UK EXPLOSION LIAISON GROUP

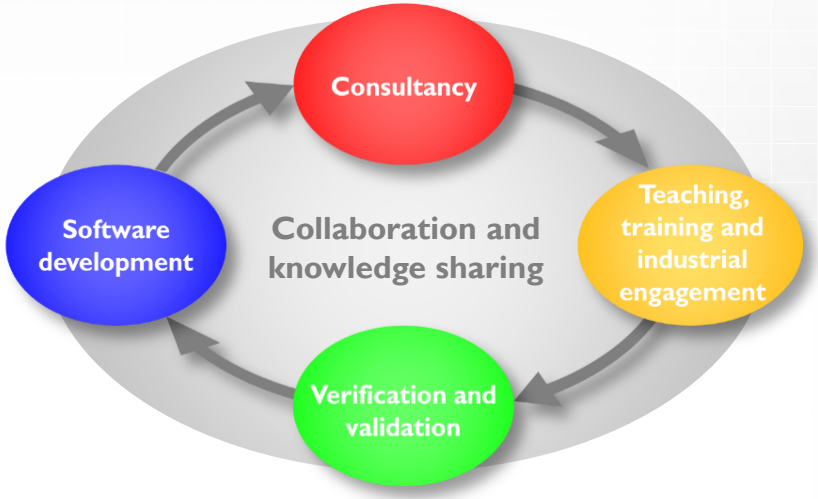
Explosion research of yesterday, today and tomorrow: Trust and VVUQ for explosion simulations with CFD

Steve Howell, Prankul Middha and Francesco Chillè (Abercus)
Kees van Wingerden and Remi Martini (Vysus Group)

Abercus 7 Queen's Gardens Aberdeen AB15 4YD www.abercus.com

Steve Howell (Abercus)

Steve is a chartered engineer with 30 years' experience in the application and development of CFD. He founded Abercus, an **independent**, privately-owned consultancy specialising in **advanced engineering simulation**, in 2010.



Steve is an active member of the CFD (Chair) and SGM* working groups at NAFEMS, the international organisation for engineering simulation.

NAFEMS

* Simulation governance and management

Co-authors

Prankul Middha
Francesco Chillè

Kees van Wingerden
Remi Martini

Agenda

- Simulating vapour cloud explosions (VCE) with CFD:
  - Predominantly, this is the porosity distributed resistance (PDR) approach.

Yesterday → Today → Tomorrow?...

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[Ref. 2]: "*Analysis Origins – KFX and FLACS, Modelling Explosions and Combustion and the Impact of Piper Alpha*", NAFEMS, 2018 (Link).
[Ref. 3]: Hisken H et al, (2025), "*45 Years of Modelling Gas Explosions with the PDR Concept – Current Status and Future Prospects*", 2nd Olympiad in Engineering Science – OES 2025 (Link).

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- Simulating vapour cloud explosions (VCE) with CFD:
  - Predominantly, this is the porosity distributed resistance (PDR) approach.
- Meet PeDRo, our black-box friend who will help us explore this journey:
  - Yesterday: what is the PDR approach?
  - Today: how to earn trust in the PDR approach (VVUQ*).
    - VVUQ framework – NAFEMS/ASME.
    - User VVUQ.
  - Tomorrow?...

*VVUQ – Verification, Validation and Uncertainty Quantification

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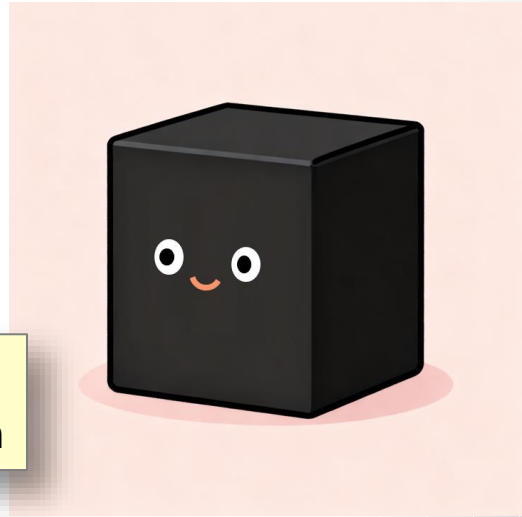

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Agenda

This presentation is hyperlinked. Click on the title bar to return to this slide. Click on the relevant words below to jump to the associated slides later in the presentation.

- Simulating vapour cloud explosions (VCE) with CFD:
  - Predominantly, this is the porosity distributed resistance (PDR) approach.
- Meet PeDRo, our black-box friend who will help us explore this journey:
  - Yesterday: what is the PDR approach?
  - Today: how to earn trust in the PDR approach (VVUQ*).
    - VVUQ framework – NAFEMS/ASME.
    - User VVUQ. – Revisit today.
  - Tomorrow?... – Closing remarks. – The way forward…

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Yesterday

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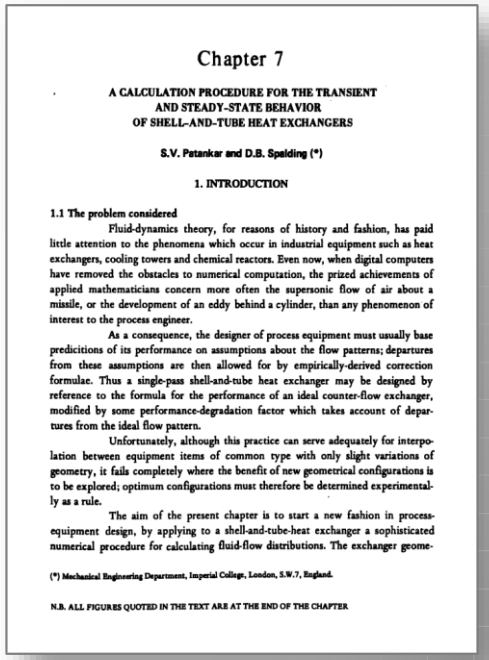

Chapter 7

A CALCULATION PROCEDURE FOR THE TRANSIENT AND STEADY-STATE BEHAVIOR OF SHELL-AND-TUBE HEAT EXCHANGERS

S.V. Patankar and D.B. Spalding (*)

1. INTRODUCTION

1.1 The problem considered

Fluid-dynamics theory, for reasons of history and fashion, has paid little attention to the phenomena which occur in industrial equipment such as heat exchangers, cooling towers and chemical reactors. Even now, when digital computers have removed the obstacles to numerical computation, the prized achievements of applied mathematicians concern more often the supersonic flow of air about a missile, or the development of an eddy behind a cylinder, than any phenomenon of interest to the process engineer.

As a consequence, the designer of process equipment must usually base predicitions of its performance on assumptions about the flow patterns; departures from these assumptions are then allowed for by empirically-derived correction formulae. Thus a single-pass shell-and-tube heat exchanger may be designed by reference to the formula for the performance of an ideal counter-flow exchanger, modified by some performance-degradation factor which takes account of departures from the ideal flow pattern.

Unfortunately, although this practice can serve adequately for interpolation between equipment items of common type with only slight variations of geometry, it fails completely where the benefit of new geometrical configurations is to be explored; optimum configurations must therefore be determined experimentally as a rule.

The aim of the present chapter is to start a new fashion in process-equipment design, by applying to a shell-and-tube-heat exchanger a sophisticated numerical procedure for calculating fluid-flow distributions. The exchanger geome-

(*) Mechanical Engineering Department, Imperial College, London, S.W.7, England.

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Yesterday Today Tomorrow?...

