Application of Grid Convergence Index Estimation for Uncertainty Quantification in V&V of Multidimensional Thermal-Hydraulic Simulation

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High Cycle Thermal Fatigue around CIP at Bottom of UIS in JSFR

Thermal fatigue caused by thermal mixing (thermal striping) between
- Hot sodium from fuel subassemblies and
- Cold sodium from control rod channels and blanket fuel subassemblies

Target areas related to thermal fatigue

Primary Control Rod (PCR) Channel

Backup Control Rod (BCR) Channel
In extrapolated estimation of high cycle thermal fatigue in JSFR,
- Confirmation of consistency of two methods to ensure the credibility.

(1) Analytical estimation method based on the experimental data
- Suitable for the design work and it is easy to handle
- Difficulties to integrate and generalize experimental data
  by sub-scale experiments in view point of scaling effect

(2) Direct estimation method using numerical simulations
- Direct estimation from thermal-hydraulics to structural response
- Requirement of comprehensive procedure for V&V and prediction
  ▽ Implementation of V&V (establishment of practical procedure)
  ▽ Appropriate arrangement of experiments for V&V
  ▽ Uncertainty quantification for each examination in V&V
  and integration of uncertainties for prediction
  ▽ Prediction (extrapolation) for the JSFR
V2UP (Verification and Validation plus Uncertainty quantification and Prediction)

1-1) Implementation of PIRT analysis
1-2) Establishment of assessment matrix and conceptual model

2-1) Plan of code development or code selection (in-house/CFD)
2-2) Mathematical model
2-3) Code (model) development and numerical scheme detection
2-4) Verification and uncertainty quantification

2-5) Validation and uncertainty quantification
   a) Fundamental validation (FP & SET)
   b) Validation (CET & IET)

3-1) Physical modeling
3-2) Scale analysis
3-3) Exploratory experiments (if necessary)
3-4) Review of existing database applicable to validation
3-5) Arrangement and implementation of experiments for validation, and uncertainty quantification
   a) Fundamental problems (FP)
   b) Separate effects tests (SET)
   c) Component effects tests (CET)
   d) Integrated effects tests (IET)

4-1) Quantitative comparison of results and adequacy decision for each problem
4-2) Total uncertainty and adequacy decision for prediction

5) Prediction of a specific problem and estimate uncertainty
**Conceptual Model for Numerical Estimation of High Cycle Thermal Fatigue around CIP**

1. **Thermal-hydraulics in upper plenum**
   - by RANS method (AQUA / CFD)
   - External flow for blanket fuels
   - Internal flow for control rods

   **Boundary conditions for local analysis**

2. **Unsteady thermal-hydraulics and heat conduction in structure in local areas around**
   - Control rod (CR) channels
   - Blanket fuel (BF) subassemblies

   **by fluid-structure thermal interaction simulation code (MUGTHES)**

   **Temperature information in structure**

3. **Estimation of structural integrity**
   - by thermal stress analysis (FINAS)**

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**Whole upper plenum analysis**

**External flow**

UIS

**Internal flow**

(for CRs)

(for BFs)

**Local analysis**

**Thermal stress analysis**
(Code) Verification: **Uncertainty quantification (UQ) by GCI estimation**
Comparing with the theoretical results of governing equations

2-step Validation:
Step-1) Fundamental Validation (functions of the solution verification and a part of validation processes): **UQ by GCI estimation**
(a) **Fundamental problems (FPs)**: including fundamental phenomena
(b) **Separated effect tests (SETs)**: including elemental phenomena related to the target issue

Step-2) Validation: Application of AVM (MAVM) method
(c) **Component effect tests (CETs)**: simulating subcomponent system including significant phenomena in the target issue
(d) **Integrated effect tests (IETs)**: simulating component system or subsystem of the target plant
<Integrated program for GCI estimation>

**INPUT:** Data-sets along the traverse line of the reference results and more than 3 numerical results at different mesh arrangement.

(1) Pretreatment: Setting up the numerical results for the estimation, Ref.) using spline interpolation of the numerical results to set at the position of the reference result, or Opt.) choosing the numerical result at the closest position to the reference result.

