CFD with OpenSource software

A course at Chalmers University of Technology
Taught by Håkan Nilsson

Study questions and answers for:

Implementation of growing CCM library to reduce chemistry calculation time

Author:
Yuchen Zhou
Lund University
yuchen.zhou@energy.lth.se

Peer reviewed by:
Xue-Song Bai
Yaquan Sun
Mohammad Hossein Arabnejad Khanouki

January 14, 2023

Study questions and answers

1. What is Chemistry Coordinate Mapping (CCM) and the basic procedure of that?

   CCM is a chemistry acceleration method. During a simulation of the reactive flow, physical grids with similar reaction states will be grouped and share an identical reaction rate. This way, the amount of points sent to the chemistry solver will be much fewer so that the calculation time is significantly shorter.

   The procedure of the CCM method will include indexing, grouping, solving, and assigning.

2. What is the basic theory behind CCM, or generally the basic theory behind a chemistry acceleration method?

   The basic idea is that the reaction rates have a low-dimensional manifold. We might choose some key variables to represent the feature of the whole manifold.

   The thought behind generally all chemistry acceleration methods is that many physical grids during different times might fall into the same places in the manifold, so we might come up with some methods to reuse them instead of re-calculating them again and again.

3. How do you choose some key variables to construct a reaction rate manifold for your simulation case?

   The general idea is to make sure the chosen variables are enough to characterize the manifold.

   For constant pressure reacting flow, temperature, progress variable, scalar dissipation, and some key species will be enough.

   For diffusion flame, adding the mixture fraction might be helpful.

4. How do you use CCM and growing CCM to accelerate the combustion simulation?

   The answer is in Chapter 4 of the report.

5. How can you modify a chemistry library?

   The answer is in Chapters 3 and 4 of the report.

6. How do you manage index/data (in this case, reaction rates) with multiple cores efficiently?

   Conclude Chapter 3 for the long answer.