1974

Yesterday

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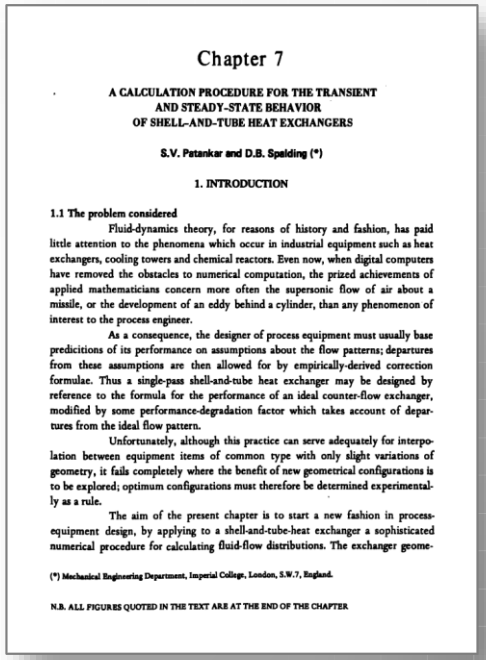
  - Originally intended for modelling the fluid domain on the shell-side of a heat exchanger without having to explicitly capture the tubes within a body-fitted CFD grid.



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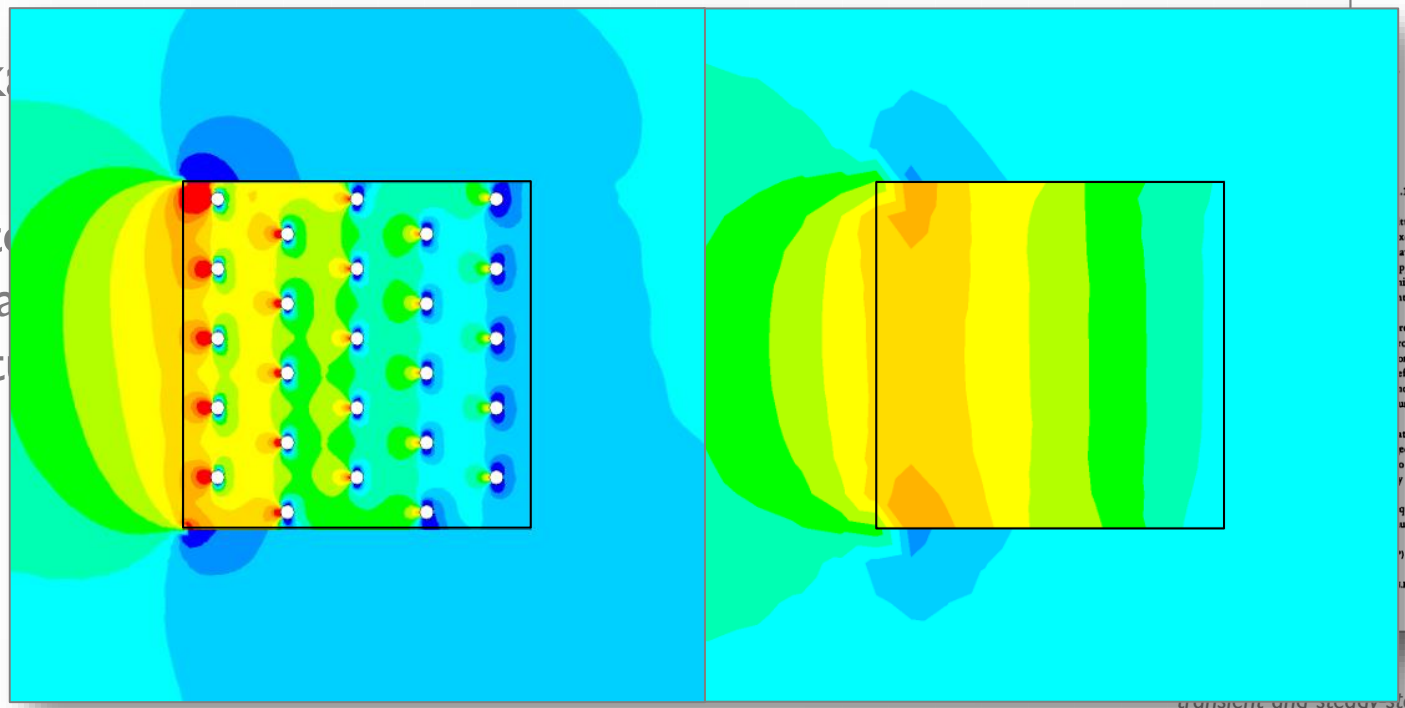

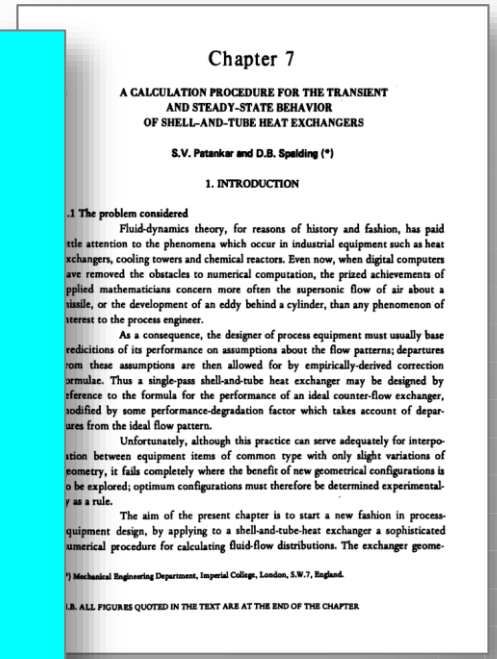

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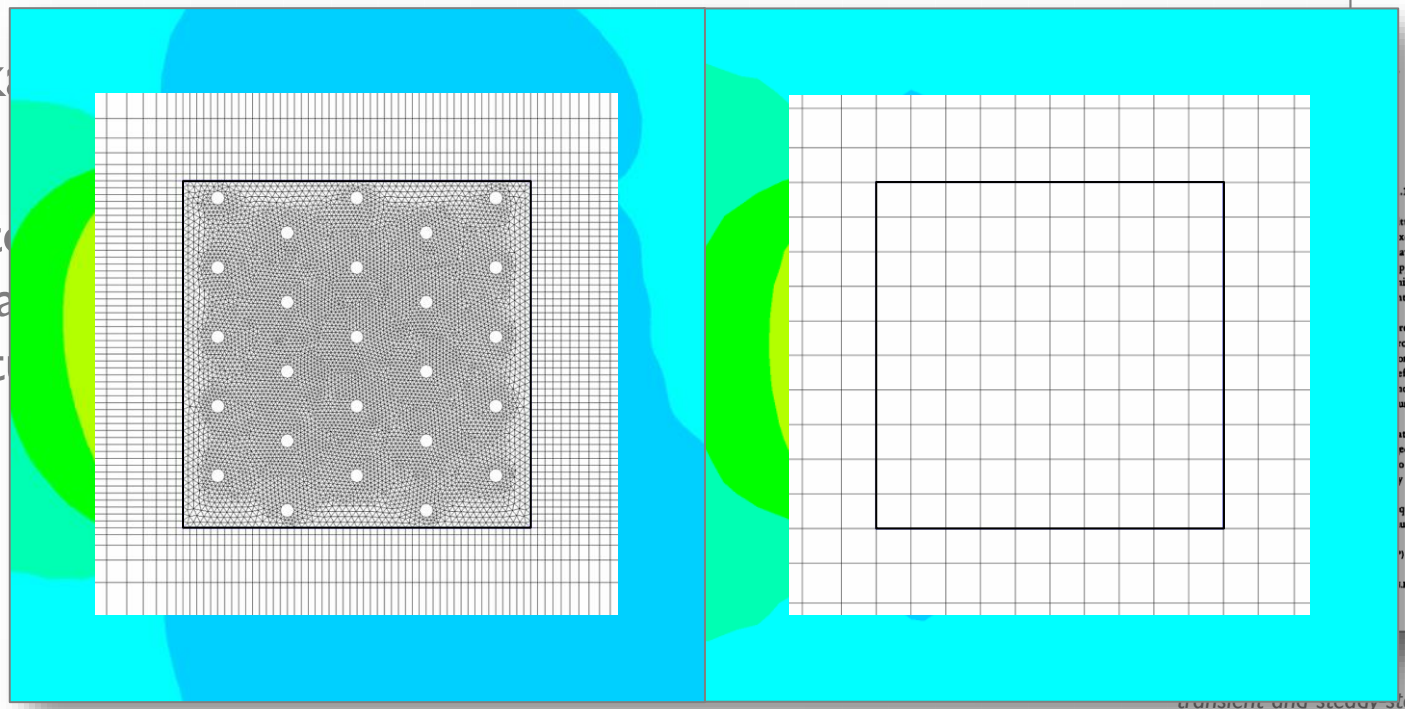