(2) GCI estimation:
- ASME V&V 20 method (Roache’s method)
- Modified ASME V&V 20 method (based on the Roache’s method)
- Global average method
- Roy’s modification method
- Eca’s least square version GCI
- **SLS-GCI (Simplified Least Square version GCI)**

OUTPUT: Uncertainty in the domain and detailed information at each position

Uncertainty Quantification (GCI estimation) ~ Modified ASME V&V 20 method ~

1. (More than) three calculations with different mesh number ($N_k : N_1 > N_2 > N_3$)
   (Better to keep a constant mesh increasing rate)
   
   \[ r_{21} = \frac{N_1}{N_2}, \quad r_{32} = \frac{N_2}{N_3} \]

2. Prediction of convergence rate $p_j$.
   
   \[
   \tilde{p}_j = \ln \left[ \frac{(\varepsilon_{32})_j}{(\varepsilon_{21})_j} + q(\tilde{p}_j) \right] / \ln (r_{21}), \quad (\varepsilon_{32})_j = (f_3)_j - (f_2)_j, \quad (\varepsilon_{21})_j = (f_2)_j - (f_1)_j
   \]
   \[
   q(\tilde{p}_j) = \ln \left[ \frac{(r_{21}\tilde{p}_j - s_j)}{(r_{32}\tilde{p}_j - s_j)} \right], \quad s_j = 1 \times \text{sign} \left[ \frac{(\varepsilon_{32})_j}{(\varepsilon_{21})_j} \right]
   \]

   - Modification: $p_j = \max(p_l, \tilde{p}_j)$  ($p_l=1.0$)

3. Prediction of extrapolation solution $(f_c)_j$
   
   \[
   (f_c)_j = \frac{r_{21}^p (f_1)_j - (f_2)_j}{(r_{21})^p - 1}
   \]

4. GCI estimation (safety coefficient: $F_S$)
   
   \[
   (u_G)_j = F_S \times \left| \frac{(\varepsilon_{21})_j}{(r_{21})^p - 1} \right|
   \]
   \[
   = F_S \times |f_c - f_1|
   \]

   \[
   f_c - f_1 = \frac{f_1 - f_2}{r_{21}^p - 1}
   \]

   (ASME: $F_S=1.25$)

   Fs=1.25 in $p_l < p_j \leq p_f$  ($p_f=2.0$)
   Fs=3.0 in $p_j \leq p_l$ or $p_f < p_j$
Proposal of Least Square (LS) method modified from Eca’s LS method

- Without judgment of convergence condition
  (as the first step of Eca’s method)
  - Dispersed results around the theoretical curve
  - Limited data to judge the convergence condition

- Solve equation on $(\alpha, p, f_c)$ by the LS method
  \[ \tilde{f}_k = f_c + \alpha (h_k)^p \]

- Estimations of the GCI using estimation values $\tilde{f}$
  and the error in the curve

1) $p_1 (=1) < p$
\[ u_{GCI} = \frac{F_s |\tilde{f}_2 - \tilde{f}_1|}{(h_2/h_1)^p - 1}, \quad u_s = \sqrt{\frac{1}{n} \sum_{k=1}^{n} [f_k - \{f_c + \alpha (h_k)^p\}]^2} \]
\[ \begin{cases} F_s=1.25 & p_1 (=1) < p \leq p_f (=2) \\ F_s=3.0 & p > p_f (=2) \end{cases} \]

2) $0 < p \leq p_1 (=1), \quad p = p_t = 1$
\[ u_{GCI} = \frac{3.0 |\tilde{f}_2 - \tilde{f}_1|}{(h_2/h_1) - 1}, \quad u_s = \sqrt{\frac{1}{n} \sum_{k=1}^{n} [f_k - \{f_c + \alpha h_k\}]^2} \]

3) $p \leq 0$ or $p$ is not converged.
\[ u_{GCI} = 0, \quad u_s = \sqrt{\frac{1}{n} \sum_{k=1}^{n} (f_k - f_c)^2}, \quad f_c = \frac{1}{n} \sum_{k=1}^{n} f_k \]

(GCI can not be defined)
Estimation of Combined Standard Uncertainty in Domain

Combined standard uncertainty \( (C_e = 1) \) in the domain by root sum square (RSS) method.

