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 & Reactor Safety

- **Use of CFD results for safety-critical analyses**
- **Requirements:**
  - Reliability
  - Quality
- **Definition of <u>'CFD Quality'</u>:**
  - 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

Real vs. Ideal

Best Practice Guidelines

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- 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
  - <u>Data</u>
- **Accuracy expectations vs. assumptions?**

Structure of ECORA BPG's

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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**

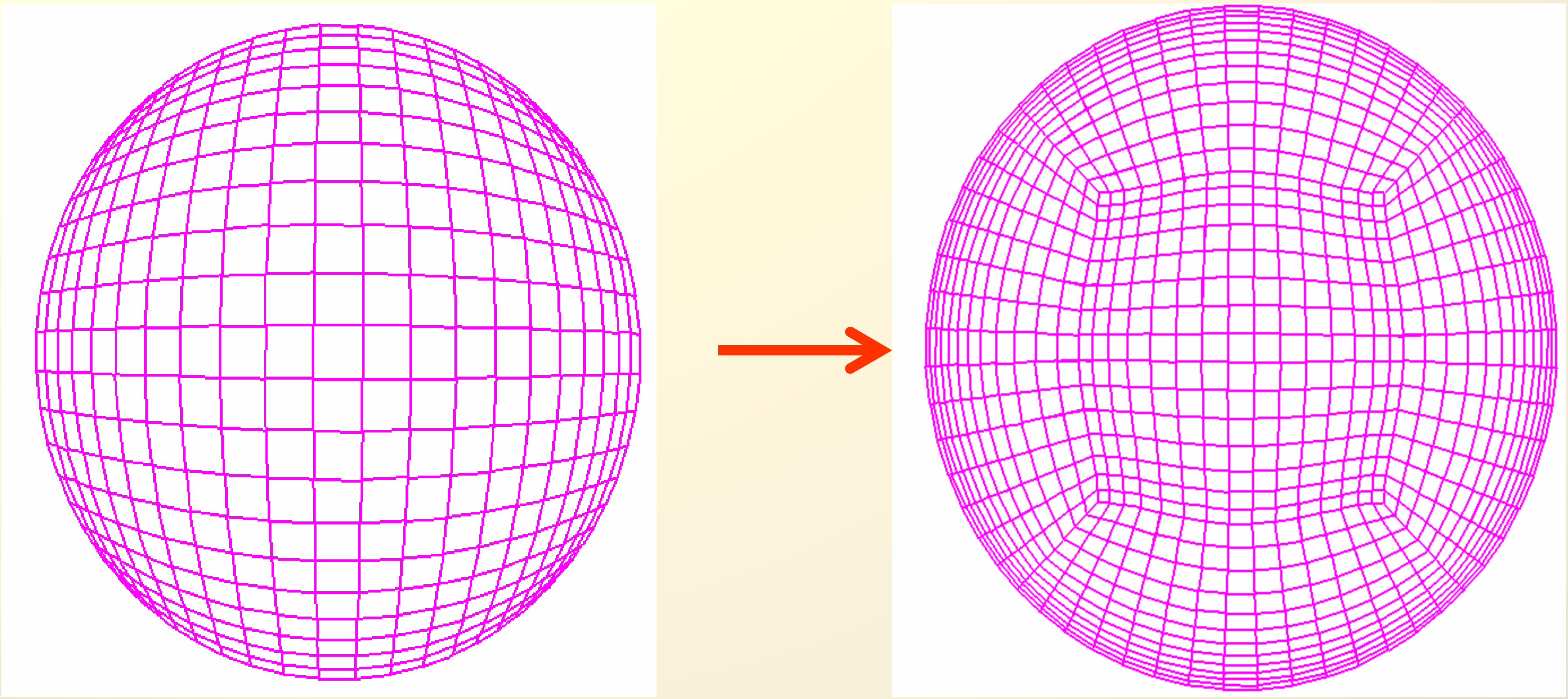
Investigated ECORA testcases

- **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:**
  - <u>Scalable grids</u>
  - Grid angles > 20° and < 160° (accuracy, convergence)
  - Aspect ratios < 1,000 on 32-bit computers
  - Expansion ratios < 1.5 …2
  - Capture physics
- **Grid refinement:**
  - Manual, based on error estimate
  - Automatic adaptive based on ‘error sensor’