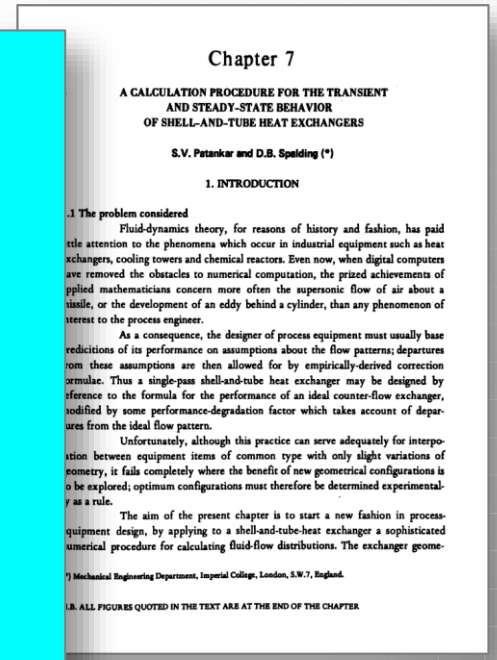

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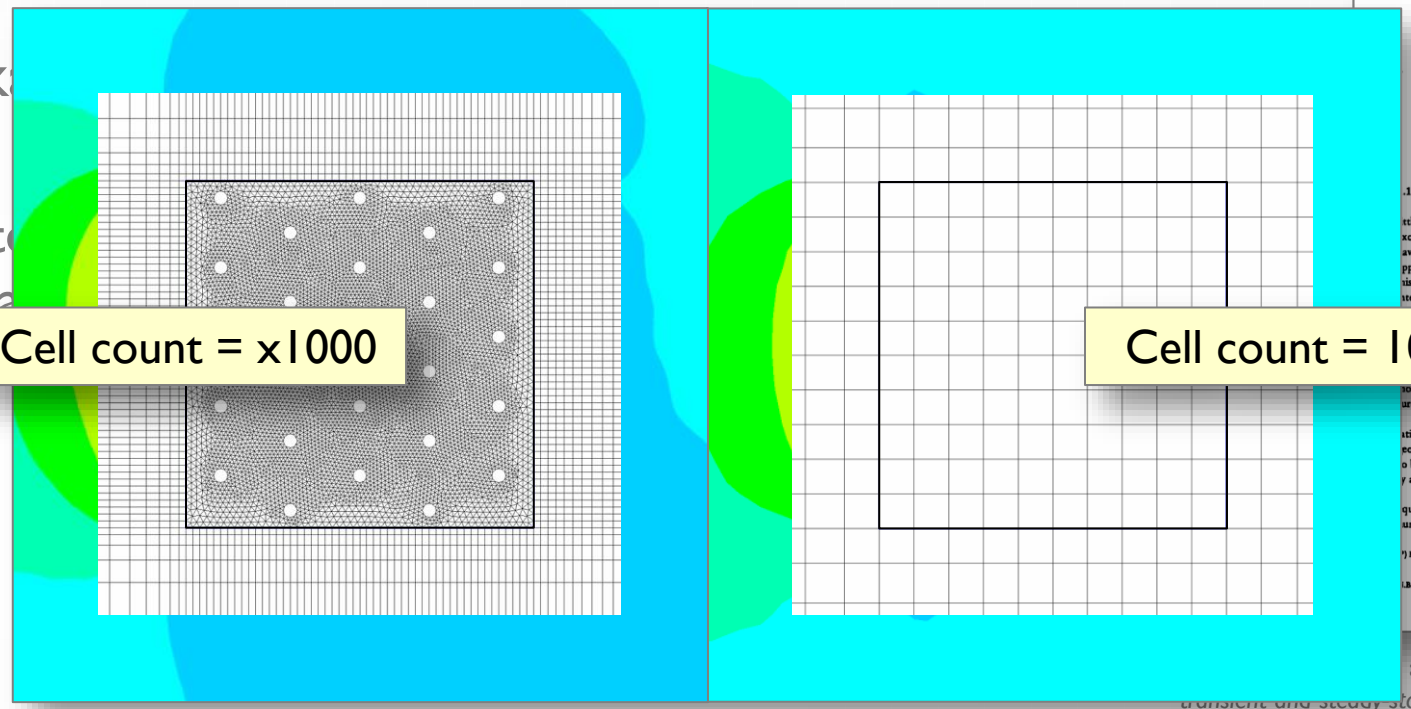

