Development and Application of BPG in the EU-Project ECORA for the Evaluation of CFD-Simulations in NRS

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Contents

• CFD Quality
• Overview of Best Practice Guidelines (BPG)
• Error estimation techniques
• Practicality considerations
• Review & recommendations
• Summary
Use of CFD results for safety-critical analyses

Requirements:
- Reliability
- Quality

Definition of ‘CFD Quality’:
- Quantification of numerical errors
- Minimization of numerical errors
- Quantification of model errors
- Quantification of application uncertainties
- Application and collection of ‘Best Practices’
- Continuous improvement → Kaizen
Best Practice Guidelines

- Techniques for quality assurances in CFD
- Importance for validation
- Hierarchies
  - Error hierarchy
  - ’Exact‘ methods → ’empirical‘ methods
- Practicality ↔ progress in computer hardware & algorithms
- Awareness
- No checks → no errors?
Best Practice Guidelines

• Knowledge management
  – Document
  – Foster use of good practices
  – Build expertise
BPG: Main Topics

- Understand application
- Document and defend assumptions:
  - Geometry
  - Boundary conditions
  - Flow regime
  - Sources of systematic error
  - Approximations
  - Data
- Accuracy expectations vs. assumptions?
Structure of ECORA BPG’s

Definition of errors in CFD simulations:

1. **Numerical errors**
   - Solution error
   - Spatial discretisation error
   - Time discretisation error
   - Iteration error
   - Round off error
   - Solution error estimation

2. **Modelling errors**
3. **User errors**
4. **Application uncertainties**
5. **Software errors**
Structure of ECORA BPG’s

General Best Practice Guidelines:

1. Avoiding user errors
2. Geometry generation
3. Grid generation
4. Model selection and Application
   • Turbulence models
   • Heat transfer models
   • Multi-phase models
5. Reduction of application uncertainties
6. CFD simulation
   • Target variables
   • Minimising iteration errors
   • Minimising spatial discretisation errors
   • Minimising time discretisation errors
   • Avoiding round-off errors
7. Handling software errors
Further Topics of ECORA BPG’s

• Guidelines for evaluation of existing CFD simulations

• Selection and evaluation of experimental data
  – Verification experiments
  – Validation experiments
  – Demonstration experiments

• Specific consideration for ECORA

• Structure of Evaluation and Validation Reports
Investigated ECORA testcases

- **Verification tests**
  - Oscillating manometer (PSI, CEA)
  - Centralized sloshing (CFX, CEA)

- **Validation tests**
  - Impinging air jet with heat transfer (CFX)
  - Impinging water jet in air (GRS)
  - Impinging water jet on free surface (CEA, NRG)
  - Contact condensation in stratified flow (EDF, CFX)

- **Demonstration tests**
  - UPTF Test 1 (single-phase mixing) (NRG, EDF)
  - UPTF Test 8 (GRS)
  - UPTF TRAM C1 (GRS, EDF)
BPG: Recommendations

• Grid generation:
  – Scalable grids
  – Grid angles $> 20^\circ$ and $< 160^\circ$ (accuracy, convergence)
  – Aspect ratios $< 1,000$ on 32-bit computers
  – Expansion ratios $< 1.5 \ldots 2$
  – Capture physics

• Grid refinement:
  – Manual, based on error estimate
  – Automatic adaptive based on ‘error sensor’
Scalable Grids
BPG: Recommendations

- **Iteration error:**
  - Apply procedure in BPG to define convergence criterion
  - Monitor residual norms
  - Monitor global balances
  - Check on monotonic convergence
Iteration Error Control
BPG: Recommendations

- **Discretisation error:**
  - 1\textsuperscript{st} order schemes require *very, very fine grids* for most 3-D applications
  - Start with 1\textsuperscript{st} order scheme
  - Switch to 2\textsuperscript{nd} order scheme
  - Compare target variables for both schemes
  - **Error estimation at little extra cost**
Richardson Extrapolation

- Impinging jet flow with heat transfer
- 2-D, axisymmetric
- Grids:
  - $50 \times 50 \rightarrow 800 \times 800$
- Practical in 2-D
<table>
<thead>
<tr>
<th>Grid</th>
<th>Nu Scheme 1</th>
<th>Nu Scheme 2</th>
<th>Error Scheme 1</th>
<th>Error Scheme 2</th>
<th>R.E.</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 × 50</td>
<td>190.175</td>
<td>176.981</td>
<td>22.1 %</td>
<td>13.6 %</td>
<td></td>
</tr>
<tr>
<td>100 × 100</td>
<td>170.230</td>
<td>163.793</td>
<td>9.3 %</td>
<td>5.1 %</td>
<td>8.1 %</td>
</tr>
<tr>
<td>200 × 200</td>
<td>162.664</td>
<td>159.761</td>
<td>4.4 %</td>
<td>2.6 %</td>
<td>2.5 %</td>
</tr>
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<tr>
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</tr>
<tr>
<td>∞ × ∞</td>
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<td>155.777</td>
<td></td>
<td></td>
<td></td>
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</table>
Discretisation Error