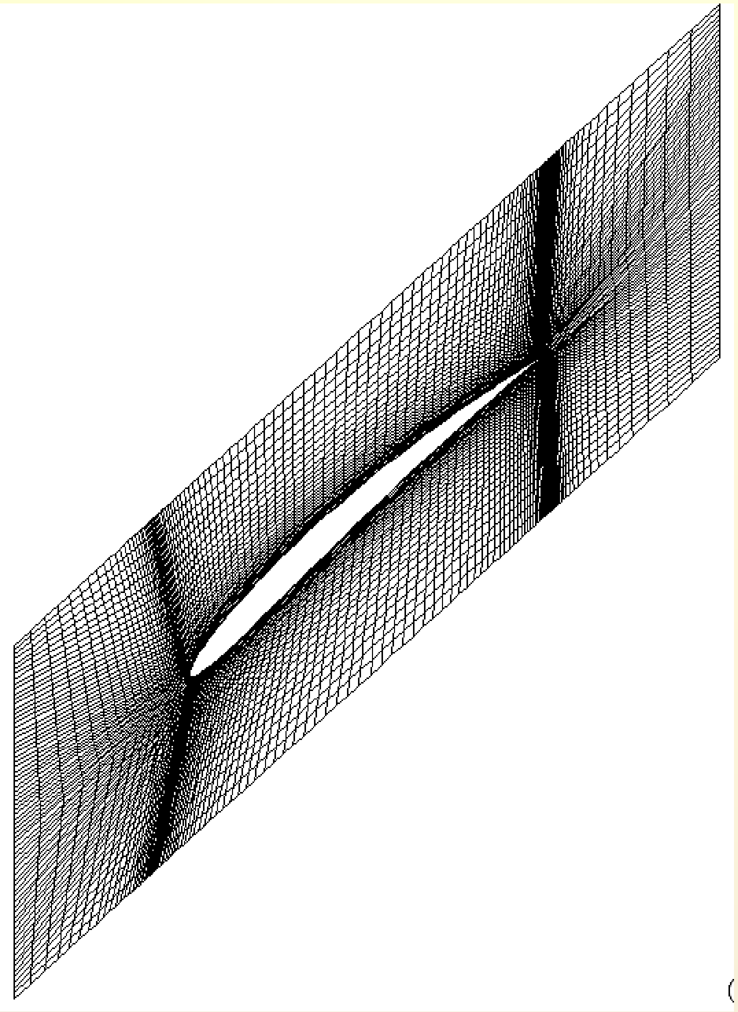
Scalable Grids

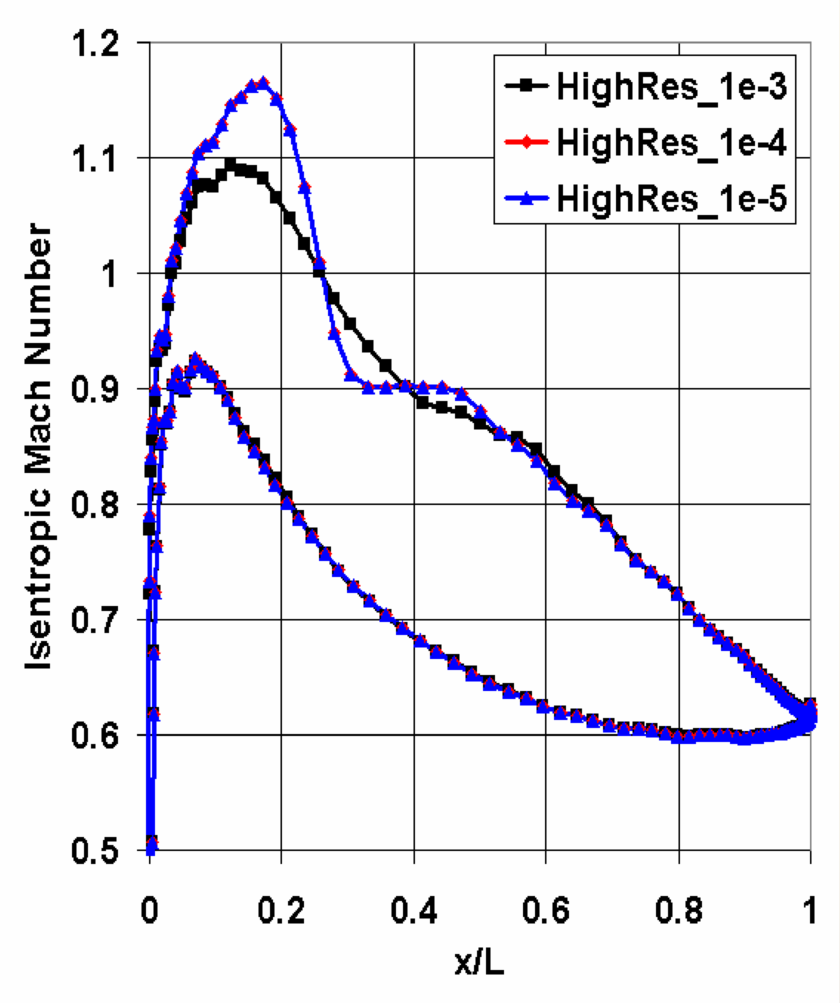


BPG: Recommendations

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

Iteration Error Control



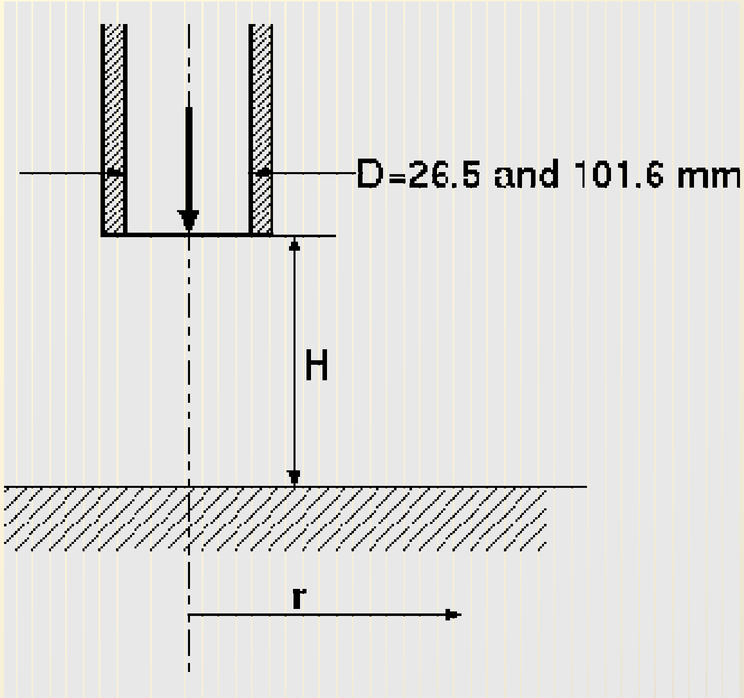


BPG: Recommendations

- **Discretisation error:**
  - 1st order schemes require <u>very, very fine</u> grids for most 3-D applications
  - Start with 1st order scheme
  - Switch to 2nd order scheme
  - Compare target variables for both schemes
  - <u>Error estimation at little extra cost</u>

Richardson Extrapolation

- Impinging jet flow with heat transfer
- 2-D, axisymmetric
- Grids:
  - $50 \times 50 \rightarrow 800 \times 800$
- Practical in 2-D