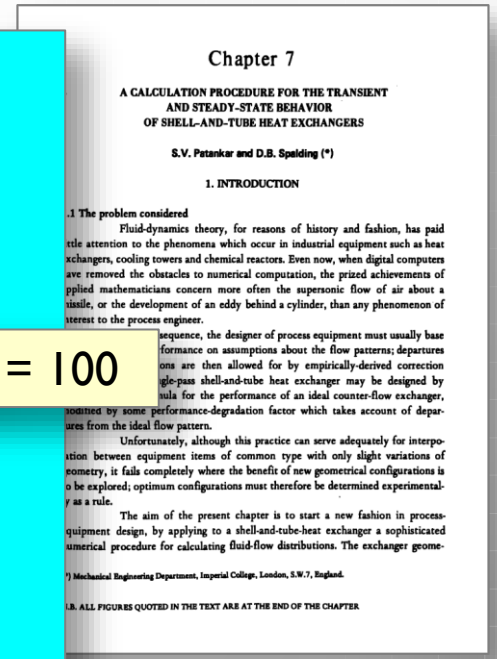

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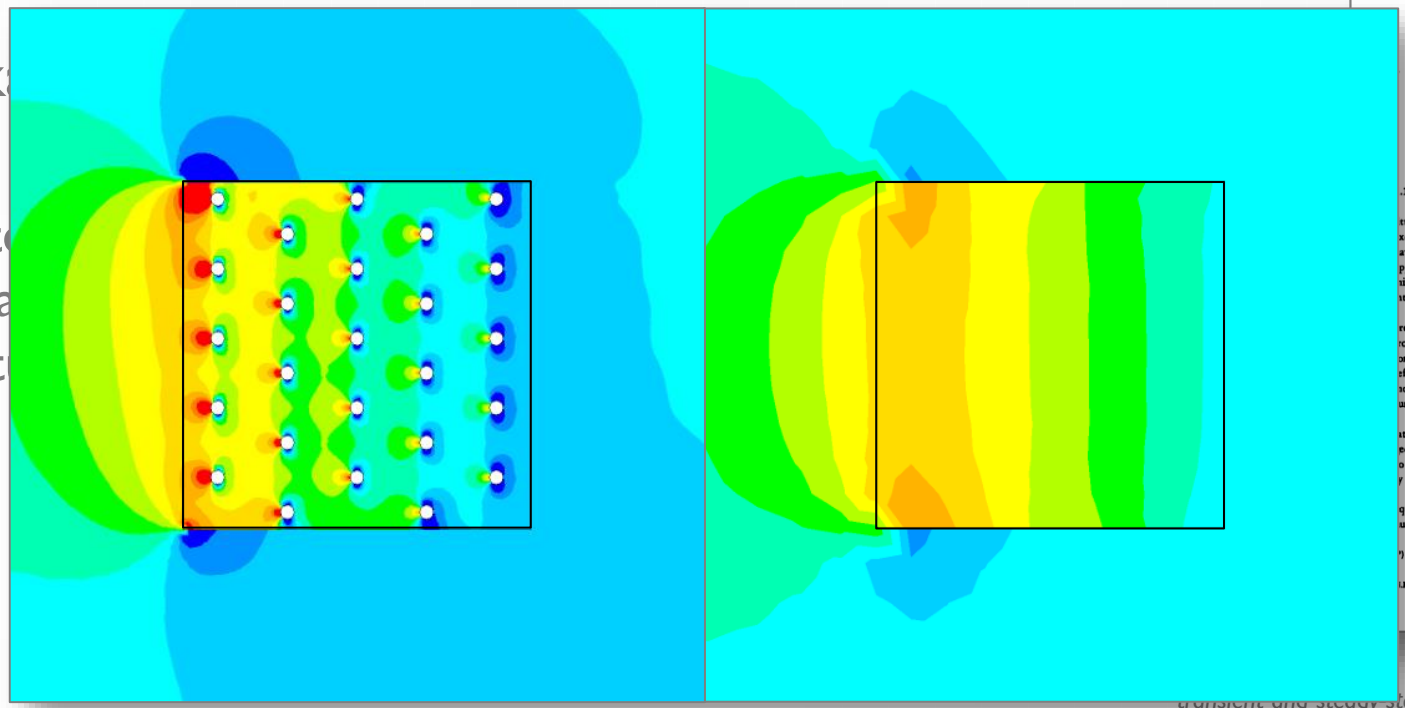

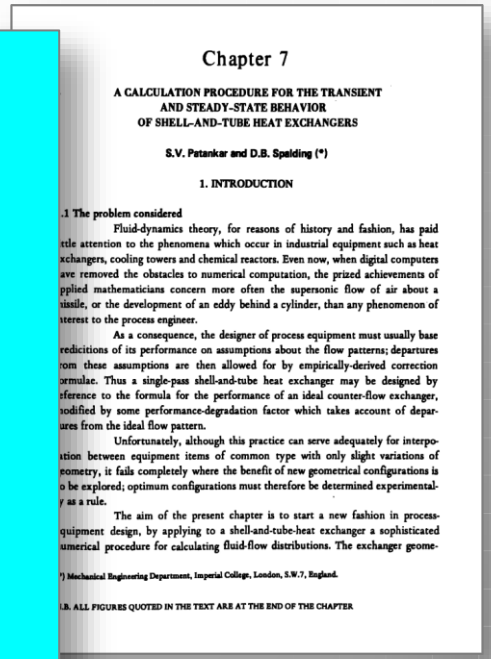

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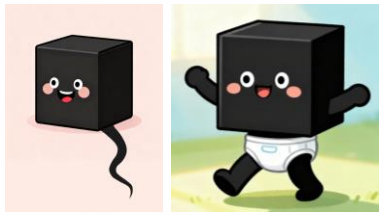
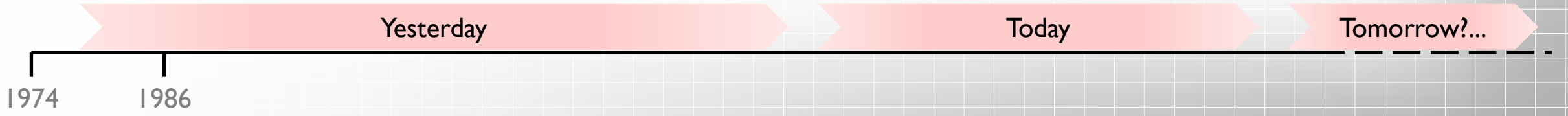
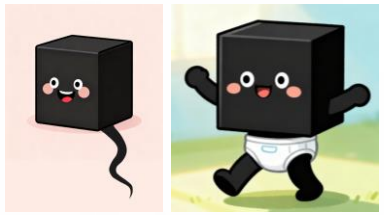


*GEP 80-86, Gas Explosion Programme sponsored by BP, Elf, Esso/Exxon, Mobil, Norsk Hydro and Statoil, running from 1980 to 1986.



Yesterday

- **1986**: The first PDR-CFD code is developed for simulating vapour cloud explosions (through a JIP*):
  - The strength of a vapour cloud explosion is known to be strongly dependent upon the level of small-scale congestion due to pipework and other obstructions within the flammable cloud, which are often too small to resolve with body-fitted meshing.
  - With the PDR approach, the effect of small-scale congestion is instead captured at the sub-grid level through equivalent porosity source terms and empirical turbulent combustion corrections.



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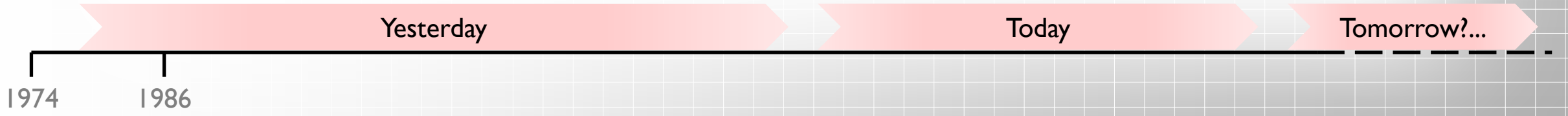
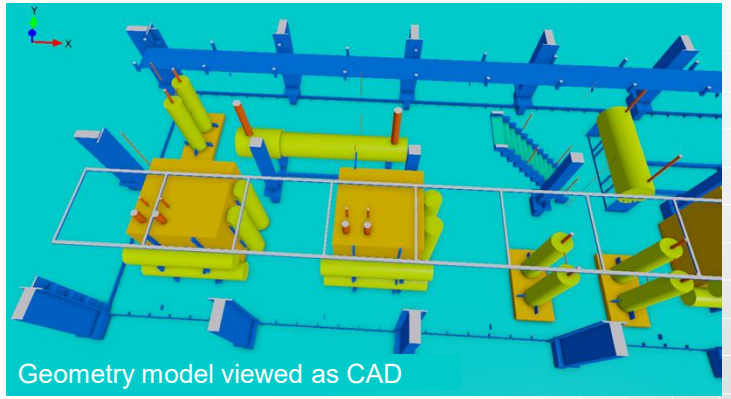
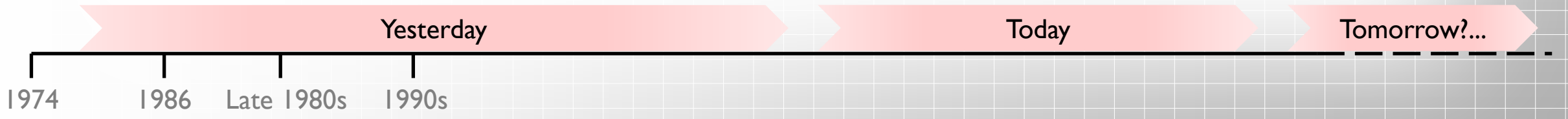


Yesterday

- **Late 1980s/1990s**: Several PDR-based CFD codes are developed for modelling hydrocarbon vapour cloud explosions, primarily in the offshore sector:
  - The PDR codes are commercial, black-box codes.
  - Geometry is represented in terms of the equivalent boxes/cylinders approach.


