2025 Helmholtz – OCPC – Program

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Jacobian-Free Newton-Krylov Approach for 3D Fully-Implicit Coupled Multiphysics Simulation of Hydrogen-based Energy Systems

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT), Institute for Thermal Energy Technology and Safety (ITES)

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Description of the project (max. 1 page):

Introduction:

The utilization of hydrogen as a clean and sustainable energy source has gained significant attention in recent years due to its potential to reduce greenhouse gas emissions and dependence on fossil fuels. Combustion of hydrogen, however, presents unique challenges due to its high reactivity and the resulting numerical stiffness in computational fluid dynamics (CFD) simulations. Efficient and accurate numerical methods are essential for modeling fully-coupled multi-physical phenomena in innovative hydrogen applications, particularly when dealing with stiff systems that arise from the coupling of turbulence, chemical kinetics, heat transfer and fluid dynamics.

This project aims to explore the feasibility of and develop a Jacobian-Free Newton-Krylov (JFNK) approach to tackle the numerical challenges associated with three-dimensional fully-implicit coupled multi-physics simulation relevant to advanced hydrogen-based technologies. The proposed method will leverage high-order numerical schemes, embedded boundaries and adaptive mesh refinement (AMR) to enhance the computational accuracy and efficiency.

Objectives:

1. **Development of a JFNK Method**: Develop a Jacobian-Free Newton-Krylov method to solve the non-linear systems arising from multi-physics CFD simulation of innovative hydrogen energy applications. The JFNK approach significantly minimizes memory requirements and computational cost, thereby enabling the simulation of complex hydrogen energy systems with enhanced fidelity and reduced computational cost.
2. **High-Order Numerical Schemes**: Incorporate high-order spatial and temporal discretization schemes to improve the accuracy of the simulations. High-order schemes are particularly beneficial for capturing the complex dynamics of compressible flows.
3. **Adaptive Mesh Refinement (AMR)**: Develop an AMR strategy to dynamically adjust the computational grid based on local flow features. This will ensure that regions with high gradients or complex chemistry are resolved with sufficient accuracy while minimizing computational effort in less critical areas.
4. **Verification and Validation**: Validate the developed method against traditional methods, benchmark cases and experimental data, with a specific emphasis on conducting high-fidelity and efficient multi-physics simulations for hydrogen-based energy systems.

Expected Outcomes:

1. **Efficient Solver for Non-linear Stiff Systems**: The development of a JFNK-based approach will provide an efficient, fully-implicit and coupled solution for simulating multi-physics, particularly for hydrogen-based energy systems.
2. **Improved Efficiency and Accuracy**: The integration of high-order numerical schemes and AMR will significantly improve the accuracy of the simulations, enabling the capture of complex features in multi-physics simulations.
3.

Keywords:
Hydrogen-based energy system, Computational Fluid Dynamics (CFD), Jacobian-Free Newton-Krylov (JFNK) method, multi-physics simulation, Adaptive Mesh Refinement (AMR).

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

Tsinghua University is one of the Chinese Universities which have developed direct cooperations with the Karlsruhe Institute of Technology.
Tsinghua University, located in Beijing, China, is renowned globally for its academic excellence, innovative research, and commitment to fostering international partnerships that drive knowledge exchange and collaboration. As one of China's top-tier universities, Tsinghua University has a rich history dating back to its establishment in 1911 and has consistently ranked among the world's leading academic institutions. Tsinghua University is a comprehensive research university and a base for training high-level talents and scientific and technological research in China. As of August 2022, the university covers an area of 462.74 hectares, with a construction area of 3.0267 million square meters. The university offers 12 discipline categories, including science, engineering, literature, art, history, philosophy, economics, management, law, education, medicine, and interdisciplinary studies, with 21 colleges, 59 teaching departments, and 87 undergraduate majors. With a diverse and vibrant community of students, scholars, and researchers from across the globe, Tsinghua University offers a dynamic and multicultural environment that encourages cross-cultural learning and intellectual growth.

Required qualification of the postdoc:

- A Ph.D. in applied physics or a related engineering field.
- Demonstrated experience in applying the Jacobian-Free Newton-Krylov (JFNK) Method.
- Proficiency in programming with open-source scientific computation libraries like PETSc, Sundials, and Trilinos.
- Proficiency in programming languages such as C++, Fortran 90, and Python.
- Experience with Computational Fluid Dynamics (CFD) software, including OpenFOAM, ANSYS Fluent, PeleC, or GASFLOW, is advantageous.
- Strong collaborative skills to work effectively with diverse teams and communicate research findings.
- Excellent proficiency in both written and oral English.