Richardson Extrapolation

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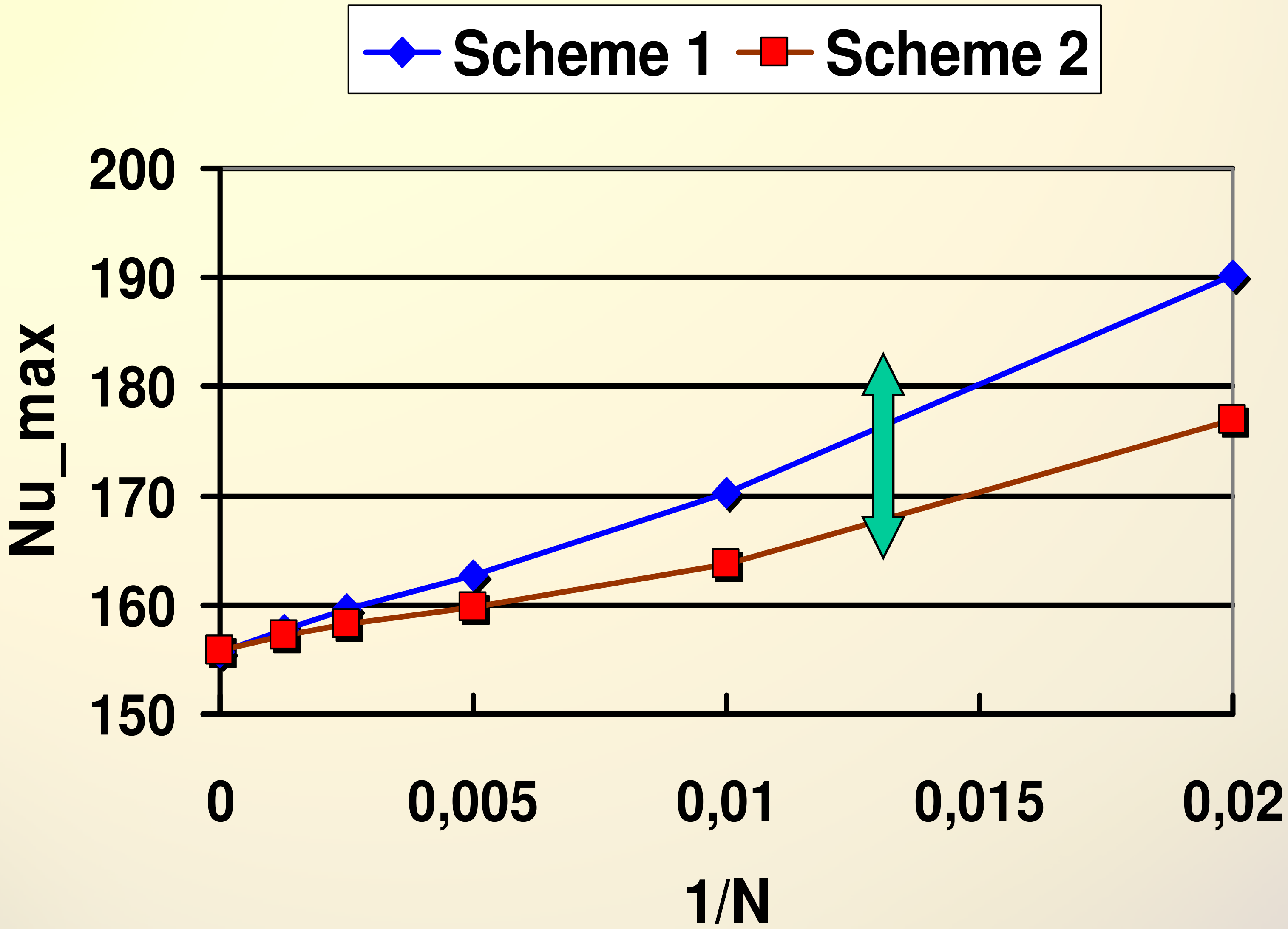
Grid	Nu		Error		
	Scheme 1	Scheme 2	Scheme 1	Scheme 2	R.E.
50×50	190.175	176.981	22.1 %	13.6 %	
100×100	170.230	163.793	9.3 %	5.1 %	8.1 %
200×200	162.664	159.761	4.4 %	2.6 %	2.5 %
400×400	159.646	158.296	2.3 %	1.4 %	0.9 %
800×800	157.808	157.168	1.1%	0.7 %	0.7 %
$\infty \times \infty$	155.751	155.777			