Geometry model viewed as CAD

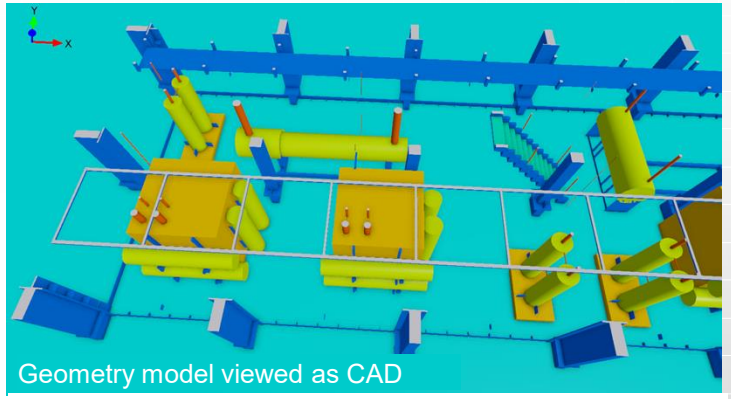


Yesterday

- **Late 1980s/1990s**: Several PDR-based CFD codes

While an explosion model may look impressive within the CFD modelling software, it is important to remember that under the hood, the PDR CFD model is actually very simple:

- It is generally a *Lego*-style geometry captured on a structured orthogonal grid, with varying shades of grey representing the volume and area porosity for the local level of congestion.
- Correspondingly, empirical parameters for turbulent combustion are assigned at each cell.



Corresponding PDR model (actually used by CFD solver)

Yesterday | Today | Tomorrow?...

1974 1986 Late 1980s 1990s

Yesterday

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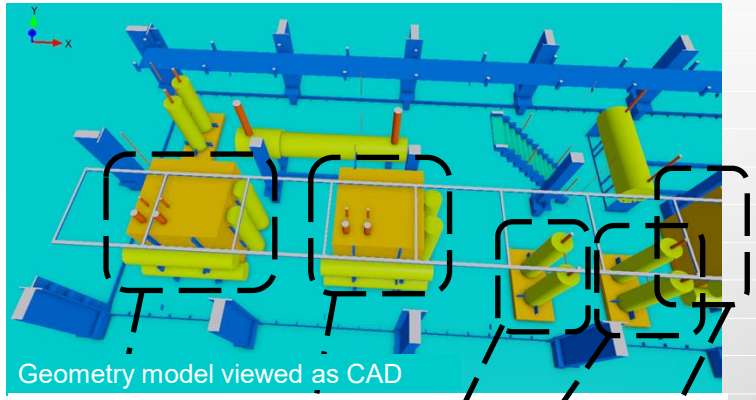

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- **Late 1980s/1990s**: Several PDR-based CFD codes

The PDR-CFD approach is an <u>imperfect but pragmatic</u> approach for modelling vapour cloud explosions – it allows us to consider explosion dynamics in an *engineering* way.

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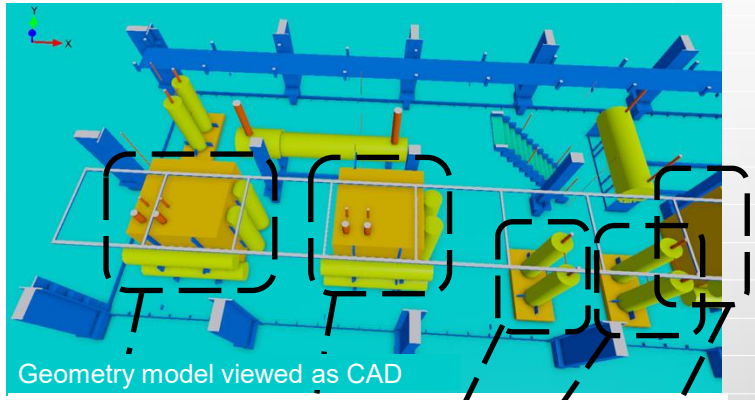

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  - The PDR-CFD approach is an imperfect but pragmatic approach for modelling vapour cloud explosions – it allows us to consider explosion dynamics in an *engineering* way.
  - Geometry is represented in terms of the equivalent boxes/cylinders approach.
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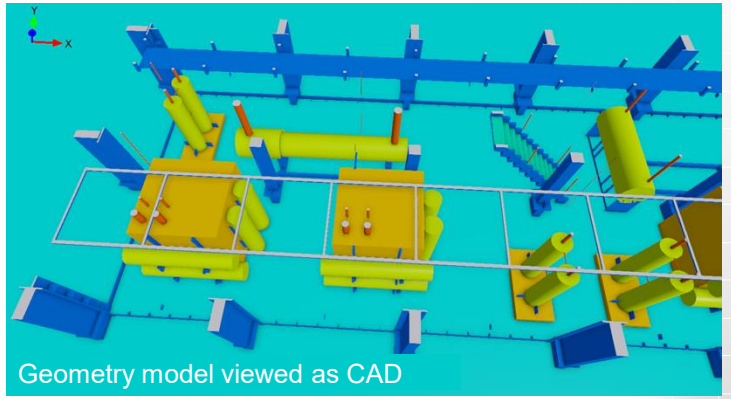
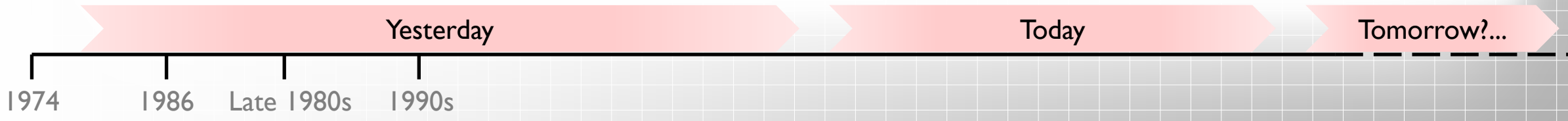

