TECHNISCHE UNIVERSITÄT DARMSTADT

High Performance Computing of Stratified Burner using ATF and FGM models

NuSim

Numerical Simulation on High Performance Computer

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16.04.2012

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Outline

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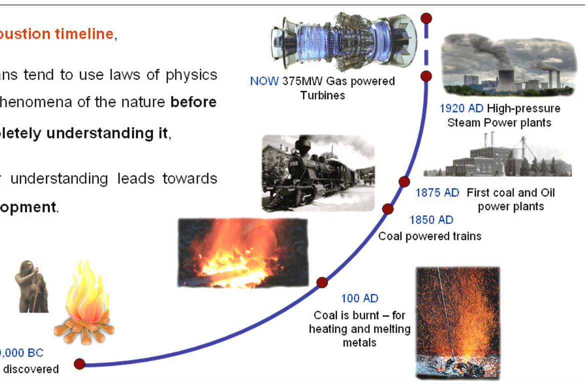
Introduction

- Combustion timeline,
- Humans tend to use laws of physics and phenomena of the nature **before completely understanding it**,
- Better understanding leads towards **development**.



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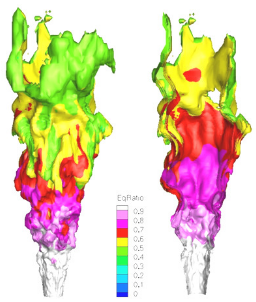
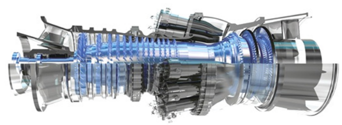
Motivation

- Trend of using **lean stratified combustion** (IC-engines, lean-burn gas turbines), gaining deeper understanding into the **physics** by means of **numerical modeling**,





- **Stratified conditions** in **practical combustion processes** – have reduced **harmful emissions** and improved combustion efficiency for reduced **fuel consumption**,

Perfectly premixed reactants — Stratified conditions — **Perfectly non-premixed reactants**

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Numerical modeling

Governing equations | Combustion modeling | Coupling

Favre Filtered Governing equtions

Modeling

i. Closing the equations
ii. Combustion Modeling

- Conservation of mass

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0$$

- Conservation of momentum

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right) = \frac{\partial}{\partial x_j}\left[\bar{\rho}\nu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\bar{\rho}\nu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij} - \bar{\rho}\tau_{ij}^{SGS}\right] - \frac{\partial \bar{p}}{\partial x_j} + \bar{\rho}g_i$$

Smagorinsky sub-grid scale model

- Species transport equations

Eddy-diffusivity model

$$\frac{\partial\left(\bar{\rho}\tilde{Y}_k\right)}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\tilde{Y}_k\right) = \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{D}_k\frac{\partial \tilde{Y}_k}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}J_i^{SGS}\right) + \bar{\dot{\omega}}_k \quad \text{for } k = [1, 2, \ldots, n]$$

~100 of species and 1000 of reactions

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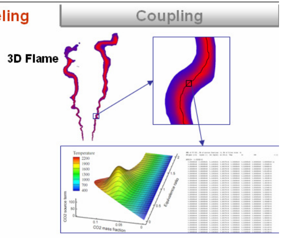
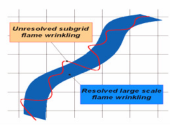
Numerical modeling

Governing equations | Combustion modeling | Coupling

i. **Flamelet Generated Manifold (FGM)**
   - **Idea:** Multidimensional turbulent flame can be divided into large amount of 1D laminar flames
   - Describing **detailed chemistry** by only **two controlling variables** computed by transport equations
     - **progress variable** & **mixture fraction**

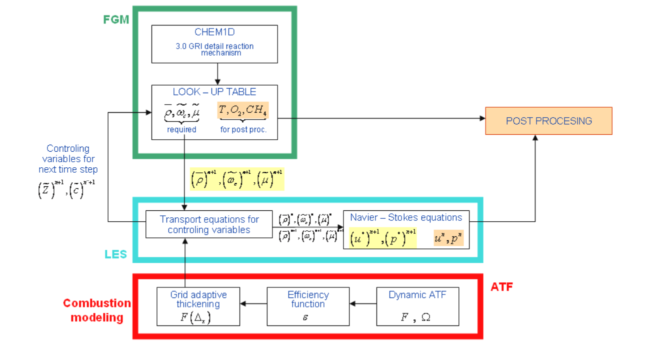


ii. **Artificially Thickened Flame (ATF)**
   - **capturing flame front** on standard Large Eddy Simulation (LES) grid size of 1 mm [G. Kuenne et al.]