Discretisation Error



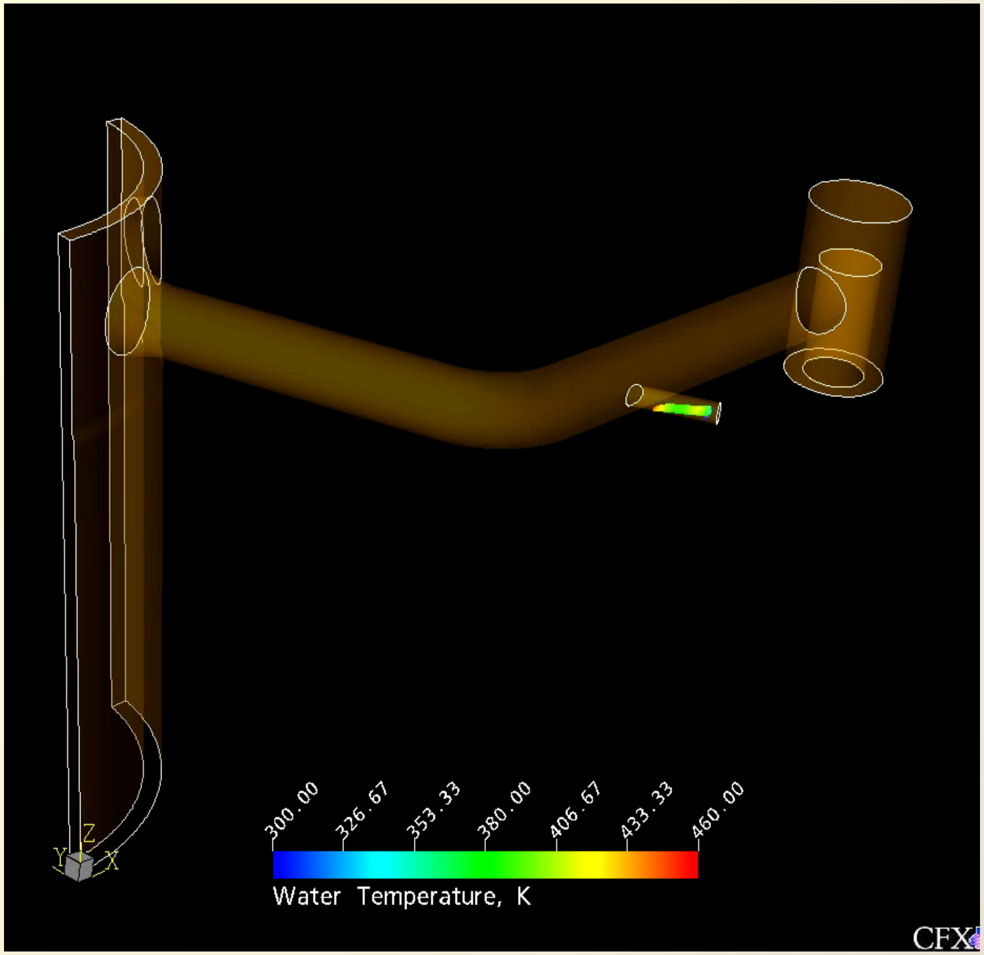
Discretisation Error

ANSYS

Equivalent 3-D	Grid	Nu		Error		
		Scheme 1	Scheme 2	Scheme 1	Scheme 2	Diff.
125,000	50 × 50	190.175	176.981	22.1 %	13.6 %	8.5 %
1,000,000	100 × 100	170.230	163.793	9.3 %	5.1 %	4.1 %
8,000,000	200 × 200	162.664	159.761	4.4 %	2.6 %	1.9 %
64,000,000	400 × 400	159.646	158.296	2.3 %	1.4 %	0.9 %
512,000,000	800 × 800	157.808	157.168	1.1%	0.7 %	0.4 %
	∞ × ∞	155.751	155.777			

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



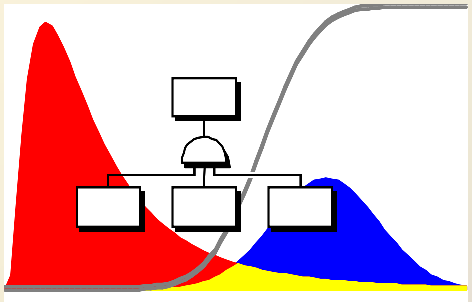
UPTF test, ECC injection below water level, courtesy M. Scheuerer, GRS

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

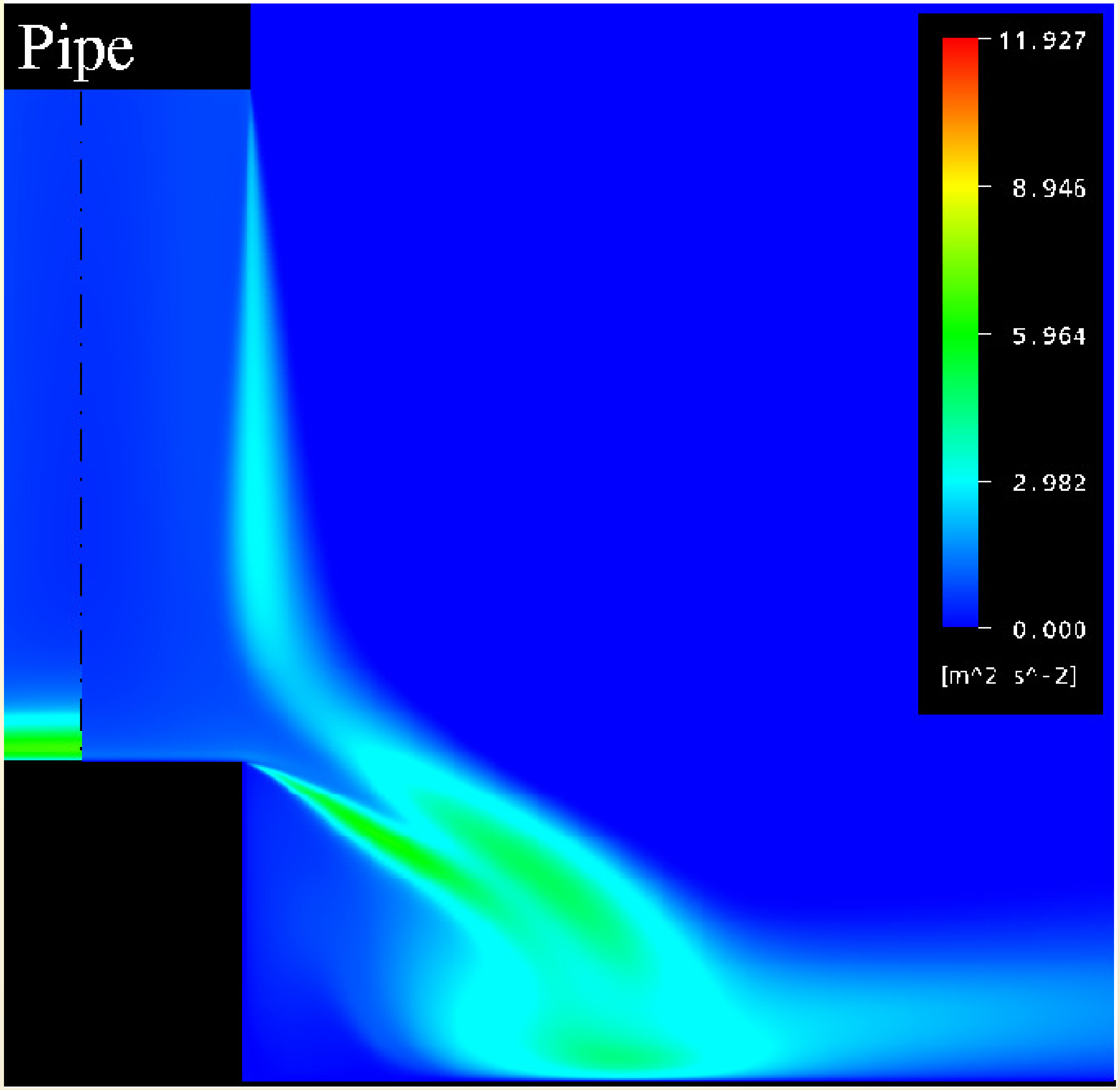
- **Uncertainties:**
  - Uncertainty analysis for both the experiments and CFD solutions
  - Systematic variation of uncertain parameters (e.g. turbulence boundary conditions, MPF length scales,…)
  - Generate response surfaces
- **General 'Quality Assurance' and PSA techniques applicable**
  - Statistics
  - Design of Experiments (DOE)
  - Probabilistic Safety Analysis