Geometry model viewed as CAD



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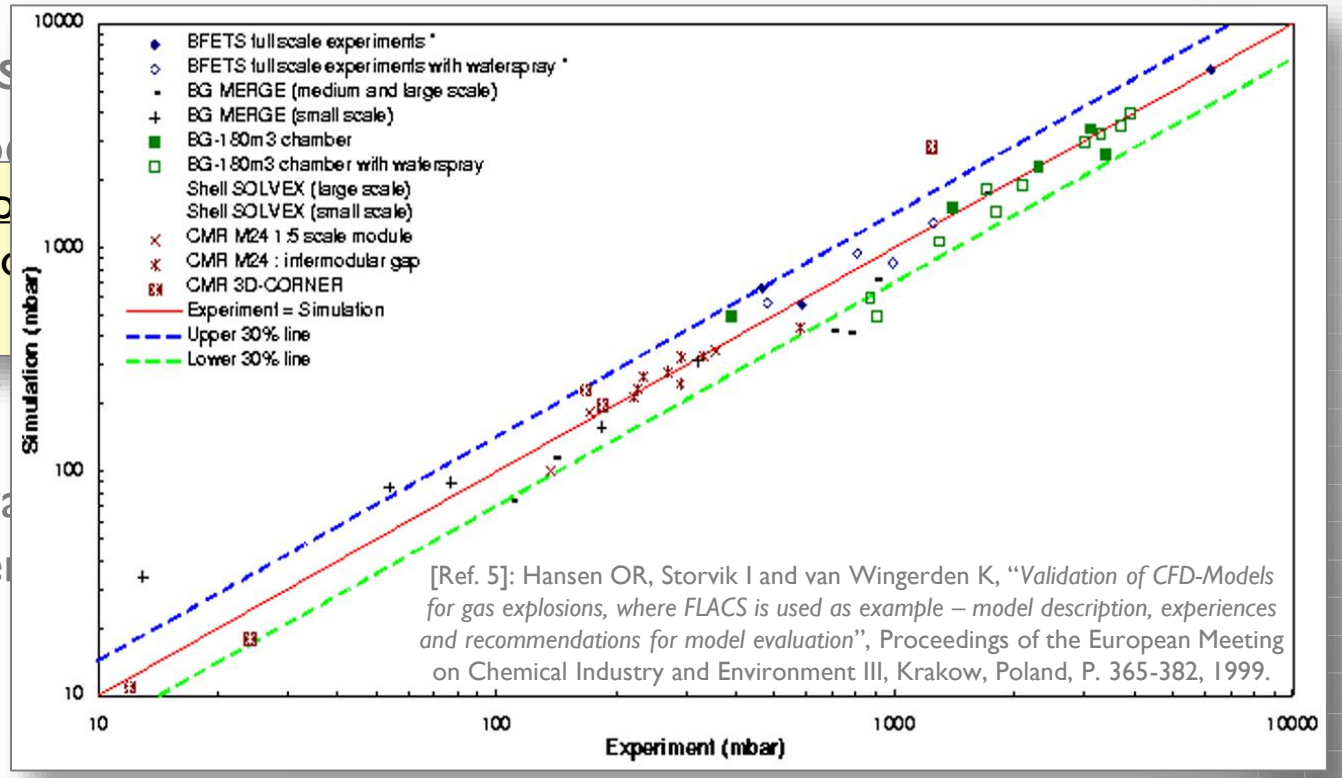

[Ref. 5]: Hansen OR, Storvik I and van Wingerden K, "*Validation of CFD-Models for gas explosions, where FLACS is used as example – model description, experiences and recommendations for model evaluation*", Proceedings of the European Meeting on Chemical Industry and Environment III, Krakow, Poland, P. 365-382, 1999.

Yesterday Today Tomorrow?...

1974 1986 Late 1980s 1990s

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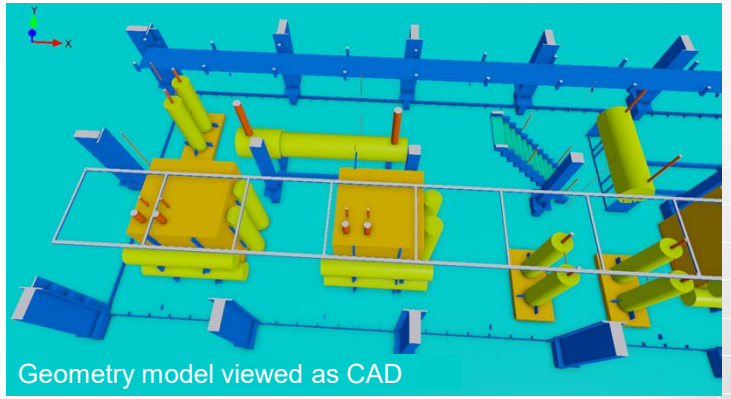
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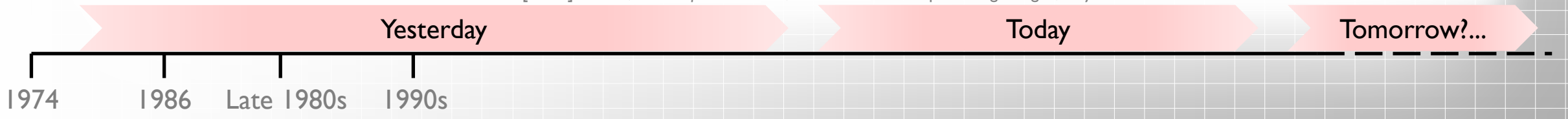
- Industry validation campaigns (for example, MERGE and BFETS) are undertaken to provide a basis for earning trust in the PDR-CFD tools.
- Blind comparison exercise in 1998 (part of BFETS) – poor predictive performance led to further improvements in the PDR-CFD codes.

[Ref. 6]: Tam V, "*Once upon a time…*", FLACS User Group meeting, Bergen, May 2014.



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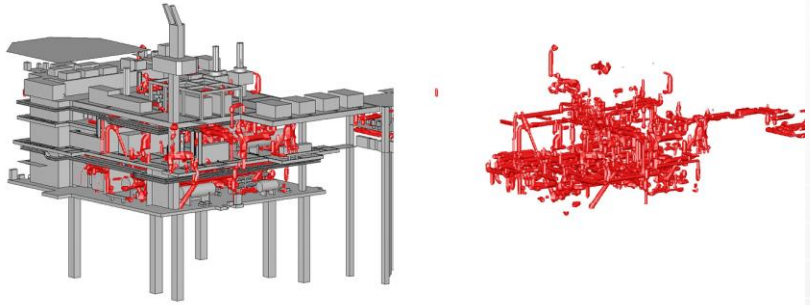
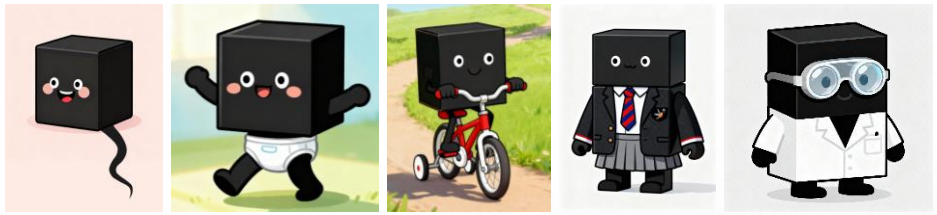
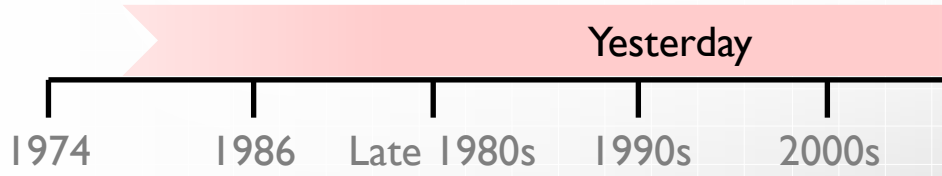
- **2000s**: PDR approach starts to mature:
  - Research into explosions with other fuels, such as hydrogen.
  - Development of the PDR approach on an unstructured mesh.
  - Fluid–structure interaction – direct coupling with FEA.



[Ref. 7]: ACE Method (2004) – PDR implementation on an unstructured mesh (http://www.abercus.com/SoftwareSolutions_ACEMethod.aspx).





