Oral presentation | Higher order methods

## Higher order methods-III

Tue. Jul 16, 2024 2:00 PM - 4:00 PM Room C

# [5-C-03] Robust and Efficient Numerical Schemes for LES of Liquid Rocket Engine Combustor

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Keywords: High-order, Limiter, Time integration, Turbulent Combustion

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# Robust and Efficient Numerical Schemes for LES of Liquid Rocket Engine Combustor

Takanori HAGA
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ICCFD12
Kobe, Japan, July 14-19, 2024

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## Outline

1. **Introduction**
2. **Physics modeling for Liquid Rocket Engine (LRE) simulation**
3. **Numerical schemes**
   - Robust entropy-based limiter
   - Paired explicit Runge-Kutta (P-ERK) scheme
4. **Summary/Ongoing work**

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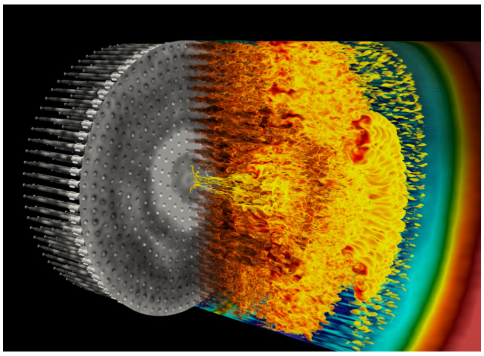
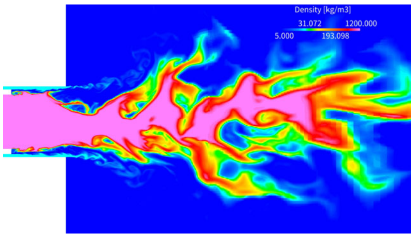
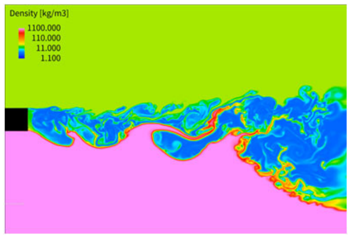
## Toward Full-Scale Simulation of LRE



**Full-scale chamber**
＞500 injectors
～1 m length



**Single-element (Co-axial)**
Diameter ～10 mm



**Injector tip**
Thickness <1 mm

**Grid to resolve small scales near the tip**

- Minimum grid spacing at tip ～10 μm (50-100 points)

**Sound speed** inside chamber ＞1,000 m/s

- Time step size ～10 ns （CFL～1)
- 1-10 million steps for 10-100 ms (target freq. ≧ 1 kHz)

**【Goal】**

To predict combustion instability by high-fidelity simulation → Compressibility

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## LES Solver "LS-FLOW-HO"

**Massively parallel combustion LES solver for Exa-scale**
(Development started in 2012)

**Step 1. To reduce the cost (the number of grid points)**

- HO scheme : Resolves turbulence/acoustics with fewer grid points
- Flamelet table : Models flame structure (diffusion flame) without resolving on a grid

**Step 2. To ensure numerical stability**

- Limiter for trans-critical interface

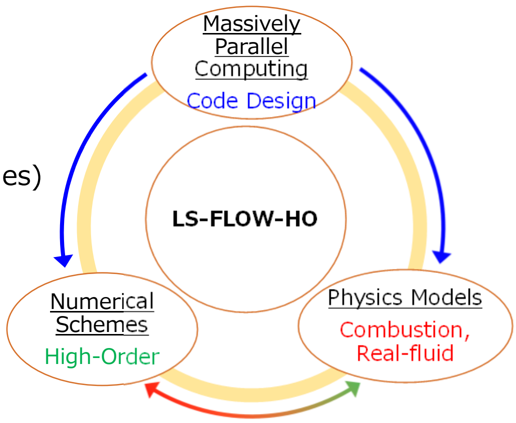
**Step 3. To speed-up the full-scale simulation**

- Code tuning
- Regression model (Cubic EoS, Transport Properties)

**Step 3′. Speed-up more!**

**Supercomputer Fugaku**
**Industrial Access Projects (FY2024, Prof. Kurose)**

- 8,000,000 Node Hours
- Full-scale LRE combustor simulation

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## Research Objectives

**Objectives:**
Develop the flux reconstruction (FR) method for liquid rocket engine (LRE) combustor simulations

**Approach:**

- Robust discontinuous capturing scheme for trans-critical interface of liquid oxygen (LOX)
  - Positivity-preserving limiter based on the local entropy (Zhang et al. 2010, Dzanic and Witherden, 2022)
- Efficient time integration algorithms suitable for massively parallel computation
  - Paired Explicit Runge-Kutta (P-ERK) Scheme (Vermeire, JCP 2019)

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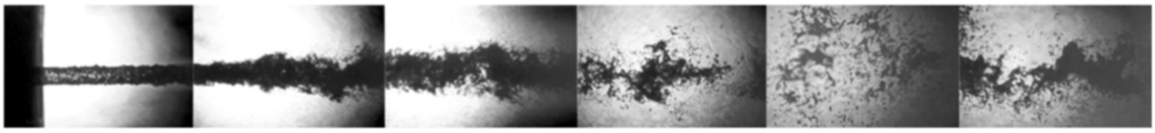
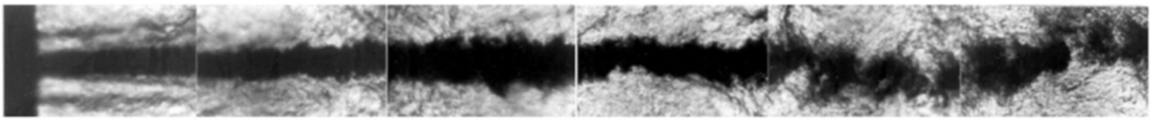
# LOX/GH2 Mixing and Combustion



