Next-generation space–time integration methods with error control for highly compressible reactive Navier–Stokes flows

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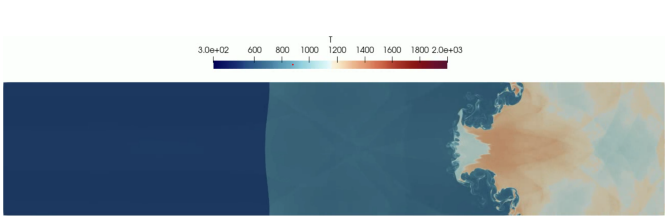
Abstract

Direct numerical simulation of hydrogen safety scenarios requires resolving highly compressible reactive flows with strong moving discontinuities, multi-scale turbulence and stiff chemistry, under time steps of a few nanoseconds to microseconds. The WALL-HY platform, developed jointly by CEA, CMAP and EM2C, combines adaptive multiresolution (library `samurai`), a high-order one-step monotonicity-preserving (OSMP) scheme for the Euler operator with complex equations of state, and the time-integration library `ponio`. This post-doctoral project aims at designing, analysing and implementing a new generation of space–time integration strategies for the reactive Navier–Stokes equations, in which the coupling between convection, diffusion and stiff reaction is controlled rather than merely split. The core of the project is the numerical analysis of partitioned implicit–explicit stabilised integrators of PIROCK type, in collaboration with Gilles Vilmart (University of Geneva), their coupling with a one-step space–time convection scheme and with multiresolution-based mesh adaptation, and the quantification of the accuracy/efficiency trade-off of CFL- and Fourier-constraint relaxation strategies. Applications target hydrogen risk in extreme thermodynamic conditions.

1 Context

Hydrogen raises multiple safety issues in industrial and domestic contexts: H_2 is odourless and colourless, leaks and ignites easily in air, and readily undergoes deflagration-to-detonation transition. Controlling hydrogen risk is essential for new nuclear reactor designs and for the deployment of low-carbon energy technologies. Its simulation at DNS resolution requires solving highly compressible reactive flows involving strong moving discontinuities (shock waves), turbulence over a wide range of scales and time steps severely constrained by the CFL condition, together with the very broad spectrum of time scales of combustion chemistry [13, 27]. This calls for numerical methods that are accurate, robust, efficient and portable on parallel architectures.

The WALL-HY platform, the result of a collaboration between CEA, CMAP and EM2C, has demonstrated its ability to resolve such flows beyond the state of the art, in particular for strongly turbulent shock–interface interactions (reactive Richtmyer–Meshkov instabilities, Fig. 1, left). WALL-HY is a finite-volume code built on the adaptive multiresolution framework `samurai` [6] developed at CMAP, which relies on an algebra of intervals and a wavelet decomposition of the discrete solution [7, 17]; it typically removes about 90–95 % of the cells while controlling the error (Fig. 1, right). The Euler operator is solved with the OSMP scheme [8], extended to thermodynamically complex multi-species equations of state [21], which provides a high-order space–time coupling, a much lower dissipation of contact discontinuities than WENO-type schemes [5, 19], and up to a sixfold speed-up with respect to WENO5. WALL-HY is interfaced with the time-integration library `ponio` [23], which offers a broad range of explicit, implicit, ImEx, splitting and stabilised schemes, including PIROCK [4], still largely unexplored for reactive flows in which convection, diffusion and reaction act simultaneously.



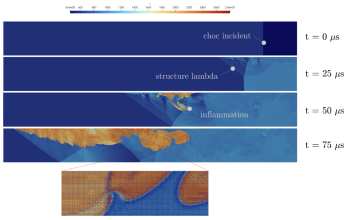


Figure 1: WALL-HY simulations. Left: reactive Richtmyer–Meshkov instability ($Xe/H_2/O_2$ mixture with an upstream N_2 material interface, single-mode perturbation evolving towards turbulence; $\phi = 1$, $P_0 = 1\,\text{atm}$, $T_0 = 298\,\text{K}$, $\text{Ma}_{\text{shock}} = 1.83$). Right: ignition of a lean H_2/air premixture behind a reflected shock in a closed tube ($\phi = 0.5$, $\text{Ma}_{\text{shock}} = 2.5$): 67 M cells at the finest level, at most 3.5 M cells during the computation (∼95 % compression), minimum cell size 2.4 µm, time step $\sim 9 \times 10^{-10}$ s.

2 Objectives

The project pursues the development of numerical methods for the space–time integration of the reactive Navier–Stokes equations along four main objectives:

1. **Next-generation time integrators with controlled operator coupling.** Improve the quality of the solution by analysing finely the coupling between convection, reaction and diffusion, whose stiffness varies widely: reaction and diffusion are integrated in a coupled way by new-generation partitioned ImEx stabilised integrators of PIROCK type implemented in `ponio` [23], combined with the one-step OSMP treatment of convection, with an explicit control of the coupling errors instead of full operator splitting.
2. **Performance through constraint relaxation.** Relax the CFL time-step constraint by exploiting operator splitting (Lie, Strang [25]) and stabilised explicit treatment of diffusion on the finest levels, where the Fourier constraint scales as Δx^{-2}; the impact of these accelerations on accuracy must be quantified both theoretically and numerically.
3. **Physics in extreme thermodynamic conditions.** Adapt the equations of state to high pressures and temperatures, which significantly modifies the hyperbolic structure of the underlying Euler system and requires its rigorous re-derivation; ionisation and strongly non-equilibrium thermodynamics (vibrational, translational and electronic temperatures) may be explored.
4. **Support of the `samurai` platform [6].** Boundary conditions, GPU porting and complex geometries (immersed boundaries, cell warping).