BPG: Model Recommendations

- Statistical turbulence models
  - k-ε → k-ε/k-ω turbulence models with shear-stress limiter (SST)
  - Improved results for
    - Separation
    - Re-attachment
- Wall treatment
  - Standard logarithmic wall laws → Combined linear/logarithmic wall laws
  - Resolution of viscous sublayer, if possible

Example: Impinging Jet Flow



Example: Impinging Jet Flow

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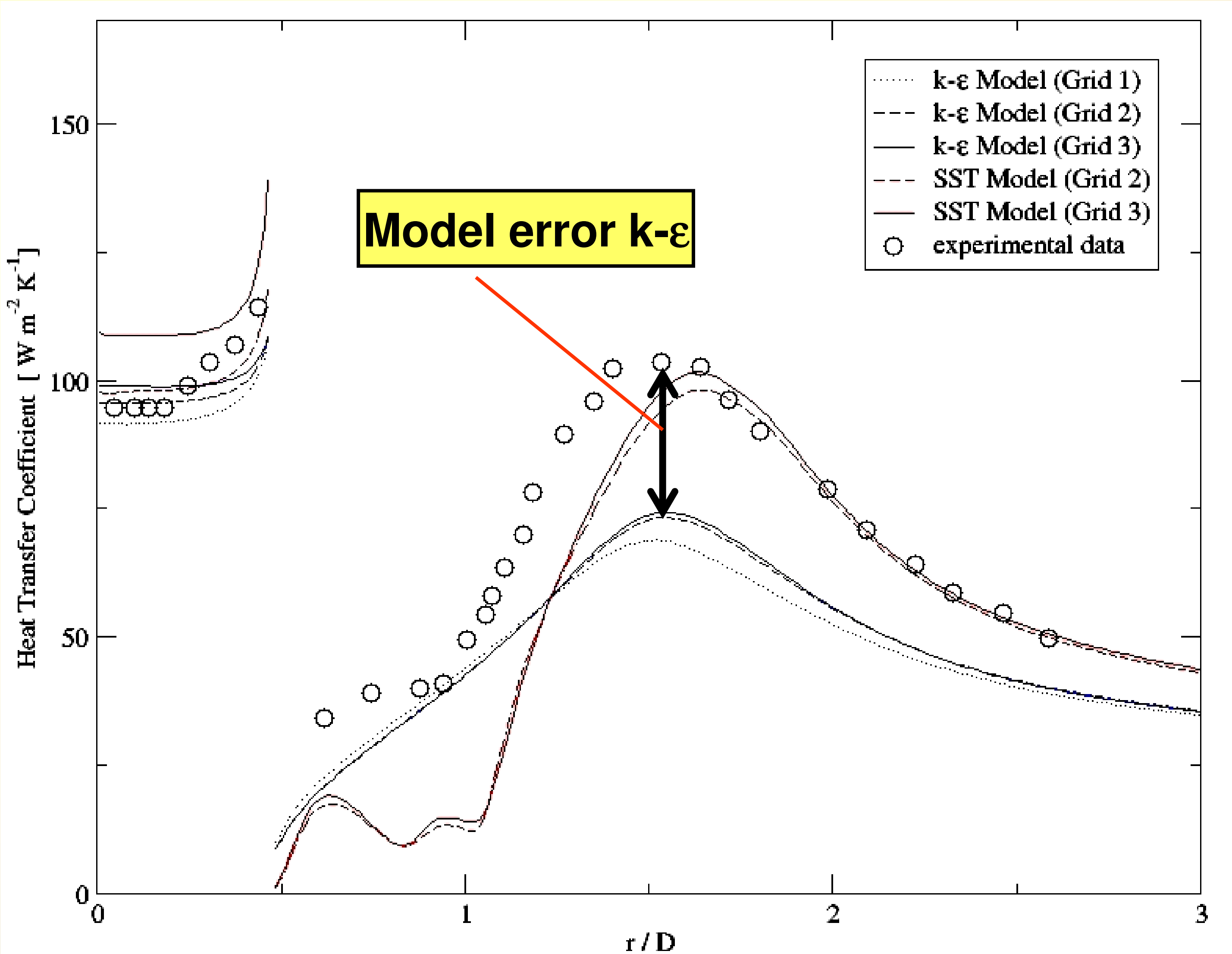
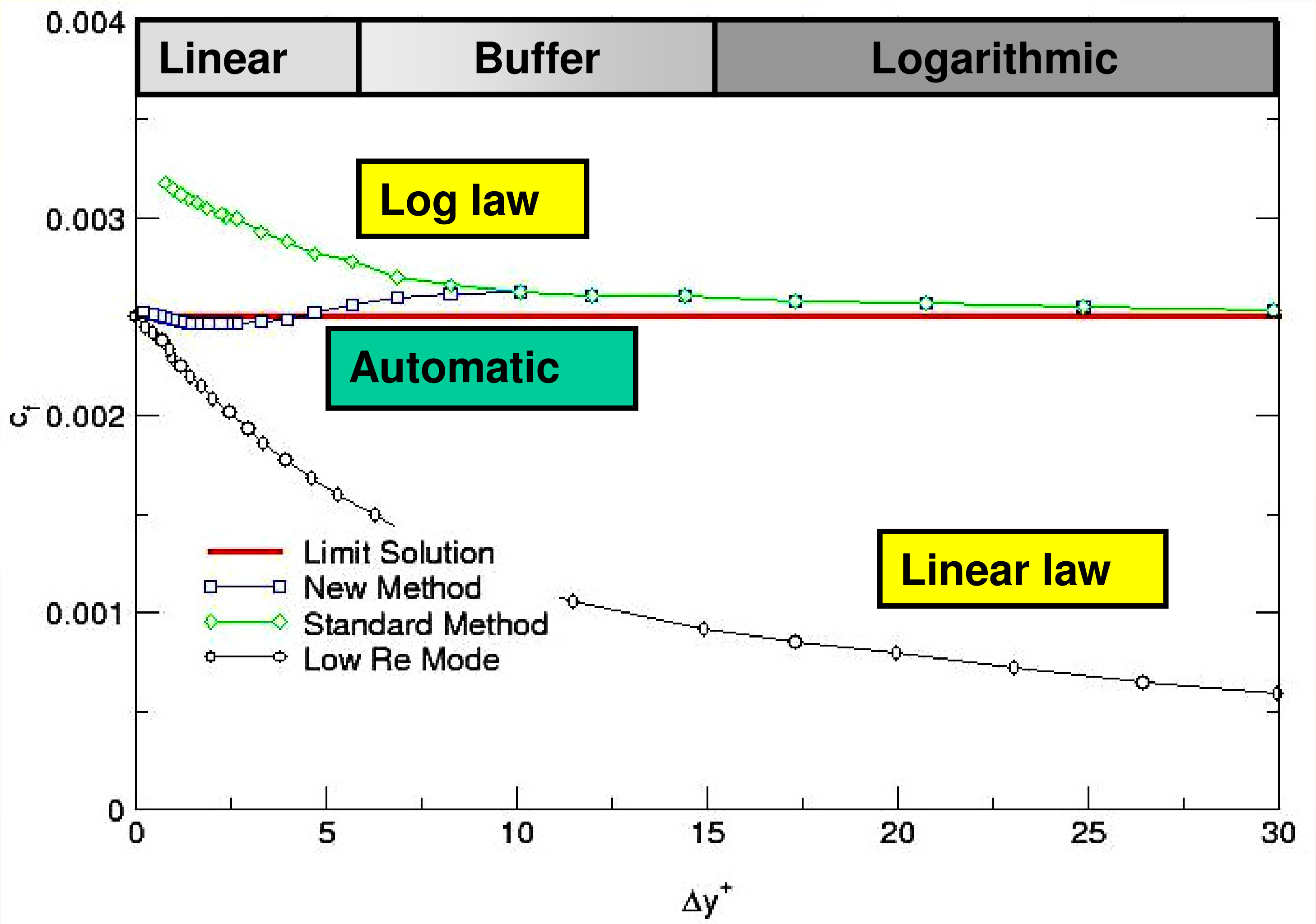