(a) Subcritical Pressure, 1.5 MPa Combustion



(b) Supercritical Pressure, 10 MPa Combustion

*Mayer and Tamura (1996)*

| | $T_C$ [K] | $P_C$ [MPa] |
|---|---|---|
| $O_2$ | 155 | 5.1 |
| $H_2$ | 33 | 1.3 |

- "**Gas like mixing**" under the **supercritical pressure**
  - ➢ Surface tension and latent heat of evaporation are assumed to be negligible. → **single phase model**
- Liquid oxygen is usually injected at **subcritical temperature <155 [K].**
  - ➢ Real fluid effects should be considered. → **SRK EoS**

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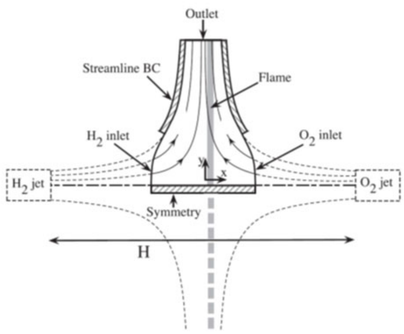
# Flamelet Progress Variable Model

- Turbulent diffusion flame is modeled as an aggregate of laminar flamelets by assuming:
  - ➢ Low Mach number, Da>1, Le=1
- Counterflow diffusion flame (1D) is solved by ***FlameMaster*** (Prof. H. Pitsch)
- Standard gas properties (ideal gas EoS, transport model) is used for LOX/GH2 diffusion flame[1]
- FPV（Flamelet Progress Variable）table is generated by ***FLGenerator*** (Prof. R. Kurose)

Progress Variable: $C \equiv Y_{H_2O}$
Table of species mass fraction: $Y_k = f(Z, C)$
Table of production rate of $C$ : $\dot{\omega}_C = f(Z, C)$




Counterflow diffusion flame[2]

Input:
- Temperatures (Fuel, Oxidizer)
- Mass flow rates (Fuel, Oxidizer)
- Pressure
- Reaction mechanism: UT-JAXA *[Shimizu et al., JPP, 2011]*

Output: FPV Table of $f(Z, C)$
- Table size: nZ=501, nC=41

[1] Mizobuchi et al., Trans. Japan Soc. Aero. Space Sci, (2013)
[2] Lacaze and Oefelein, Combustion and Flame, (2012)

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## Governing Equations

**Compressible NS +Scalars :**

- ・Implicit LES（no SGS model）
- ・Lewis number $Le = 1$ assumed

(Mass) $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

(Momentum) $$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + P \underline{\boldsymbol{\delta}} - \underline{\boldsymbol{\tau}}) = 0$$

(Energy) $$\frac{\partial \rho e_t}{\partial t} + \nabla \cdot [\rho e_t \boldsymbol{u} + (P \underline{\boldsymbol{\delta}} - \underline{\boldsymbol{\tau}}) \boldsymbol{u} + \boldsymbol{q}_e] = 0$$

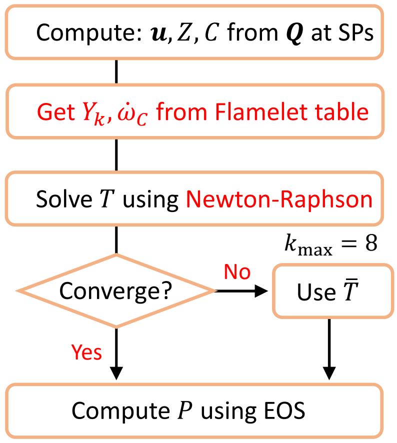
(Mixture fraction) $$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} Z - \rho D \nabla Z) = 0$$

(Progress variable) $$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} C - \rho D \nabla C) = \rho \dot{\omega}_C$$

Assuming $Le = 1$, heat flux becomes simple:

$$\boldsymbol{q}_e = -\lambda \nabla T - \rho \sum_{k=1}^{N} h_k D_k \nabla Y_k = -\frac{\lambda}{c_p} \nabla h$$

How to compute primitive variables




Converge? $Res_{Newton} \leq 1e-6$

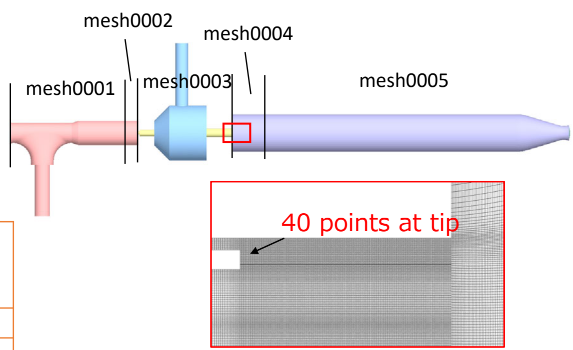


## Models and Schemes

| | |
|---|---|
| Governing eqs. | Compressible Navier-Stokes eqs. + Scalar Transport (Z, C) |
| SGS model | None（implicit LES） |
| Combustion | Flamelet progress variable (FPV) |
| Cp, EoS | NASA-7 Polynomial, SRK |
| Transport Coefficients | Chung's model + Chemkin hybrid |

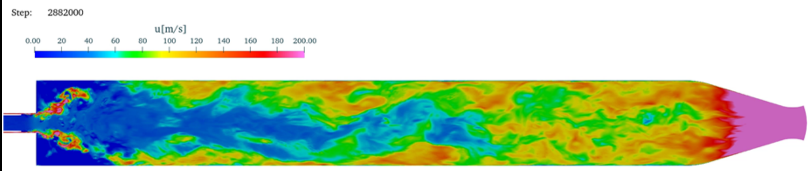
| | |
|---|---|
| Discretization | FR (conservative form), Gauss Points, gDG correction P1-P4 ($2^{nd}$-$5^{th}$ order) |
| Mesh | Hex (P1/P2 hybrid), Overset |
| Inviscid Flux | SHUS/SLAU |
| Viscous Flux | BR2 |
| Time Integration | 4-Stage TVD Runge-Kutta（$3^{rd}$-order） |
| Limiter | Positivity preserving limiter with entropy constraint |