\[
U_S = C_e \times \sqrt{\left( \frac{U_G}{1.15} \right)^2 + \varepsilon_c^2 + U_e^2}
\]

- Mean GCI \( (U_G) \) by root mean square (RMS)

\[
U_G = \sqrt{\frac{1}{m} \sum_{j=1}^{m} (u_G)_j^2} \quad (m : \text{Number of reference positions})
\]

- Mean difference \( (\varepsilon_c) \) between the reference \( (f_0) \) and the extrapolation \( (f_c) \) values

\[
\varepsilon_c = \sqrt{\frac{1}{m} \sum_{j=1}^{m} [(f_c)_j - (f_0)_j]^2}
\]

- Mean error \( (U_S) \) in the LS

\[
U_e = \sqrt{\frac{1}{m} \sum_{j=1}^{m} (u_e)_j^2} \quad u_e = \sqrt{\frac{1}{n} \sum_{k=1}^{n} \left[ f_k - \left( f_c + \alpha (h_k)^p \right) \right]^2}
\]

- The maximum difference \( (\delta_{\text{max}}) \) between the reference \( (f_0) \) and the result of \( f_1 \)

\[
\delta_{\text{max}} = \left| (f_0)_j - (f_1)_j \right|_{\text{max}}
\]

\( U_{GCI} \) as 95\% uncertainty \( (2\sigma) \) is modified to 1\% value with expansion factor of 1.15
Uncertainty quantification by GCI method is performed in verification and fundamental validation processes.

For Verification
- **Couette-Poiseuille Flow:**
  - Theoretical results of N-S equation without uncertainty
  - Verification of coupling functions of velocity and pressure fields at adverse/even/positive pressure gradient condition

For Fundamental validation with Fundamental Problem and SET
- **Back-Facing Step Flow as a Fundamental Problem:**
  - Denman’s Experimental result at Re=229
  - Influence of set of mesh density conditions on the uncertainty
- **WATLON experiment as a SET:**
  - Water experiment in T-junction piping system
  - Typical problem for thermal mixing in turbulence conditions
Uncertainty Quantification in Verification
~ Couette-poiseuille Flow Problem ~

<Couette-Poiseuille Flow in Parallel Cannel at Re=10>
\(U_0=0.001 \text{ m/s, } H=0.01 \text{ m, Water at 20 °C}\)

\[
u(y) = U_0 \left(\frac{y}{H}\right) + \frac{H^2}{2\mu} \left[-\frac{dP}{dx}\right] \left[\frac{y}{H} \left(1 - \frac{y}{H}\right)\right]
\]

<Mesh arrangements>
- **Ny (Vertical direction)** for \(H\): 10, 20, 40 (Ref.), 80
- **Nx (Depth direction)** for \(2H\): 49 (Periodic condition)
- **Nz (Axial direction)** for \(5H\): 101 (Periodic condition)

Case1: \(U_m=0\) \((-dP/dx)<0\)
Case2: \(U_m=0.5U_0\) \((-dP/dx)=0\)
Case3: \(U_m=U_0\) \((-dP/dx)>0\)
## Uncertainty Quantification in Verification