Wall Function Behaviour



BPG: Model Recommendations

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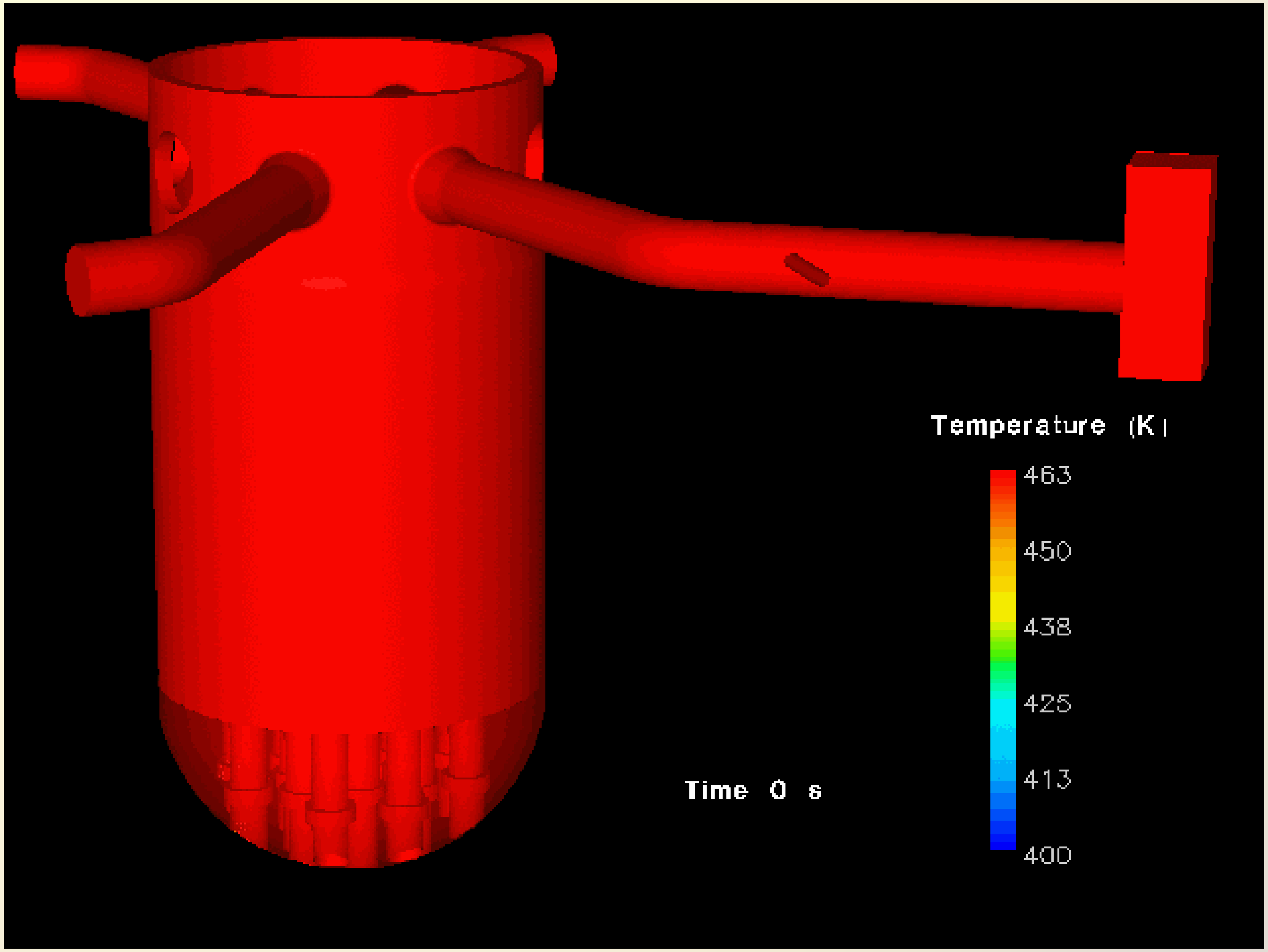
- Steady-state vs. unsteady-state flows
- Turbulence models?
  - URANS
  - LES
  - DES & SAS
    - Combination of URANS & LES
- Research & validation required