Overset Grids of a Single-Element Combustor

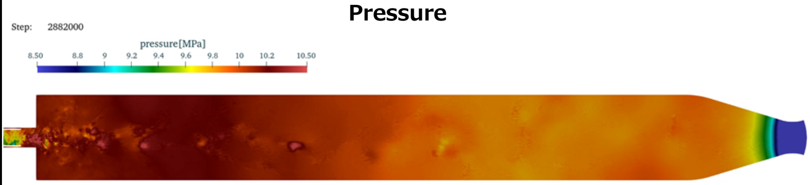


# LOX/GH2 Single Element Combustor

**Axial Velocity**

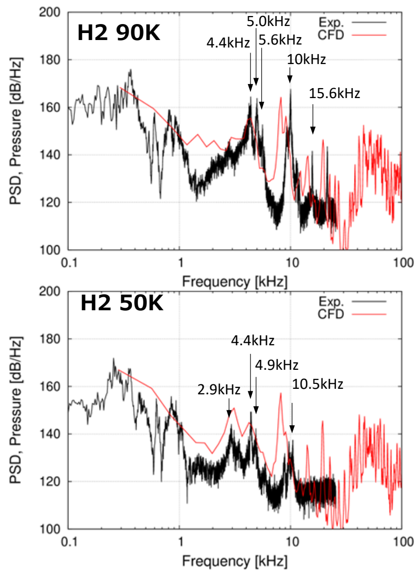



**Pressure**




**Cost: ~1 week/case with 500 A64fx CPUs (x48 cores)**

**PSD of LOX Injection Pressure**



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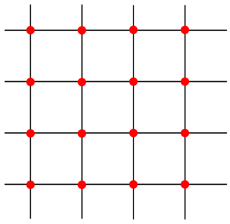
# Flux Reconstruction and Discontinuity

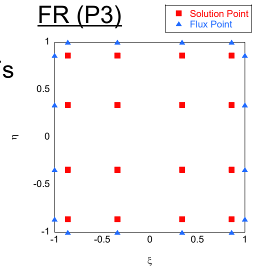
- “Solution points” (SPs, degrees of freedom) inside the computational cell

Finite Difference Method



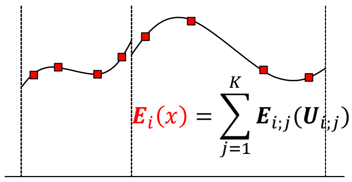
The same DoFs

FR (P3)

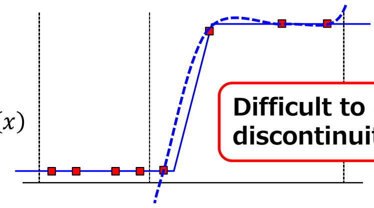



- It is desirable to capture discontinuities inside the cell.. but

Smooth solution




Discontinuous solution (shock, contact surface etc.)



**Difficult to approximate discontinuities by polynomials**

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# Localized Artificial Diffusivity (LAD)

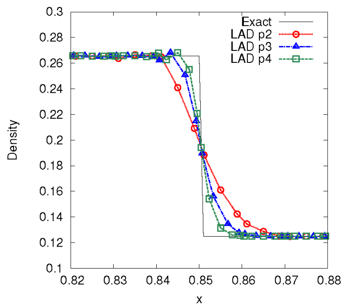
- Adding artificial dissipation specifically to shocks $\nabla \cdot \boldsymbol{u}$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot \left(\rho \boldsymbol{u}\boldsymbol{u} + p\underline{\boldsymbol{\delta}} - \beta_{\mathrm{art}}(\nabla \cdot \boldsymbol{u})\underline{\boldsymbol{\delta}}\right)$$

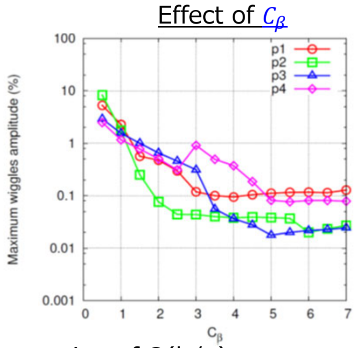
$$\beta_{\mathrm{art}} = C_\beta \rho \overline{\left|\frac{\partial^r(\nabla \cdot \boldsymbol{u})}{\partial x^r}\Delta x_p^{r+2}\right|}$$

Kawai & Lele, JCP 2008, 2010, Mani et.al., JCP 2009 Haga & Kawai, JCP 2019

Sod’s shock tube




Effect of $C_\beta$




✓ Sub-cell shock capturing of O(h/p)

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# Positivity-Preserving and Entropy Limiter

**Replacing the DoFs by blending:** Zhang & Shu, JCP 2010, Jiang & Hailiang, JCP 2018

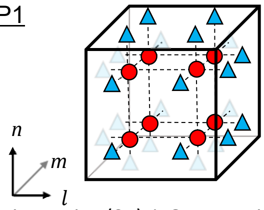
$$\hat{\mathbf{u}}_j(\boldsymbol{x}) = \theta \mathbf{u}_j(\boldsymbol{x}) + (1-\theta)\bar{\mathbf{u}}_j$$

HO polynomial    Cell-average

$$\theta = \min(1, \boldsymbol{\theta}^+, \boldsymbol{\theta}^-),$$

$$\boldsymbol{\theta}^+ = \frac{\mathcal{U}(\bar{\mathbf{u}}_j) - \mathcal{U}^{sup} - \varepsilon}{\mathcal{U}(\bar{\mathbf{u}}_j) - \mathcal{U}_j^{max} - \varepsilon}, \boldsymbol{\theta}^- = \frac{\mathcal{U}(\bar{\mathbf{u}}_j) - \mathcal{U}^{inf} + \varepsilon}{\mathcal{U}(\bar{\mathbf{u}}_j) - \mathcal{U}_j^{min} + \varepsilon}$$

