University of Stuttgart

Institute for Nonlinear Mechanics

Bachelor's thesis
Term paper
Master's thesis

Runge–Kutta methods for implicit differential equations on parallel computers

Topic Areas:	numerics, algorithms, implementation
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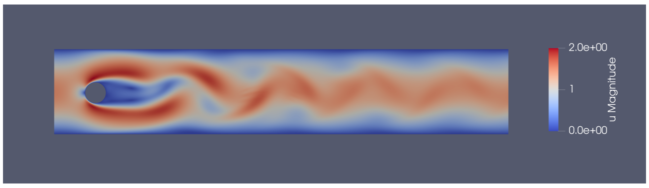
Prerequisites/Prior Knowledge:	interest in numerical algorithms

This thesis explores the numerical time integration of implicit differential-algebraic equations (DAEs) of the form:

$$\boldsymbol{f}(t, \boldsymbol{y}, \dot{\boldsymbol{y}}) = \boldsymbol{0}\,,$$

with given initial conditions. Such systems are fundamental across a wide range of physical modeling applications, including constrained mechanical systems, electrical circuits, incompressible fluids, chemical kinetics with conservation laws, and optimal control problems.



FEM simulation of Kármán vortex street.

This thesis focuses on implicit Runge–Kutta methods, specifically investigating the Radau IIA family due to their exceptional stability characteristics and superior convergence rates.

To reduce the computational cost associated with these methods, simplified Newton iterations are employed to solve the nonlinear equations, minimizing the number of Jacobian evaluations required. Furthermore, the cost of linear algebra operations (such as LU decompositions and forward/backward substitutions) can be significantly reduced by transforming the linear systems into diagonal, block diagonal, triangular, or Jordan canonical forms. Following the approach in [1], this transformation enables the decomposition of large linear systems into smaller, independent systems that can be solved in parallel, further enhancing computational efficiency.

In addition, the effective implementation of implicit Runge–Kutta methods requires the development of advanced error estimation techniques and finely tuned step-size control mechanisms, which must work in harmony to ensure optimal performance.

The key objectives of this thesis are to

- implement a parallel Radau IIA method with adaptive step-size control and simplified Newton iterations in Python, similar to the Fortran solver proposed in [2].
- validate the implementation using a variety of benchmark problems from the literature that have known analytical solutions
- compare the work-precision of the implemented method with other methods from literature.

The scope of this project may be adapted to fit the specific type of thesis being pursued.

References

[1] P. J. van der Houwen and J. J. B. de Swart, "Parallel linear system solvers for Runge-Kutta methods," *Advances in Computational Mathematics*, 1997.

[2] J. J. B. de Swart, W. M. Lioen, and W. A. van der Veen, "Specification of PSIDE," 1998.