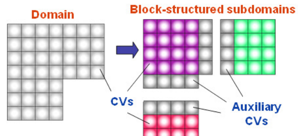
Numerical modeling

Governing equations | Combustion modeling | **Coupling**

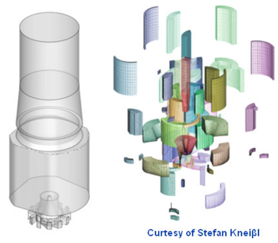


Parallel computing in FASTEST

- Concept of **block-structured grids** is used for the treatment of complex geometries,



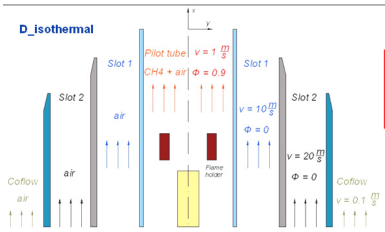
- Block structuring is also used for parallel computing by means of **grid partitioning technique**,

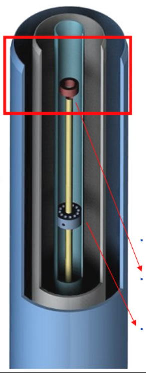


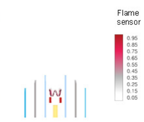
- According to a number of available processors mapping from **geometrical block-structure** into a **parallel block-structure** is performed.

Stratified Burner - Configuration

D_isothermal







Turbulent Stratified Flame D Configuration

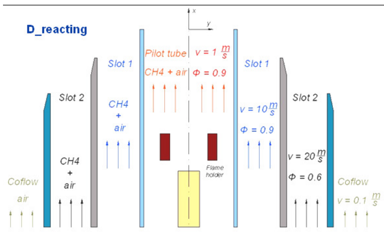
Config.	Φ_{pilot}	$v_{pilot}, \frac{m}{s}$	Φ_{Slot1}	$v_{Slot1}, \frac{m}{s}$	Φ_{Slot2}	$v_{Slot2}, \frac{m}{s}$
D_i1	0.9	1	0	10	0	20
D_r	0.9	1	0.9	10	0.6	20

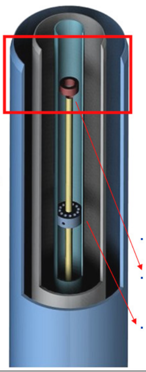
SLOT 1 SLOT 2

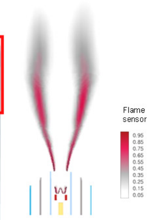
- Stratified flames are stabilized by central pilot flame,
- Central pilot flame is stabilized by central flame holder,
- Perforated plate centers the flame holder (±10%) and enhances turbulence intensity upstream.

Stratified Burner - Configuration

D_reacting







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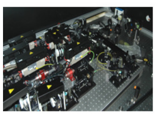
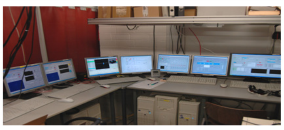
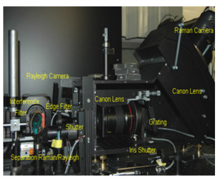
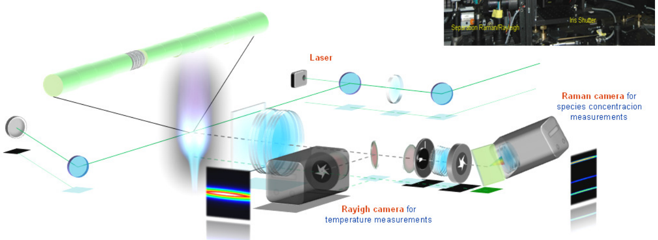
Experimental setup

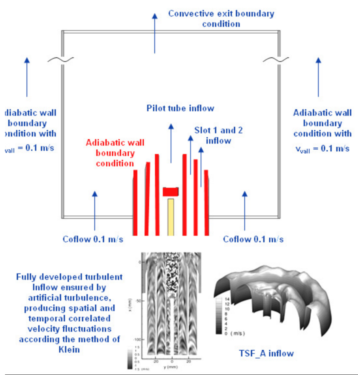




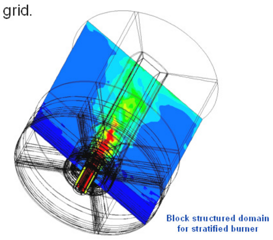




Numerical setup



- To **minimize sensitivity** related to the **boundary conditions**, details of the upstream geometry including the flame holder, are accounted for by the grid.