FR P1




Solution point (SP)：Gauss point in cell
Flux point (FP): Gauss point on face

$\mathcal{U} = (\rho, P, \rho s)$, (Entropy definition by **Dzanic and Witherden, JCP, 2022**)
$\mathcal{U}^{sup}$, $\mathcal{U}^{inf}$ from the constraints $\{\rho > 0, P > 0, s \geq s_0\}$
$\mathcal{U}_j^{max}$, $\mathcal{U}_j^{min}$ at SPs and FPs in the cell
$\varepsilon = 1\mathrm{e}-8$ (to avoid zero division and limiting in uniform region)

- For combustion case, more strict constraints on density:

$$\rho^{sup} = (1 + c_{VB}) \max_{j\in\mathcal{A}}(\bar{\rho}_j),\ \rho^{inf} = (1 - c_{VB}) \min_{j\in\mathcal{A}}(\bar{\rho}_j),\ c_{VB}\sim 0.2$$

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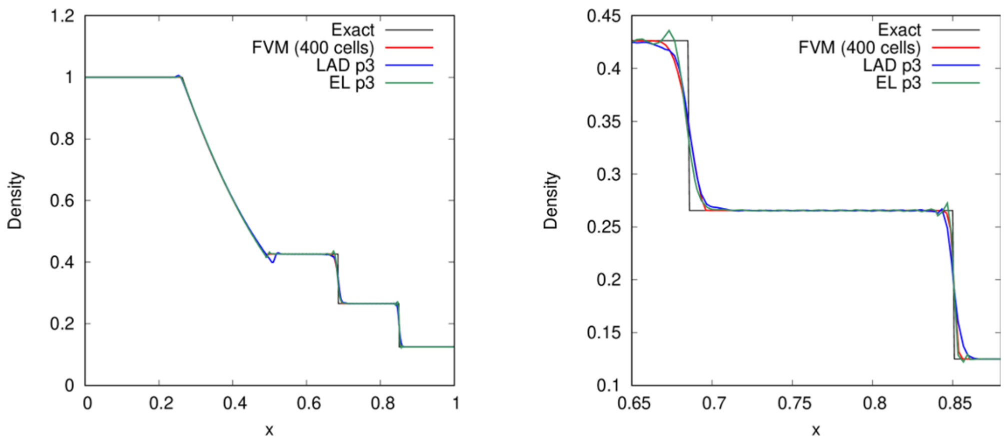
# 1D Shock Tube (Sod's Problem)

Initial condition:

$$\begin{cases} \rho_l = 1,\ u_l = 0,\ p_l = 1 & (x < 0.5) \\ \rho_r = 0.125,\ u_r = 0,\ p_r = 0.1 & (x \geq 0.5) \end{cases}$$

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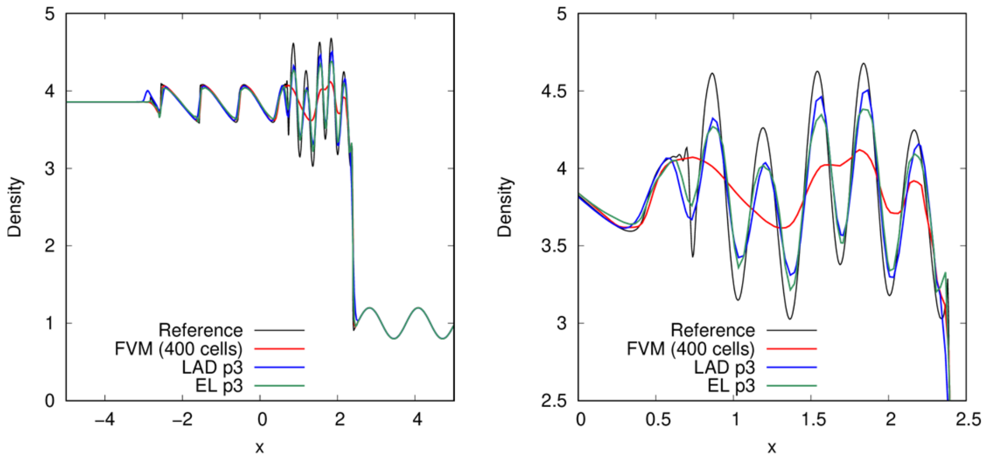
# Shu-Osher Problem

Initial condition:

$$\begin{cases} \rho_l = 3.857143,\ u_l = 2.629369,\ p_l = 10.333 \quad (x < -4) \\ \rho_r = 1 + 0.2\sin(5x),\ u_r = 0,\ p_r = 1\ (x \geq -4) \end{cases}$$

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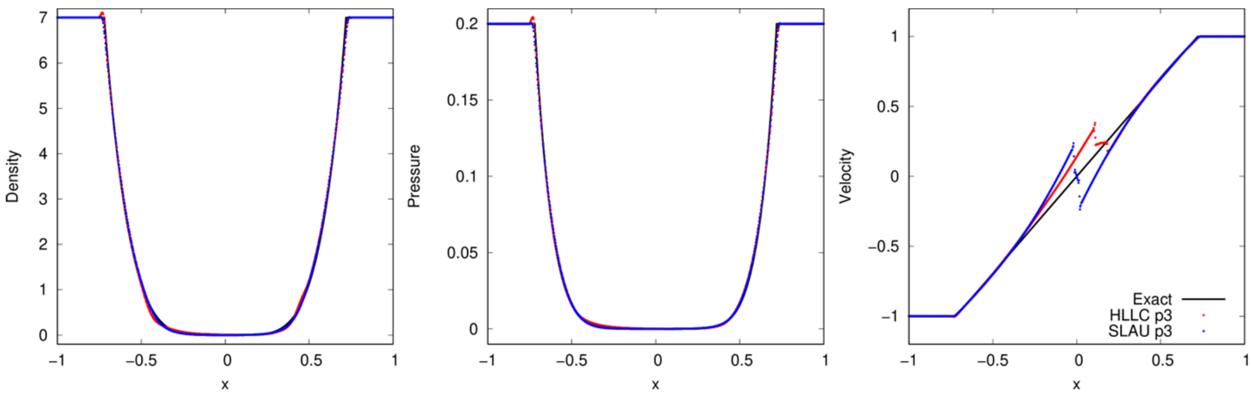
# 1D Double Rarefaction

