential combustor", *Proc. Combust. Inst.*, 2023. URL.
- [8] S. A. Shcherbanev, Q. Malé, B. Dharmaputra, R. Solana-Pérez, N. Noiray, "Effect of plasma-flow coupling on the ignition enhancement with non-equilibrium plasma in a sequential combustor", *J. Phys. D: Appl. Phys.*, 2022. URL.
- [9] Q. Malé, O. Vermorel, F. Ravet, T. Poinsot, "Jet ignition prediction in a zero-dimensional pre-chamber engine model", *Int. J. Engine Res.*, 2022. URL.
- [10] Q. Malé, O. Vermorel, F. Ravet, T. Poinsot, "Direct numerical simulations and models for hot burnt gases jet ignition", *Combust. Flame*, 2021. URL.
- [11] T. Jaravel, O. Dounia, Q. Malé, O. Vermorel, "Deflagration to detonation transition in fast flames and tracking with chemical explosive mode analysis", *Proc. Combust. Inst.*, 2021. URL.
- [12] Q. Malé, G. Staffelbach, O. Vermorel, A. Misdariis, F. Ravet, T. Poinsot, "Large Eddy Simulation of Pre-Chamber Ignition in an Internal Combustion Engine", *Flow Turbul. Combust.*, 2019. URL.
- [13] J. Lamouroux, S. Richard, Q. Male, G. Staffelbach, A. Dauptain, A. Misdariis, "On the Combination of Large Eddy Simulation and Phenomenological Soot Modeling to Calculate the Smoke Index From Aero-Engines Over a Large Range of Operating Conditions", *J. Eng. Gas Turbine Power*, 2018. URL.

Research presentations

Invited talks:

o 7 th Int. Flame Chemistry Workshop: "Integrating plasma effects into simulations []: status and challenges"	Jul 2024
• Swiss Combustion Day: "Multiphysics high performance computing of plasma-assisted combustion"	Feb 2024
 AVBP user's committee: "Large eddy simulation of plasma-assisted combustion" 	Dec 2023
• GENCI early access grant feedback at TGCC: "High performance computing for innovative engine design"	Jun 2019
• French Combustion Scientific Meeting: "Impact of rich burnt gas radicals on turbulent jet ignition: numerical study"	Mar 2018
Conference presentations:	
• Int. symposium on combustion: "Stabilization of a thermoacoustically unstable sequential combustor []"	Jul 2024
\circ Int. symposium on combustion: "The LEAF concept operated with hydrogen []"	Jul 2024
• Int. symposium on combustion: "Numerical study of plasma-assisted combustion in a sequential combustor"	Jul 2022
◦ Int. workshop on plasma-assisted combustion: "Numerical simulations of plasma-assisted combustion []"	Jun 2022
• Int. symposium on combustion: "Direct numerical simulations of jet ignition"	Aug 2018