Transient 3-D Flows

Example:

UPTF test

turbulence vs. large scale fluc-tuations



Calculations by Sander Willemsen, NRG

Turbulence & Transient Flows

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- Large-scale fluctuations vs. turbulence fluctuations

$$t_t = \frac{k}{\varepsilon} \leq T_f$$

- 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
- <u>Numerical methods</u>
  - <u>Calculation times, robustness, ...</u>

Multiple Morphologies

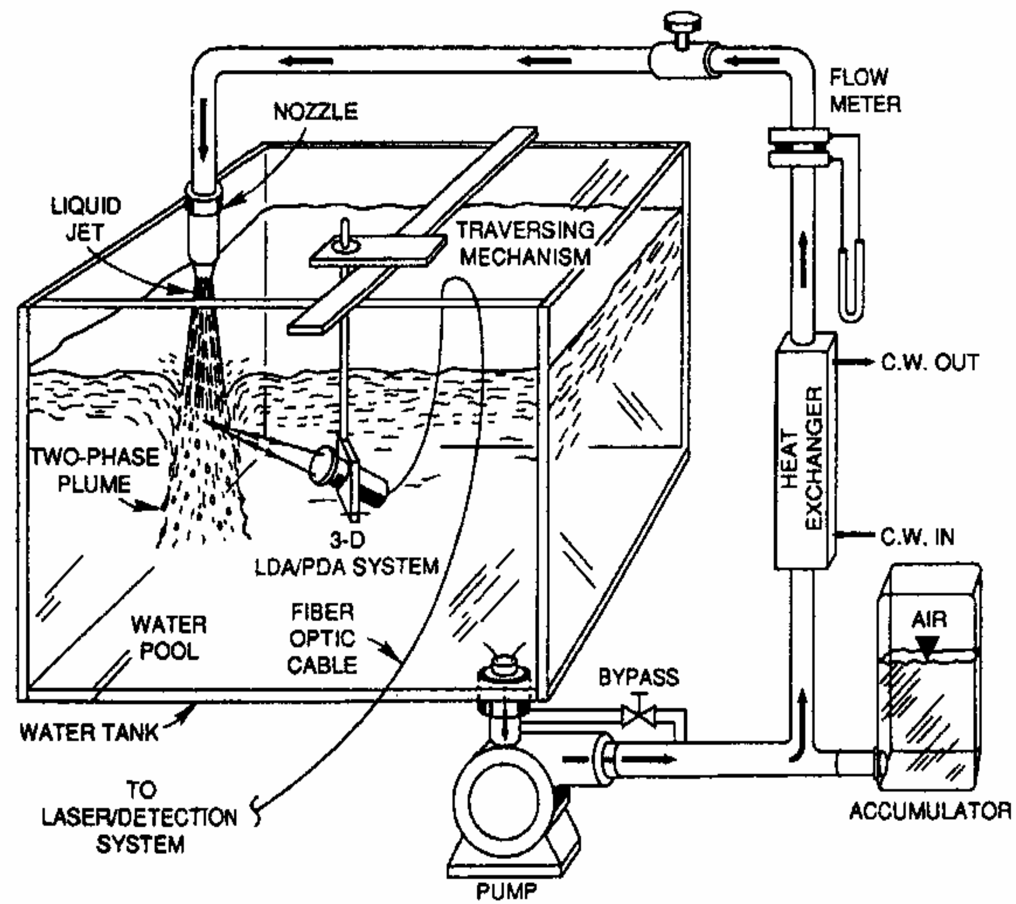
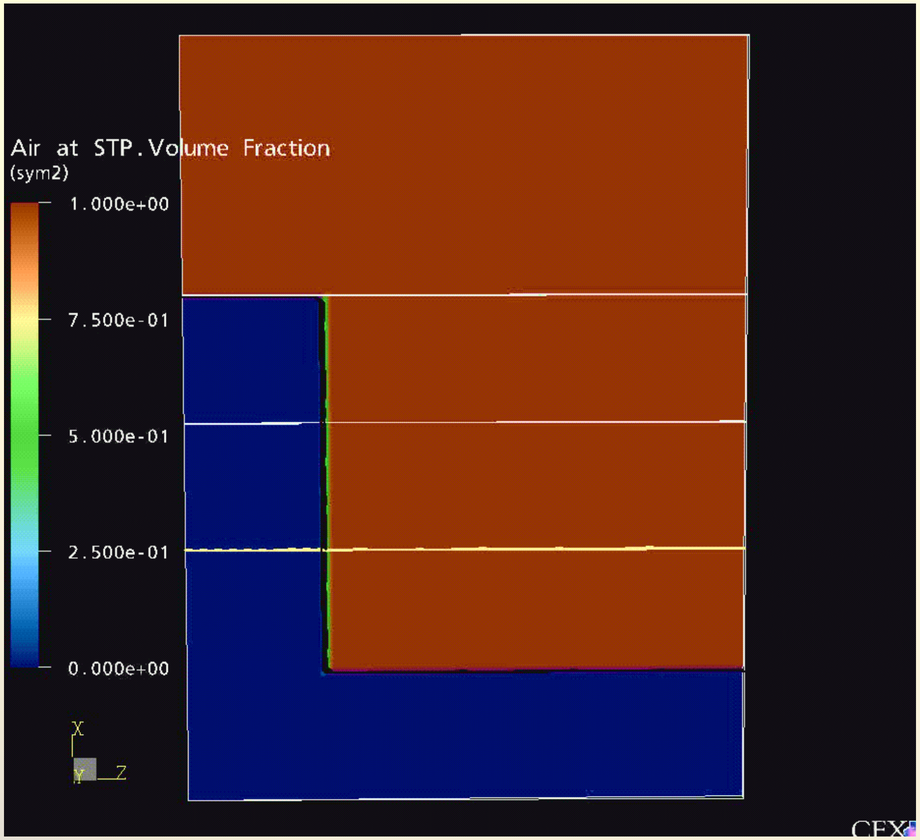


Figure 1. Schematic of the experimental apparatus.