Initial condition: Zhang & Shu, JCP 2010,

$$\begin{cases} \rho_l = 7,\ u_l = -1,\ p_l = 0.2 \quad (x < 0) \\ \rho_r = 7,\ u_r = 1,\ p_r = 0.2\ (x \geq 0) \end{cases}$$

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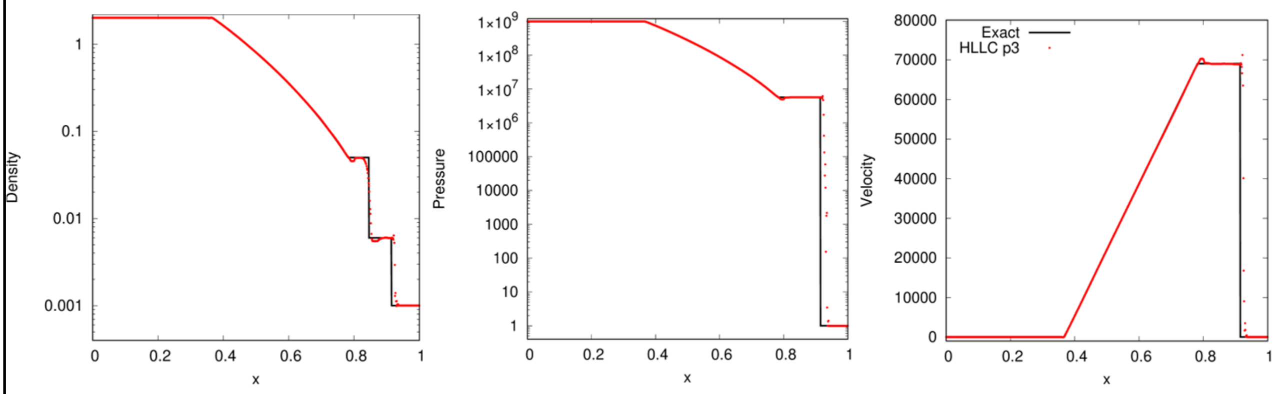
# 1D Leblanc Shock Tube Problem

Initial condition: Zhang & Shu, JCP 2010,

$$\begin{cases} \rho_l = 2,\ u_l = 0,\ p_l = 10^9 & (x < 0.5) \\ \rho_r = 0.001,\ u_r = 0,\ p_r = 1 & (x \geq 0.5) \end{cases}$$

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# Compressible Taylor-Green Vortex

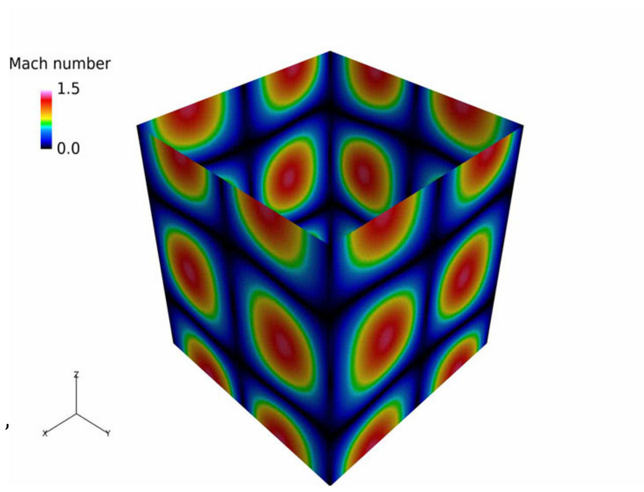
Lusher and Sandham, AIAA J. 2021

Mach Number $M_0 = 1.25$
Reynolds Number $\mathrm{Re} = 1{,}600$

Domain $(-\pi L \leq x, y, z \leq \pi L)$

Initial Condition:

$$u = V_0 \sin\left(\frac{x}{L}\right)\cos\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right),$$
$$v = -V_0 \cos\left(\frac{x}{L}\right)\sin\left(\frac{y}{L}\right)\cos\left(\frac{z}{L}\right),$$
$$w = 0,$$
$$p = p_0 + \frac{\rho_0 V_0^2}{16}\left(\cos\left(\frac{2x}{L}\right) + \cos\left(\frac{2y}{L}\right)\right)\left(\cos\left(\frac{2z}{L}\right) + 2\right),$$
$$\rho = \frac{p}{RT_0}.$$

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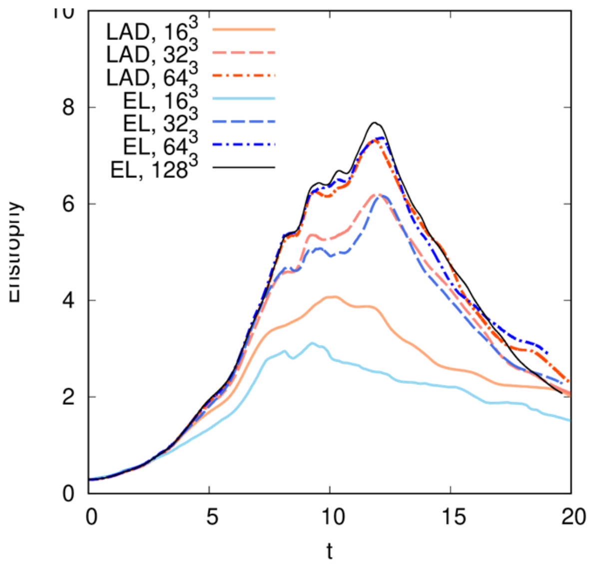
# Time History of Integrated Enstrophy