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  - Research into explosions with other fuels, such as hydrogen.
  - Development of the PDR approach on an unstructured mesh.
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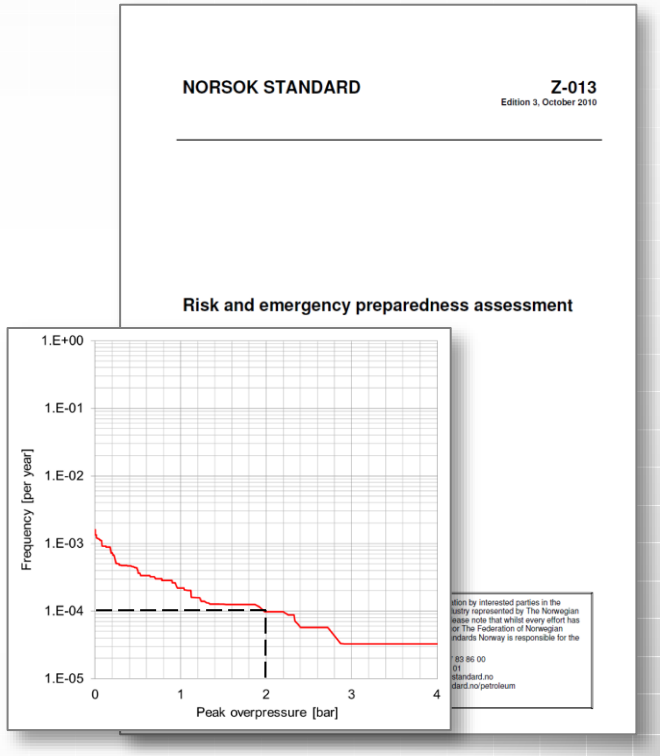
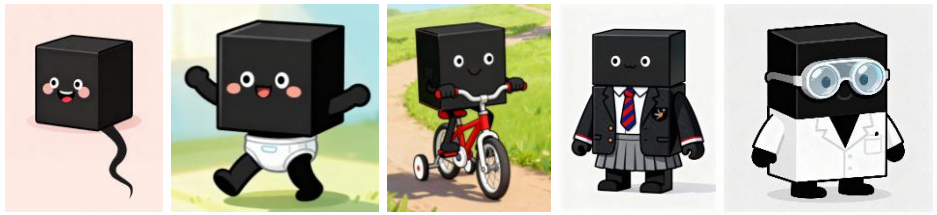
  - Increasing commercial use (following Piper Alpha).
  - NORSOK Z013 for CFD-based probabilistic ERA.



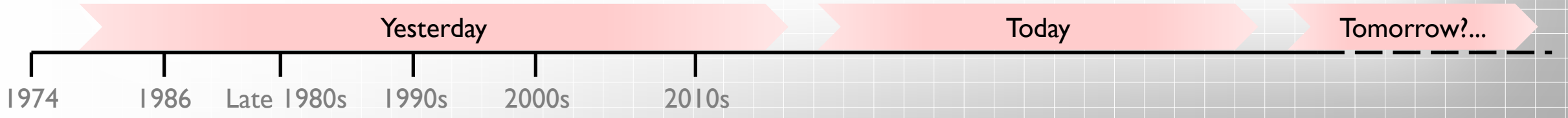


Yesterday | Today | Tomorrow?...

1974 1986 Late 1980s 1990s 2000s

Yesterday

- **2010s**: PDR approach continues to mature:
  - Growing user base of commercial PDR codes.
  - High-Performance Computing (HPC).
  - Automation/Simulation Data Management (SDM) implemented by advanced users (users develop integrated eco-system around PDR-CFD tools).
  - Open-source codes and academic in-house codes.



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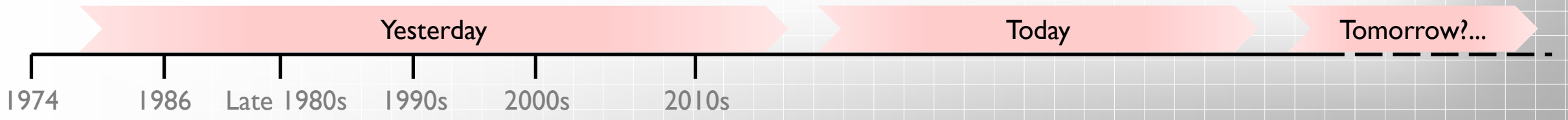
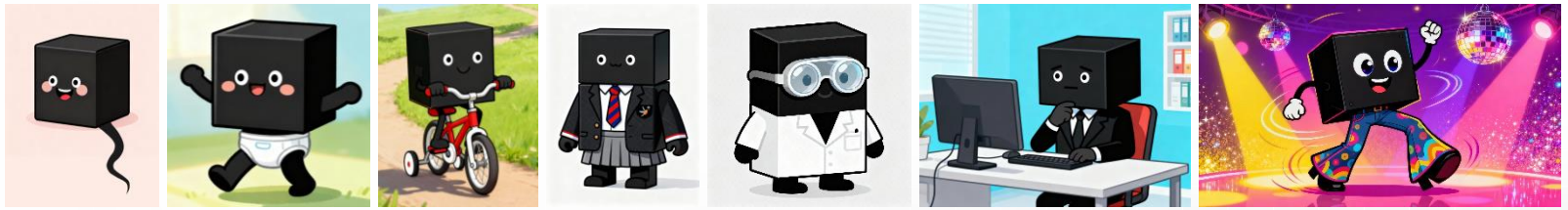
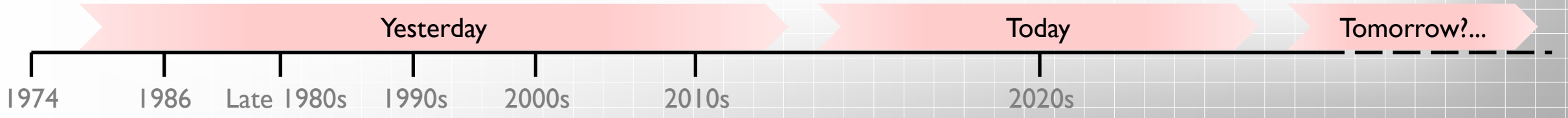
- New validation campaigns:
  - HySea.
  - MEASURE.
  - DOWSES.
  - FM Global chamber…
- Comparisons with existing data:
  - Sandia FLAME.
  - Fraunhofer LANE.
  - RUT facility
  - BakerRisk tests…
- Incident investigations:
  - Buncefield.
  - Jaipur.
  - Kjorbo.
  - …



Today

- **2020s**: Democratisation:
  - Direct CAD import.
  - Shift away from boxes/cylinders towards *generalised mesh objects*.
  - *"With* [our PDR-CFD software], *you get results you can trust to control risks and improve safety"*.





Today

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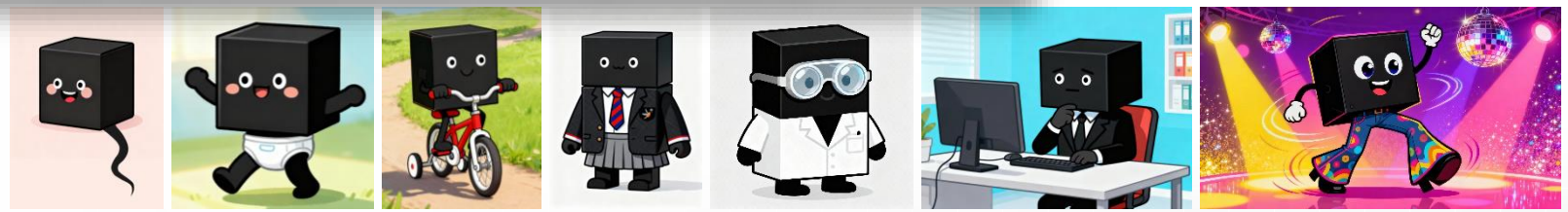

Yesterday → Today → Tomorrow?...

