EX25302

Quantum-HPC hybrid architecture toward reacting flow analysis

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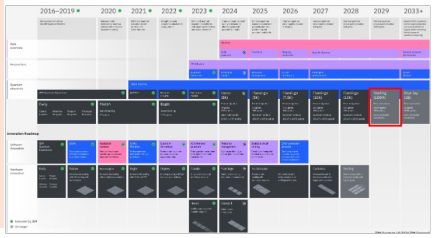
Intoroduction

Emerging technologies
- Efficient combustion
- Carbon-free combustion

→ Combustion under extreme condition and/or new fuel → Require detail analyses

Quantum computers
- Quantum acceleration
- Clear hardware roadmap[2]

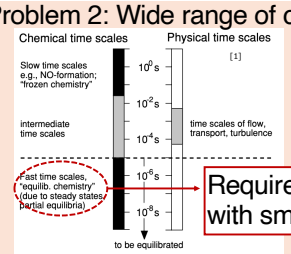


Problem 1: Huge number of variables

Physical parameter	Number of variables
Mass	1
Energy	1
Flow	1-3
Chemical species	**10-1000**

Need to handle many variables

Problem 2: Wide range of characteristic time scale



→ Requires time integration with small time step size

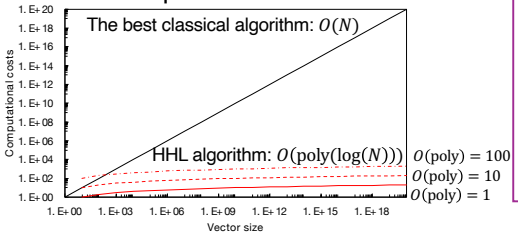
HHL: The quantum algorithm to obtain the solution vector of linear equation[3]:

A problem $A\vec{x} = \vec{b}$ → Input $A, \vec{b}$ → HHL → Solution $\vec{x}$

Non-linear problem $\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x})$

Process on HPC / Process on quantum computer

Comparison of computational costs: classical vs quantum



Carleman linearization : the method to linearize the non-linear problems[4]

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{F}(\boldsymbol{x}) = \sum_{k=1}^{K} a_k \boldsymbol{x}^{\otimes k} \qquad \boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}^{\otimes 1} \\ \boldsymbol{x}^{\otimes 2} \\ \vdots \\ \boldsymbol{x}^{\otimes K} \end{pmatrix}$$

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = A\boldsymbol{X}$$

Update $\boldsymbol{x}$ Time stepping

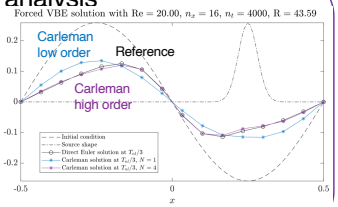
Linearized problem $A\boldsymbol{y} = \boldsymbol{b}$
→ Pre-conditioning $\tilde{A}\tilde{\boldsymbol{y}} = \tilde{\boldsymbol{b}}$
→ Post-conditioning $\tilde{\boldsymbol{y}} \longrightarrow \boldsymbol{y} \longrightarrow \boldsymbol{x}$

Input $\tilde{A}, \tilde{\boldsymbol{b}}$ → HHL → Output $\tilde{\boldsymbol{y}}$

Nonlinearity in combustion analysis

Convection term: Velocity × Variable

Reaction term → No investigation



Demonstrated with Burger's equation[5]

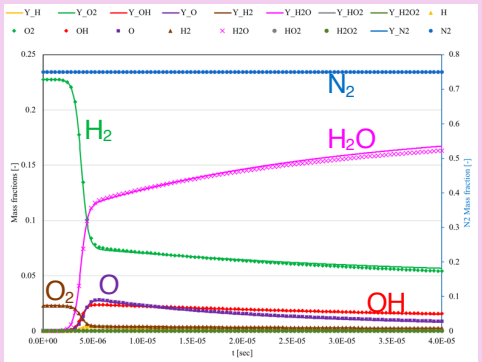
Objective: To establish the method to describe the reaction term as linear problem with Carleman linearization

Overall approach

Common settings
- Carleman linearization : SageMath[6] + extra library 'carlin[7]'
- Solution method: implicit method

Collision[11]

Concentration × Concentration



Reference data
Cantera[8] with skeletal mechanism based on USC Syngas mechanism[9] (9 species, include only H and O atoms and N_2 molecule)

Temperature dependence

$k \sim \exp(-E/RT)$

Taylor series

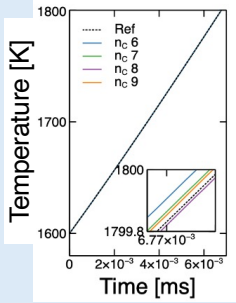
$$k(T+\Delta T) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n k}{dT^n} (\Delta T)^n$$

$$\frac{d^n k}{dT^n} = \frac{k}{T^n} \sum_{j=1}^{n} a_j^n \theta^j$$

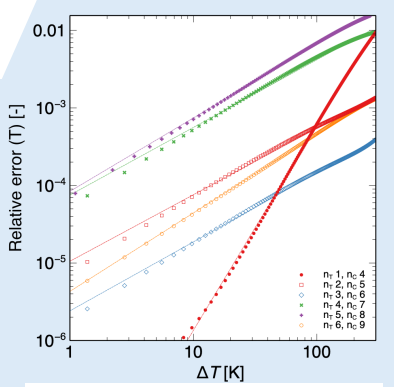
$$\theta = E/RT$$

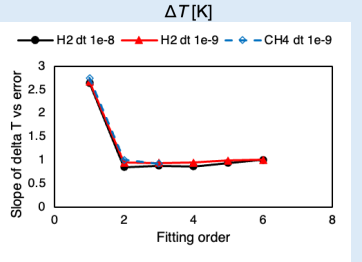
$$a_j^n = \begin{cases} a_{n-1}^{n-1} (= 1)(j = n) \\ a_{j-1}^{n-1} - (n-1+j) a_j^{n-1} \ (j \neq n) \end{cases}$$

$$a_1^1 = 1, a_0^{n-1} = 0$$



Reference data
Cantera[8] with single-step mechanism based on SanDiego mech.[10]





Conclusions

The concept to describe the non-linear reaction term as linear problem with Carleman linearization was presented. The validity of the simulation was partially given.

References
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