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# Comparison of LAD and Limiter

| Approaches | Robustness for extreme Riemann problems | Resolution for shock-vortex interaction | Time step size (explicit RK scheme) |
|---|---|---|---|
| **LAD** | △ (Small wiggles lead to negative rho or P) | ◎ | △ (Limited by large diffusivity ) |
| **PP+Entropy Limiter** **(**Dzanic and Witherden constraints**)** | ○ | ○ (Dissipative in a coarse mesh for TGV) | ○ (~10 times larger than LAD) |

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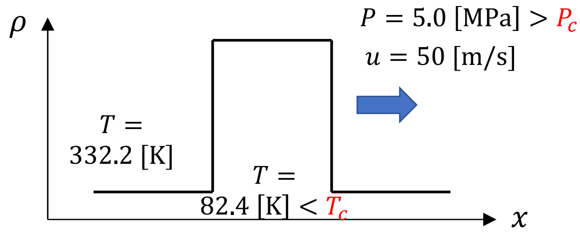
# Transcritical $N_2$ Blob (SRK EOS)




- 100 cells for $0 \leq x[\mathrm{m}] \leq 1$
- 1 cycle with periodic B.C.

| Approaches |
|---|
| **Flux-Reconstruction (FR) + Limiter** |
| **Flux-Reconstruction (FR) + Limiter (Constraints by Dzanic & Witherden 2022)** |

Critical Parameters

| Species | $T_c$ [K] | $P_c$ [MPa] | $\omega$ |
|---|---|---|---|
| $N_2$ | 126.2 | 3.40 | 0.0372 |

Constraints: $\{\rho > 0, P > 0, 0 \leq Y_k \leq 1, s \geq s_0\}$

Local minimum entropy: $s_0 = \min_{j \in \mathcal{A}}(s_j)$,
$\mathcal{A}$ is face-adjacent neighbors

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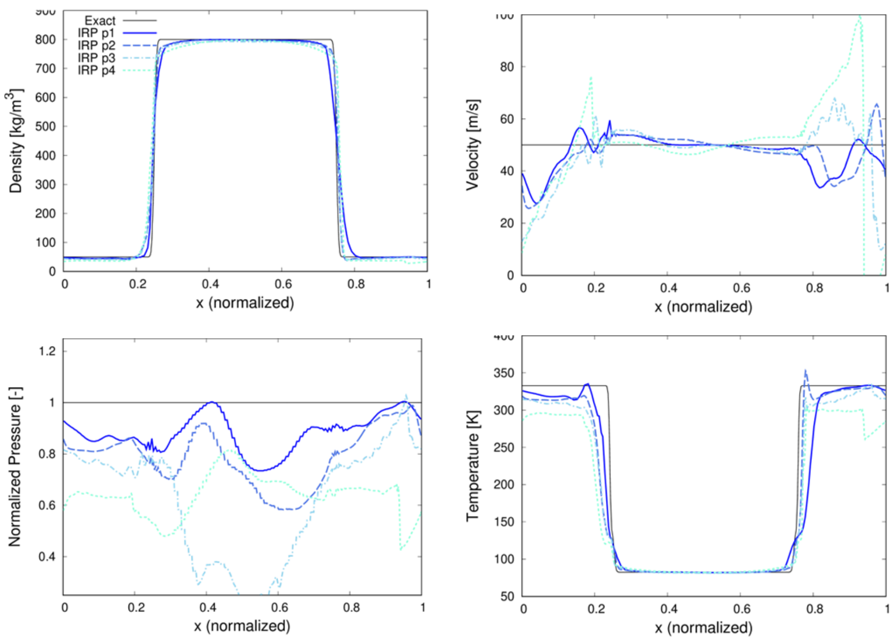
# PP+Entropy Limiter (Jiang and Hailiang 2018)

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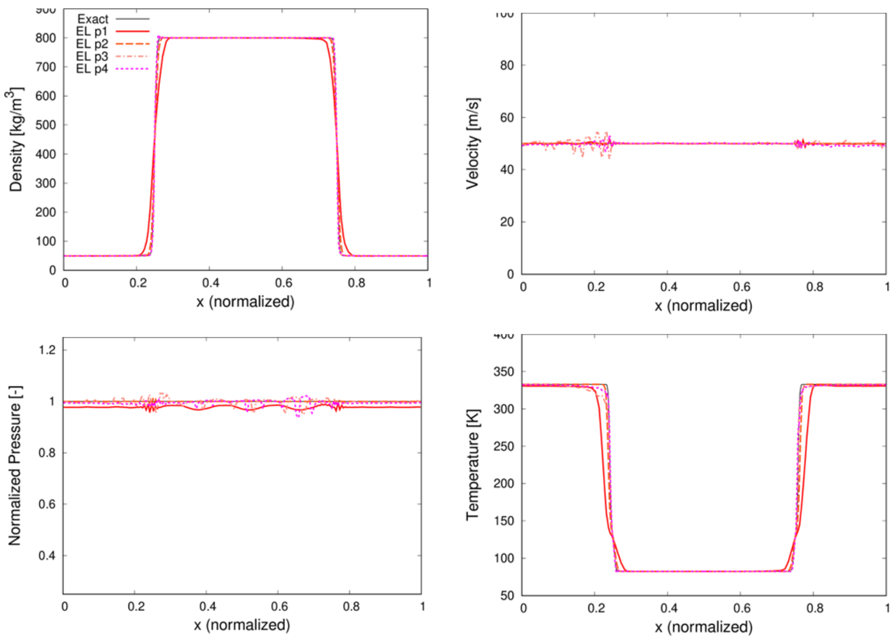
# PP+Entropy Limiter (Dzanic and Witherden 2022)

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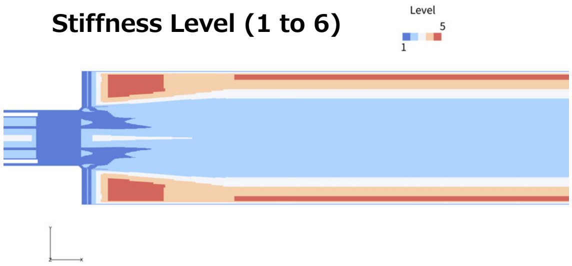
# Paired Explicit Runge-Kutta (P-ERK)