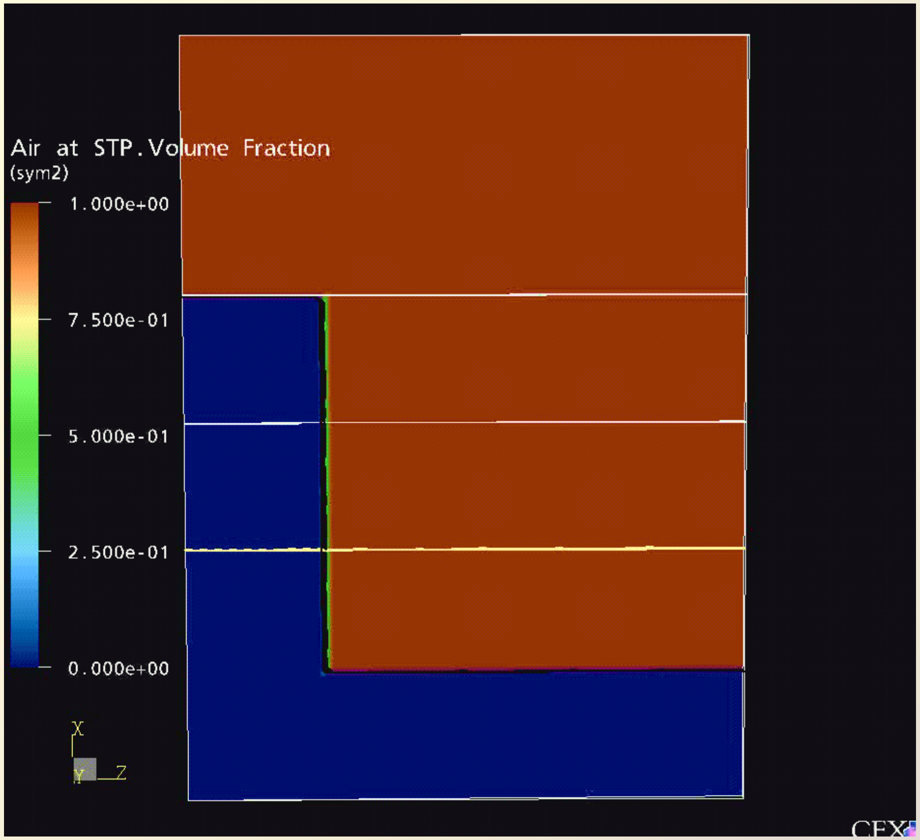
Behaviour of Model Equations

Simulation with the Grace drag model (80x80 grid):

d_P = 5mm



d_P = 0.5mm



DNS resolution of small MPF structures on grid refinement

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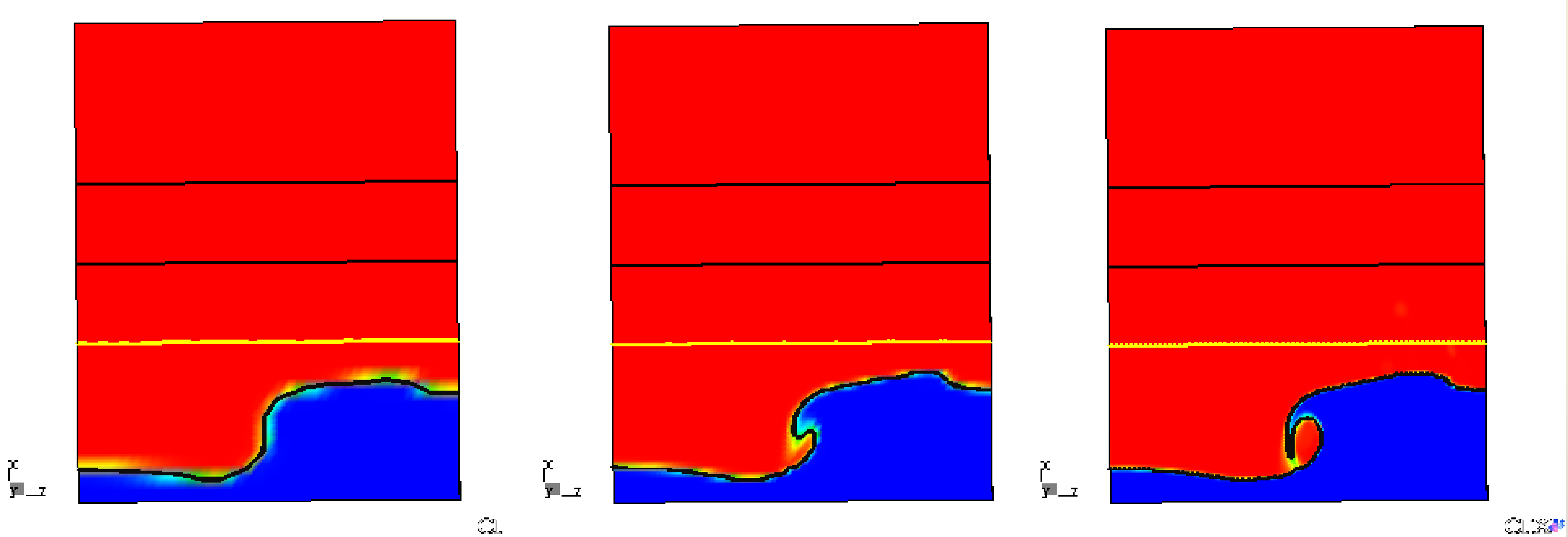
Grid dependency

water wave traveling towards the outer wall
two-phase flow model, Grace drag, d_P=5mm, time T=0.25s
→ resolution of smaller structures prevents grid convergence

40 x 40 grid **80 x 80 grid** **160 x 160 grid**



BPG: Summary & Future

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- 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

→ Large interest in BPGs from all industrial areas!