Depending on the profile and interests of the candidate, high-order discontinuous Galerkin methods and multiwavelets [14, 15, 18] may also be explored.

3 Numerical analysis

The numerical-analysis component is at the heart of the project; it builds on our earlier work on adaptive splitting, multiresolution and dedicated stiff integrators [9–12].

From operator splitting to controlled coupling. Full operator splitting is very efficient, but the splitting error forces time-step adaptation to guarantee a correct coupling of the operators [9]; it may cause order reduction, poor preservation of steady states and difficulties with boundary conditions, and it leads to prohibitively small time steps when the coupling scales between operators are very fine. Additive ImEx Runge–Kutta methods [20,24] and partitioned stabilised integrators offer an alternative in which the coupling error is controlled. The postdoctoral researcher will analyse the fully coupled approach based on extended-stability Runge–Kutta–Chebyshev methods (ROCK2/ROCK4 [1,3]) and their partitioned ImEx version PIROCK [4], in which diffusion is treated by an explicit stabilised stage, stiff reaction implicitly and advection explicitly, with an embedded error estimator. The analysis will first address scalar linear model problems to quantify coupling errors and stability regions with respect to the stiffness ratios between operators [16], and then the reaction–diffusion and full reactive Navier–Stokes systems.

Space–time coupling with a one-step convection scheme. OSMP is a one-step scheme of Lax–Wendroff type in which space and time accuracy are intrinsically coupled. Its combination with multi-stage stabilised or ImEx integrators for diffusion and reaction cannot rely on the method of lines and raises specific questions: design of intermediate strategies in which reaction and diffusion are integrated in a coupled way by PIROCK-type methods while advection is treated separately by

OSMP, analysis of the resulting order and of the splitting error at shocks and contact discontinuities, and preservation of the high-order space–time accuracy of OSMP.

Relaxing the Fourier constraint on adaptive grids. On multiresolution grids, the stiffness of diffusion is driven by the finest level. Explicit stabilised methods, whose number of stages scales as the square root of the stiffness, and multirate stabilised variants [2] that concentrate the cost on the finest cells will be analysed, together with their interaction with local time stepping across levels.

Error control in space and time. Adaptive multiresolution provides an a priori control of the space discretisation error through the thresholding parameter [7, 17]. The goal is to balance this space error with the time-integration and coupling errors, operator by operator, so as to guarantee the accuracy of the full reactive solution within a finite-volume framework of varying order, building on time–space adaptive strategies previously developed for combustion fronts [11].

Collaboration on next-generation integrators. This part will be carried out in close collaboration with Gilles Vilmart (Section de mathématiques, University of Geneva), co-author of PIROCK [4], on new-generation partitioned stabilised integrators built around PIROCK, already implemented in `ponio` [23]: analysis of their order and stability for advection–diffusion–reaction coupling with strongly varying stiffness, improved damping and stabilisation strategies, extension to higher order and to multirate settings, and design of reliable error estimators for adaptive time stepping. Research visits to Geneva are planned.

4 Work programme

1. **Analysis of ImEx and PIROCK-type schemes** on model problems: coupling errors, order conditions, stability with respect to the stiffness of each operator, embedded error estimators; comparison with Lie/Strang splitting.
2. **Space–time coupling with OSMP** and stabilised treatment of diffusion on the finest multiresolution levels, with theoretical and numerical quantification of the accuracy/efficiency trade-off of CFL and Fourier relaxation.
3. **Implementation and validation in `ponio`/`samurai`/WALL-HY** on reactive test cases of increasing complexity: auto-ignition of a diffusion flame [26], shock-induced ignition of H_2/air mixtures and reactive Richtmyer–Meshkov instabilities, including full multi-component and thermo-diffusive (Soret, Dufour) transport.
4. **Extreme thermodynamic conditions**: high-pressure, high-temperature equations of state, re-derivation of the hyperbolic structure and adaptation of the OSMP scheme and of the boundary conditions treated through ghost cells, for which stabilisation methods at singular (zero-velocity and sonic) points have recently been developed [22].

The developments will be integrated into the open-source libraries `samurai` and `ponio`, and the results disseminated through publications and communications at international conferences.

5 Candidate profile

PhD in applied mathematics, numerical analysis and scientific computing. Solid background in numerical analysis of PDEs and stiff differential equations is expected; knowledge of compressible and reactive flows is appreciated. Good programming practice (modern C++ preferably) and an interest in high-performance computing are expected.

6 Supervision and environment

- **Supervision:** Marc Massot (CMAP), Pierre-Alexandre Masset (CEA) and Christian Tenaud (EM2C and Fédération de Mathématiques de CentraleSupélec).
- **Host laboratories:** CMAP (HPC@Maths team) and LE2H (CEA); partners: EM2C and FdM CentraleSupélec.
- **Collaborations:** Gilles Vilmart (Section de mathématiques, University of Geneva); Laurent Séries, Loïc Gouarin and Josselin Massot (HPC@Maths, CMAP).

The work will be carried out at CMAP (HPC@Maths team), in close interaction with CEA, EM2C and the Fédération de Mathématiques de CentraleSupélec, and with the HPC@Maths research engineers who develop `samurai` and `ponio`.

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