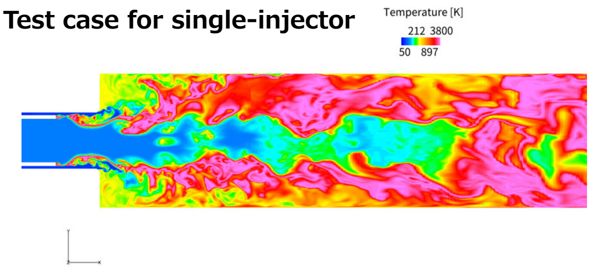
**Paired explicit Runge-Kutta (P-ERK)** (Vermeire, JCP 2019)

1. Increase RK-stages where the local stiffness is high (cell-size, acoustic speed, etc.)
2. Each grid cell is labeled (Level) depending on the local stiffness
3. Vermeire 2019 shows 4-5 times speed-up for turbulent airfoil flow comparing to 3-stage TVD RK

**Stiffness Level (1 to 6)**




**Test case for single-injector**




- It is recommended to divide the grid into 3 levels for every 2x cell size. Use 16, 8, and 3 stages. (Communication with B. Vermeire)
- P-ERK coefficients for P=1 to P=8 FR schemes are provided in text data (Vermeire 2019)

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# Paired Explicit Runge-Kutta (P-ERK)

**Butcher tableau :** P-ERK(10,6) (s: Stages, e: RHS evaluations)

Vermeire, JCP 2019

$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b} \end{array} =$

| $c$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{1}{18}$ | $\frac{1}{18}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{1}{9}$ | $\frac{1}{9}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{1}{6}$ | $\frac{1}{6}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{2}{9}$ | $\frac{2}{9}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{5}{18}$ | $\frac{5}{18}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $\frac{1}{3}$ | $\frac{1}{3} - a_{7,6}$ | 0 | 0 | 0 | 0 | $a_{7,6}$ | 0 | 0 | 0 | 0 |
| $\frac{7}{18}$ | $\frac{7}{18} - a_{8,7}$ | 0 | 0 | 0 | 0 | 0 | $a_{8,7}$ | 0 | 0 | 0 |
| $\frac{4}{9}$ | $\frac{4}{9} - a_{9,8}$ | 0 | 0 | 0 | 0 | 0 | 0 | $a_{9,8}$ | 0 | 0 |
| $\frac{1}{2}$ | $\frac{1}{2} - a_{10,9}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $a_{10,9}$ | 0 |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

In these stage $(i = 3,4,5,6)$, $a_{i,i-1} = 0$, thus RHS evaluation can be skipped

Since $a_{i,1} \neq 0$, $\boldsymbol{k}_1$ is used for every stages to update solution

**Update of solution vector :**

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \Delta t \sum_{i=1}^{s} b_i \boldsymbol{k}_i = \boldsymbol{u}_n + \Delta t \boldsymbol{k}_s$$

$$\boldsymbol{k}_1 = RHS(t_n, \boldsymbol{u}_n)$$

$$\boldsymbol{k}_i = RHS\left(t_n + c_i \Delta t, \boldsymbol{u}_n + \Delta t \sum_{j=1}^{i-1} a_{i,j} \boldsymbol{k}_j\right), i = 2, \ldots, s.$$

This study uses 3 levels:
P-ERK(16,16) , P-ERK(16,8) , P-ERK(16,3)

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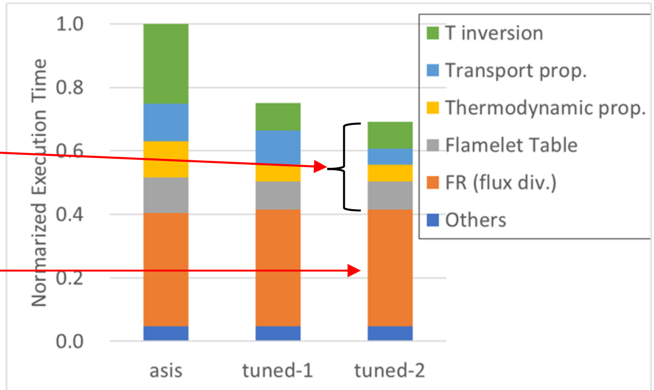
## RK Stepper Algorithm

```
Set_Initial_Condition()

Do n=1,n_final_step
    Compute_Primitive()
    Compute_Thermo()
    Compute_Transprop()
    Do k=1, k_max_stage
        Compute_FR_RHS()
        Update_Solution()
    EndDo
EndDo
```

**Computation Cost (P1-scheme)**




Note: In this study, P-ERK is applied to `Compute_FR_RHS()` only

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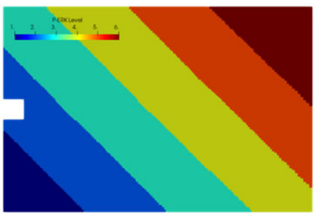
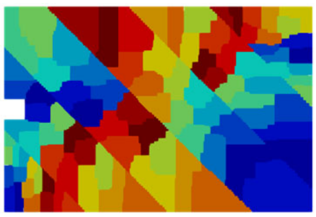
## Domain Decomposition for P-ERK

- Modified domain decomposition for P-ERK
  - 2D mesh
  - P-ERK level distribution is assumed for test