~ Couette-poiseuille Flow Problem ~

<table>
<thead>
<tr>
<th>Case-1 ((U_m=0, (-dP/dx)&lt;0))</th>
<th>Data</th>
<th>(U_G)</th>
<th>(\varepsilon_p)</th>
<th>(U_e)</th>
<th>(U_S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASME</td>
<td>30</td>
<td>0.004</td>
<td>0.003</td>
<td>-</td>
<td>0.005</td>
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<tr>
<td>Modified ASME</td>
<td>40</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
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<tr>
<td>GA</td>
<td>31</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>Roy’s GCI</td>
<td>40</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>SLS-GCI</td>
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<td>0.000</td>
<td>0.001</td>
<td>0.001</td>
<td>0.002</td>
</tr>
<tr>
<td>Eca’s LS GCI</td>
<td>24</td>
<td>0.012</td>
<td>0.001</td>
<td>-</td>
<td>0.011</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Case-2 ((U_m=0.5U_0, (-dP/dx)=0))</th>
<th>Data</th>
<th>(U_G)</th>
<th>(\varepsilon_p)</th>
<th>(U_e)</th>
<th>(U_S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASME</td>
<td>0</td>
<td>N/A</td>
<td>N/A</td>
<td>-</td>
<td>N/A</td>
</tr>
<tr>
<td>Modified ASME</td>
<td>40</td>
<td>0.000</td>
<td>0.000</td>
<td>-</td>
<td>0.000</td>
</tr>
<tr>
<td>GA</td>
<td>20</td>
<td>0.002</td>
<td>0.002</td>
<td>-</td>
<td>0.003</td>
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<tr>
<td>Roy’s GCI</td>
<td>40</td>
<td>0.000</td>
<td>0.000</td>
<td>-</td>
<td>0.000</td>
</tr>
<tr>
<td>SLS-GCI</td>
<td>40</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Eca’s LS GCI</td>
<td>0</td>
<td>N/A</td>
<td>N/A</td>
<td>-</td>
<td>N/A</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case-3 ((U_m=U_0, (-dP/dx)&gt;0))</th>
<th>Data</th>
<th>(U_G)</th>
<th>(\varepsilon_p)</th>
<th>(U_e)</th>
<th>(U_S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASME</td>
<td>30</td>
<td>0.002</td>
<td>0.002</td>
<td>-</td>
<td>0.002</td>
</tr>
<tr>
<td>Modified ASME</td>
<td>40</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>GA</td>
<td>31</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>Roy’s GCI</td>
<td>40</td>
<td>0.001</td>
<td>0.000</td>
<td>-</td>
<td>0.001</td>
</tr>
<tr>
<td>SLS-GCI</td>
<td>40</td>
<td>0.000</td>
<td>0.001</td>
<td>0.001</td>
<td>0.002</td>
</tr>
<tr>
<td>Eca’s LS GCI</td>
<td>24</td>
<td>0.013</td>
<td>0.001</td>
<td>-</td>
<td>0.011</td>
</tr>
</tbody>
</table>
- Denham’s Experimental result at $Re=229$
- Height of downstream duct: $3H$ ($H$: Step height)
- Uncertainty of inlet boundary condition potentially exists in the simulation.

Axial velocity profile measured at $(3/4)H$ upstream from the step edge was set at $4H$ upstream in the simulation.

<Mesh arrangements>
- **Vertical direction**: (parameter for GCI)
  
  \[ Ny \text{ (for } H) = 27, 36, 48 \text{ (} r=4/3 \text{)} \]

- **Depth direction**: (Periodic condition)
  
  \[ Nx \text{ (for } 4H) = 31 \]

- **Axial direction**:
  
  \[ Nz \text{ (for } 26H \text{ (} 4H \text{ for upstream})) = 135 \]
Uncertainty Quantification n Fundamenal Validatin
~ Back-Facing Step Flow Problems ~

0H (Step edge)

2H

4H

8H

\[ U_G, \varepsilon_c, U_S \]
Wall jet case

Main pipe Branch pipe

Inner Diameter: 0.15 m (=D_m) 0.05 m (=D_b)
Inlet Temperature: 48°C (=T_m) 33°C (=T_b)
Mean Velocity: 1.46 m/s (=W_m) 1.0 m/s (=V_b)
Reynolds number: 3.8x10^5 6.6x10^4

Measured data:
- Velocity components by PIV
- Fluid temperature by T/Cs

Flow-pattern map

Mr = M_m/M_b

0.35 < Mr < 1.35 ( ◆ ◆ ◆ : Deflecting jet)

Mr > 1.35 ( ■ ■ ■ : Wall jet)

Mr < 0.35 ( ◆ : Impinging jet)

M_m = \rho_m (D_m \cdot D_b) W_m^2

M_b = \rho_b (\pi D_b^2 / 4) V_b^2

Flow-pattern map

(Main pipe flow)