Grid

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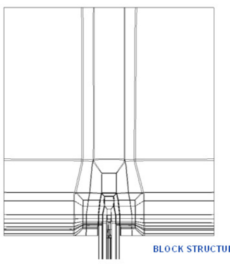
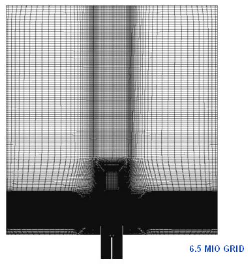
- Block structured hexahedral, boundary fitted grids, with 449 blocks to represent stratified burner geometry,
- **6.5 mio** and **0.8 mio** control volume meshes are used.





Results

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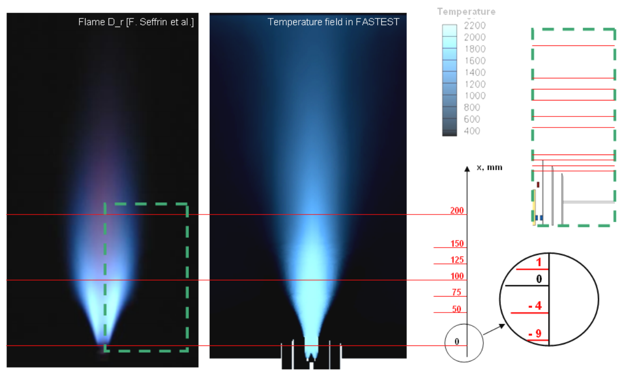

Results

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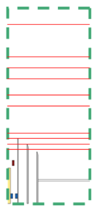
Results overview:

- **D_i1 – isothermal case with only pilot flame burning**
  - mean axial and mean radial velocities vs. experiments,
  - mean axial and mean radial fluctuating velocities.
- **D_r – reacting case**
  - mean axial and mean radial velocities vs. experiments,
  - mean axial and mean radial fluctuating velocities,
  - TSF_A vs. TSF_D reacting cases.
- **Parallelization using domain decomposition**
  - Evaluation of computation time required for TSF_D



Results

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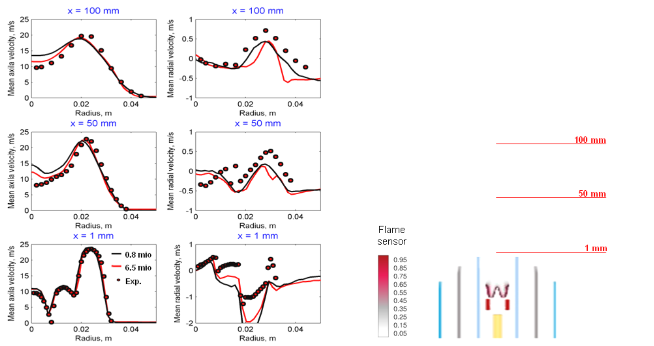
TSF_D_isothermal | TSF_D_reacting | TSF_A vs. TSF_D | Parallelization



Results

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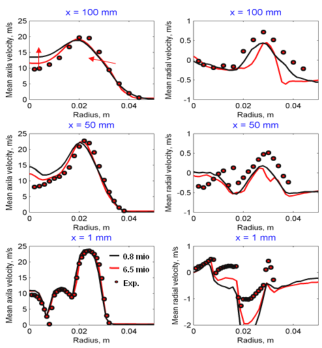
TSF_D_isothermal | TSF_D_reacting | TSF_A vs. TSF_D | Parallelization



- **Over prediction** of the mean axial velocity in the last planes close to central axis for coarse mesh,
- Axial velocity profile is **slightly shifted** towards central axis,
- Shifting toward inward can be seen with mean radial velocity **under prediction**,
- **Additional computational time** for fine grid is needed.

Results

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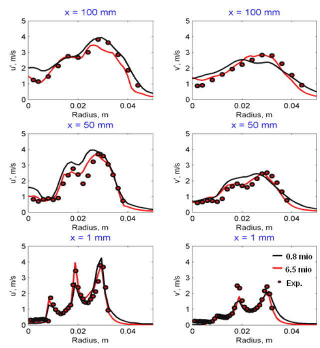
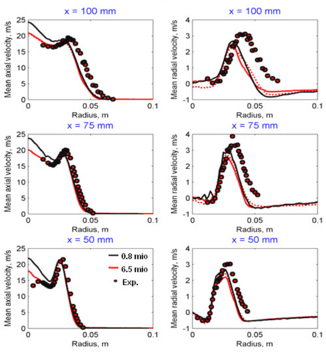
TSF_D_isothermal | TSF_D_reacting | TSF_A vs. TSF_D | Parallelization

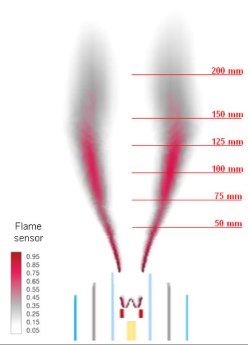
- Fluctating components of axial and radial velocity are in **good agreement** with experiments,
- Fine mesh provides better agrement, but additional computation is needed for the last planes.