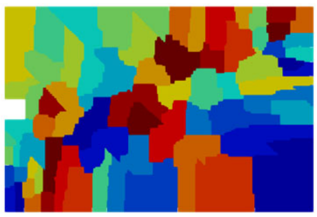


Assumed P-ERK Level

Original decomposition by METIS



METIS is applied to each P-ERK level



Detached land is reduced by reordering sub-domain ID

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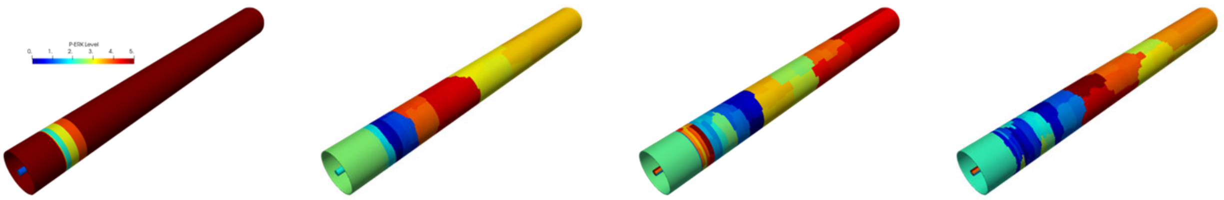
# Domain Decomposition for P-ERK

- Modified domain decomposition for P-ERK
  - 3D single-injector mesh




6 P-ERK Levels is used

Original decomposition by METIS

METIS is applied to each P-ERK level

Detached land is reduced by reordering sub-domain ID

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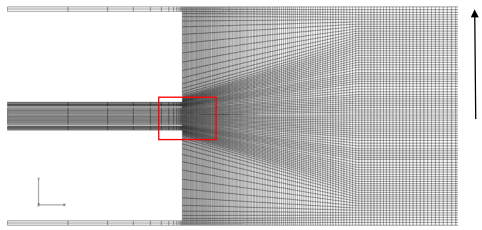
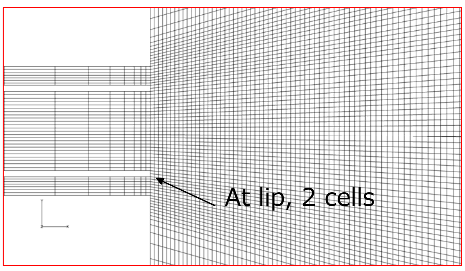
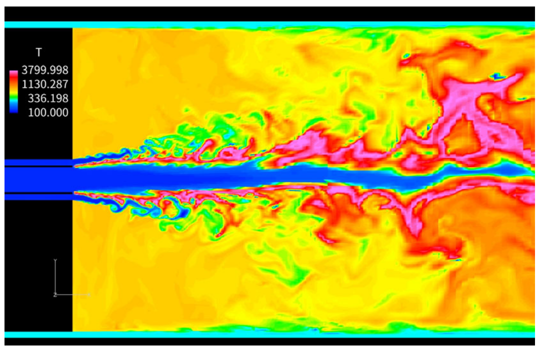
# LOX/H2 Combustor: DLR P8 @6MPa




| Mesh | Cells | FR | SPs |
|---|---|---|---|
| Coarse | 989,440 | P1 | 7,915,520 |

| Case | P | cfactor | Lv1 16-stg | Lv2 8-stg | Lv3 3-stg | Cost-ratio to 4-ERK | CFL 4-ERK | CFL PERK | CFL ratio | Speed-up (ideal) | Speed-up (actual) | Speed-up (Res) | Speed-up (Primitive_etc) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Injector | 1 | 1.2 | 0.035 | 0.104 | 0.861 | 0.99 | 1.5 | 4.5 | 3 | 3.02 | 1.13 | 2.46 | 0.75 |

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## Summary

- High-order FR method was successfully applied to sub-scale LRE combustor under realistic operating conditions (P>10MPa, T<100K)
- Entropy (considering time evolution) based limiter is robust for supercritical LOX/GH2 diffusion flames.
  - ➢ sub-cell resolution is retained for p>2 in transcritical N2 advection.
- P-ERK scheme can accelerate a single-element LRE simulation
  - ➢ 2-3x larger CFL can be taken (vs 4-stage ERK)
  - ➢ Efficiency depends on ratio of the P-ERK levels (mesh dependent)

Ongoing Works:

- ➢ Wall-model for iso-thermal walls (equilibrium/frozen composition)
- ➢ Step up to DLR-BKD combustor (42 Injectors), full-scale LE-X combustor (>500 Injectors)

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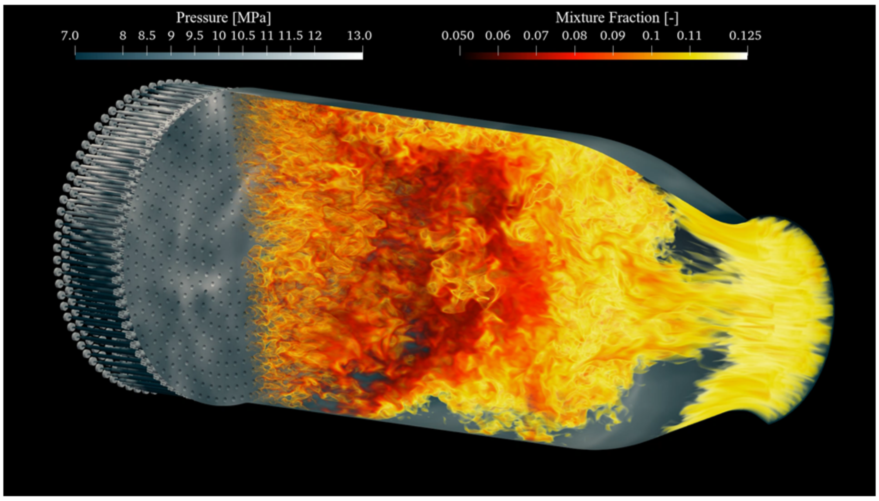
## Toward Full-Scale Engine Simulation




- Preliminary Coarse Grid LES (as of 2021):
  - ➢ 2.6 billions SPs (P1) → 2 weeks to analyze 4 msec using 960 CPUs (FX-1000)
- Estimation of a high-resolution Grid LES with improved schemes:
  - ➢ 10 billions SPs (P1) → ~2 weeks to analyze 20 msec using 10,000 CPUs (@Fugaku)

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