(Movable thermo-couples (T/Cs) tree)
Case-C: Coarse mesh
For GCI estimation

Case-M: Reference mesh

Case-F: Fine mesh

※Radial length of boundary cell on the wall: 0.5mm

<table>
<thead>
<tr>
<th>Case</th>
<th>$N_{\text{total}}$</th>
<th>$\delta_{z1}$ ((z&lt;+1.5D_m))</th>
<th>$\delta_c = \frac{D_m}{N_x}$</th>
<th>$\frac{D_m}{N_y}$</th>
<th>$h_k$ for GCI</th>
<th>($\delta_{z1} \times (\delta_c)^2)^{1/3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>602,000</td>
<td>2.5 mm</td>
<td>2.5 mm</td>
<td></td>
<td>$h_1 = 2.5$ mm</td>
<td>$\sqrt[3]{r_{21}} = 1.43$</td>
</tr>
<tr>
<td>M</td>
<td>262,480</td>
<td>3.2 mm</td>
<td>3.75 mm</td>
<td></td>
<td>$h_2 = 3.57$ mm</td>
<td>$\sqrt[3]{r_{32}} = 1.45$</td>
</tr>
<tr>
<td>C</td>
<td>91,800</td>
<td>4.2 mm</td>
<td>5.77 mm</td>
<td></td>
<td>$h_3 = 5.18$ mm</td>
<td></td>
</tr>
</tbody>
</table>

* 10 seconds transient calculation (10,000 data) for estimation
Magnitude of error bar equals to that of uncertainty of $U_s$ in the next slide.

(1) Time average

(on the symmetric cross section)

Fluctuation intensity

(near main pipe surface (1mm inside))

Axial velocity

Fluid temperature
- “Mod. ASME V&V 20” still over-estimates the uncertainty.
- “SLS-GCI” can stably use for the uncertainty quantification.

<table>
<thead>
<tr>
<th>Data (0.5D&lt;sub&gt;m&lt;/sub&gt;)</th>
<th>ε&lt;sub&gt;max&lt;/sub&gt;</th>
<th>Mod.-ASME</th>
<th>SLS-GCI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>U&lt;sub&gt;G&lt;/sub&gt;</td>
<td>U&lt;sub&gt;c&lt;/sub&gt;</td>
</tr>
<tr>
<td>T</td>
<td>0.119</td>
<td>0.200</td>
<td>0.068</td>
</tr>
<tr>
<td>T'</td>
<td>0.101</td>
<td>0.138</td>
<td>0.042</td>
</tr>
<tr>
<td>W</td>
<td>0.171</td>
<td>0.385</td>
<td>0.173</td>
</tr>
<tr>
<td>W'</td>
<td>0.126</td>
<td>0.153</td>
<td>0.078</td>
</tr>
<tr>
<td>T (1 mm)</td>
<td>0.181</td>
<td>1.069</td>
<td>0.366</td>
</tr>
<tr>
<td>T (3 mm)</td>
<td>0.274</td>
<td>0.761</td>
<td>0.303</td>
</tr>
<tr>
<td>T' (1 mm)</td>
<td>0.119</td>
<td>0.375</td>
<td>0.144</td>
</tr>
<tr>
<td>T' (3 mm)</td>
<td>0.146</td>
<td>0.375</td>
<td>0.132</td>
</tr>
</tbody>
</table>

(Uncertainty quantification using the results applying the spline interpolation)
○ Introduction of a procedure called V2UP (V&V plus Uncertainty quantification and Prediction) for a numerical estimation method for thermal mixing phenomena in a sodium-cooled fast reactors.

○ Specification of the reference GCI estimation method in the V2UP that is used in the verification and the fundamental validation processes.

○ Proposal of two modified methods,
  - Modified method from Roache’s GCI based on the ASME V&V-20 guideline
  - SLS-GCI (Simplified Least Square version GCI estimation method)

○ Examinations of the GCI estimation methods through the numerical simulations:
  - in Verification; Theoretical results of Navier-Stokes equation of Couette-Poiseuille Flows as a common benchmark problem
  - in Fundamental Validation (Fundamental Problem and Separated Effect Test): FP: Laminar flow problem over a backward-facing step
    SET: Water experiment of a T-pipe in JAEA called WATLON

○ Through the examinations, the SLS-GCI is defined as a reference method for GCI estimation method in V2UP