Results

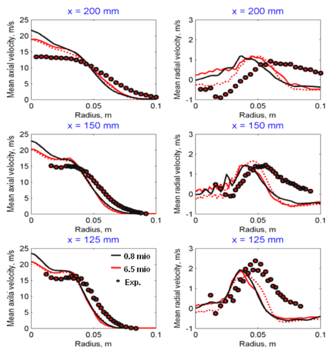
TSF_D_isothermal | **TSF_D_reacting** | TSF_A vs. TSF_D | Parallelization





Results

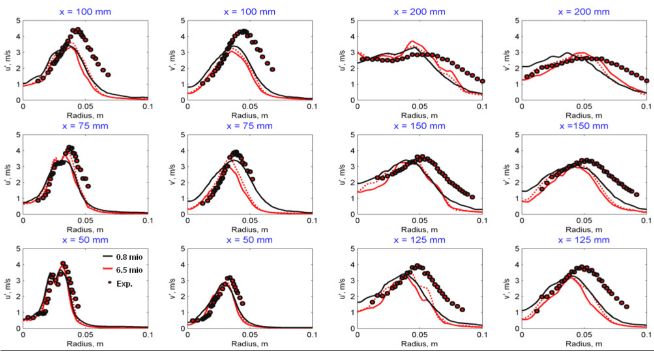
TSF_D_isothermal | **TSF_D_reacting** | TSF_A vs. TSF_D | Parallelization



- **Higher over prediction** of the mean axial velocity close to central axis comparing to D_i1,
  - **Increased axial velocity is partially most likely due to assumption that heat loss can be neglected.**
- Grid sensitivity at symmetry axis in terms of smaller mean axial velocity,
  - **Finer grid can be used for comparison.**
- Grid convergence further from the symmetry axis,
  - **Flame sensor for lean combustion should be improved to capture flame front more correctly in this region.**

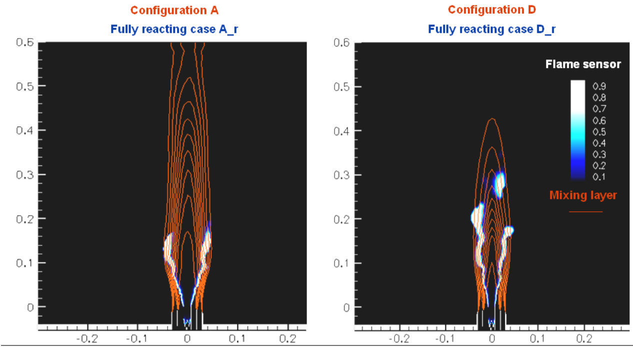
Results

TSF_D_isothermal | **TSF_D_reacting** | TSF_A vs. TSF_D | Parallelization



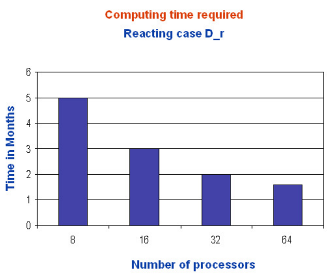
Results

TSF_D_isothermal | TSF_D_reacting | **TSF_A vs. TSF_D** | Parallelization



Results

TSF_D_isothermal | TSF_D_reacting | TSF_A vs. TSF_D | **Parallelization**



- **Evaluation :**
  - parallelization for high pressure combustor,
  - preveporized kerosene,
  - 2 million CV,
  - Same physical time simulated,
  - HHLR (IBM power6).
- More detailed investigation using Stratified Burner with complex combustion models are planned.

Summary and outlook

- Summary
  - **Combustion modeling**
    - Isothermal and reacting case for configuration A and D of stratified burner were simulated using FGM and ATF,
    - Results for velocity of TSF_D were presented where fine grid provides **good agreement** between experiments and simulation,
    - Some improvements for better prediction are suggested.
  - **Parallelization**
    - Evaluation of parallelization using domain decomposition and MPI for **complex combustion models**,
    - Preliminary data for the verification of openMP by computation for **different conditions** (TSF_A and TSF_D configurations) and with **different meshes** is being collected.

Summary and outlook

- Outlook
  - **Combustion modeling**
    - Grid refinement,
    - Include **heat losses** for better prediction,
    - Influence of stratification effects on flame sensor and its improvement for better flame front prediction in stratified region.
  - **Parallelization**
    - **Heat losses** implementation for realistic applications (combustion chambers),
    - Implementation of **openMP** strategy to achieve hybrid parallelization for combustion models in FASTEST-3D,
    - **Evaluation** of implemented hybrid parallelization.

Thank you for your attention!