- Scheme 1
- Scheme 2

\[ \frac{1}{N} \]

- \( \text{Nu}_{\max} \)

Graph showing the relationship between \( \frac{1}{N} \) and \( \text{Nu}_{\max} \) for Scheme 1 and Scheme 2.
### Discretisation Error

<table>
<thead>
<tr>
<th>Equivalent 3-D</th>
<th>Grid</th>
<th>Nu Scheme 1</th>
<th>Nu Scheme 2</th>
<th>Error Scheme 1</th>
<th>Error Scheme 2</th>
<th>Diff.</th>
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<tr>
<td>125,000</td>
<td>50 × 50</td>
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Solution Error Control → Practicality Limits

- Calculation times
  - 8 days on 6-processor parallel machine
  - ¼ geometry → 450,000 elements
  - 30 s real time

- Extrapolation to real problem
  - 2.5 mio elements (minimum)
  - 300 s real time
  - ≈ 1 year on 6 processors
  - ≈ 2 months on 36 processors

UPTF test, ECC injection below water level, courtesy M. Scheuerer, GRS
Practicality Limits

• Transient, 3-D calculations
  – Long transients
  – Complex geometry
  – Complex physics
  – ...

• Present results together with done Q&A assurance

• do ‘as much as feasible’

• Create awareness with respect to uncertainties and errors
Uncertainties

• Uncertainties:
  – Uncertainty analysis for both the experiments and CFD solutions
  – Systematic variation of uncertain parameters (e.g. turbulence boundary conditions, MPF length scales,...)
  – Generate response surfaces

• General ‘Quality Assurance’ and PSA techniques applicable
  – Statistics
  – Design of Experiments (DOE)
  – Probabilistic Safety Analysis
BPG: Model Recommendations

• Statistical turbulence models
  – $k-\varepsilon \rightarrow k-\varepsilon/k-\omega$ turbulence models with shear-stress limiter (SST)
  – Improved results for
    • Separation
    • Re-attachment

• Wall treatment
  – Standard logarithmic wall laws
    $\rightarrow$ Combined linear/logarithmic wall laws
  – Resolution of viscous sublayer, if possible
Example: Impinging Jet Flow
Example: Impinging Jet Flow

Model error $k-\varepsilon$
Wall Function Behaviour

<table>
<thead>
<tr>
<th>Linear</th>
<th>Buffer</th>
<th>Logarithmic</th>
</tr>
</thead>
</table>

- **Log law**
- **Automatic**
- **Linear law**
BPG: Model Recommendations

- Steady-state vs. unsteady-state flows
- Turbulence models?
  - URANS
  - LES
  - DES & SAS
  - Combination of URANS & LES
- Research & validation required
Transient 3-D Flows

Example:

UPTF test turbulence vs. large scale fluctuations

Calculations by Sander Willemsen, NRG
Turbulence & Transient Flows

- Large-scale fluctuations vs. turbulence fluctuations
  \[ t_t = \frac{k}{\epsilon} \leq T_f \]
- Trend towards DES, SAS, LES
- Problem areas:
  - LES wall treatment
  - DES, SAS switching criteria, CPU-time, ...
Multi-Phase Flow Models

- Progress in modelling individual flow classes
  - Bubbly flows
  - Free surface flows
- Problem and research areas
  - Different morphologies
  - Flow regime transition
  - Mathematical behaviour of model equations
- Numerical methods
  - Calculation times, robustness, ...
Multiple Morphologies

Figure 1. Schematic of the experimental apparatus.
Simulation with the Grace drag model (80x80 grid):

- \( d_P = 5\text{mm} \)
- \( d_P = 0.5\text{mm} \)
DNS resolution of small MPF structures on grid refinement

Grid dependency
water wave traveling towards the outer wall
two-phase flow model, Grace drag, $d_p=5\text{mm}$, time $T=0.25\text{s}$
$\rightarrow$ resolution of smaller structures prevents grid convergence

40 x 40 grid 80 x 80 grid 160 x 160 grid
BPG: Summary & Future

- BPG developed and successfully applied in ECORA for single phase flows and 'simple' MPF's
- Simulations with complex models/ geometries/ unsteady flows met difficulties in the application of BPG
  - strong grid sensitivity (e.g. sloshing, plunging jet)
  - strong model parameter sensitivity (e.g. sloshing, plunging jet)
  - some model formulations are grid dependent (free surface, turbulence treatment, wall boiling, ...?)
- Future topics
  - Quality control for unsteady-state flows
  - Model recommendations for unsteady-state flows
  - Model recommendations for multi-phase flows
  - Comments on practicality limits
- Worst strategy would be to continue single shot CFD in Nuclear Reactor Safety
  \[ \rightarrow \text{Large interest in BPGs from all industrial areas!} \]