[Ref. 8]: LinkedIn post: https://www.linkedin.com/posts/gexcon-as_processsafety-consequencemodelling-flacs-activity-7302633161547513858-_Dyu/?utm_source=share&utm_medium=member_desktop&rcm=ACoAAATcQoQBItzQPCgxkhqoy2vOHUZLIZrJO3I

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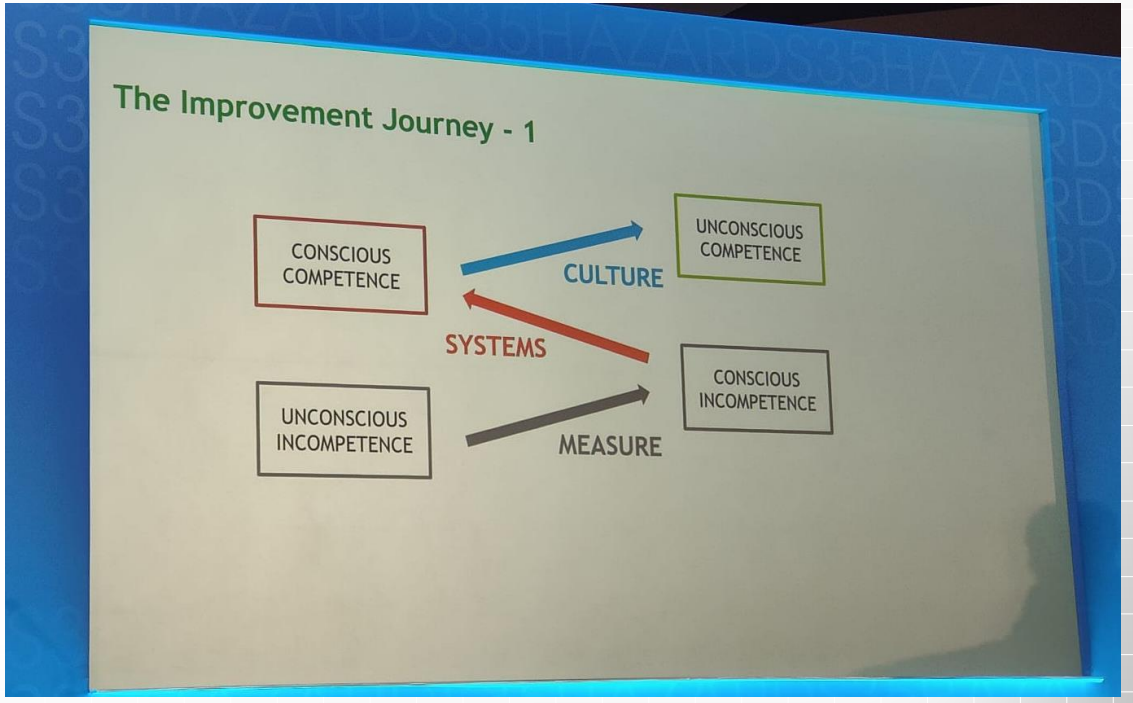

[Ref. 9]: De Phillips, Berliner and Cribbin (1960), "*Meaning of learning and knowledge*". In Management of Training Programs. Homewood, IL: Richard D. Irwin. p. 69.

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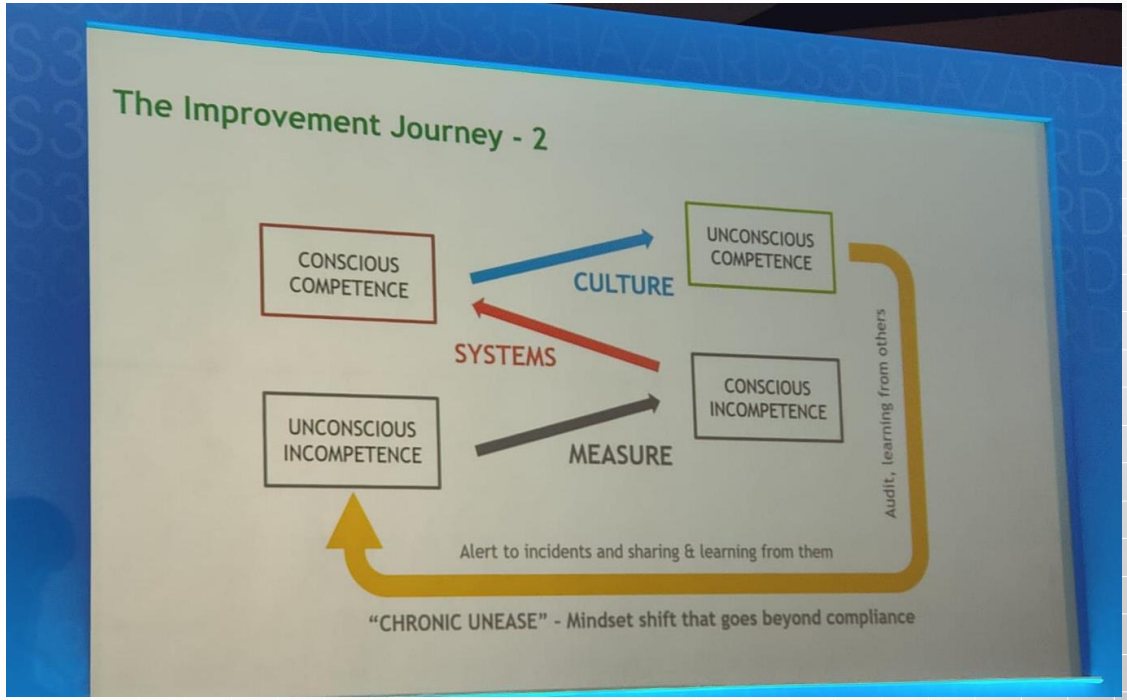

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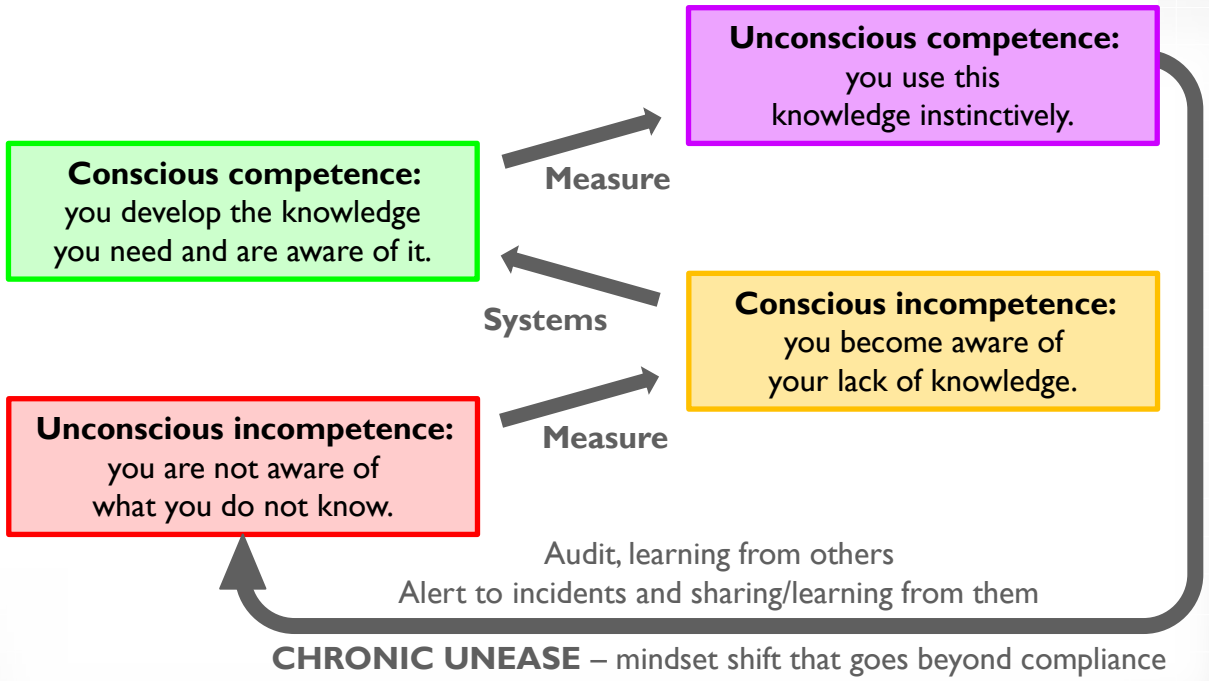

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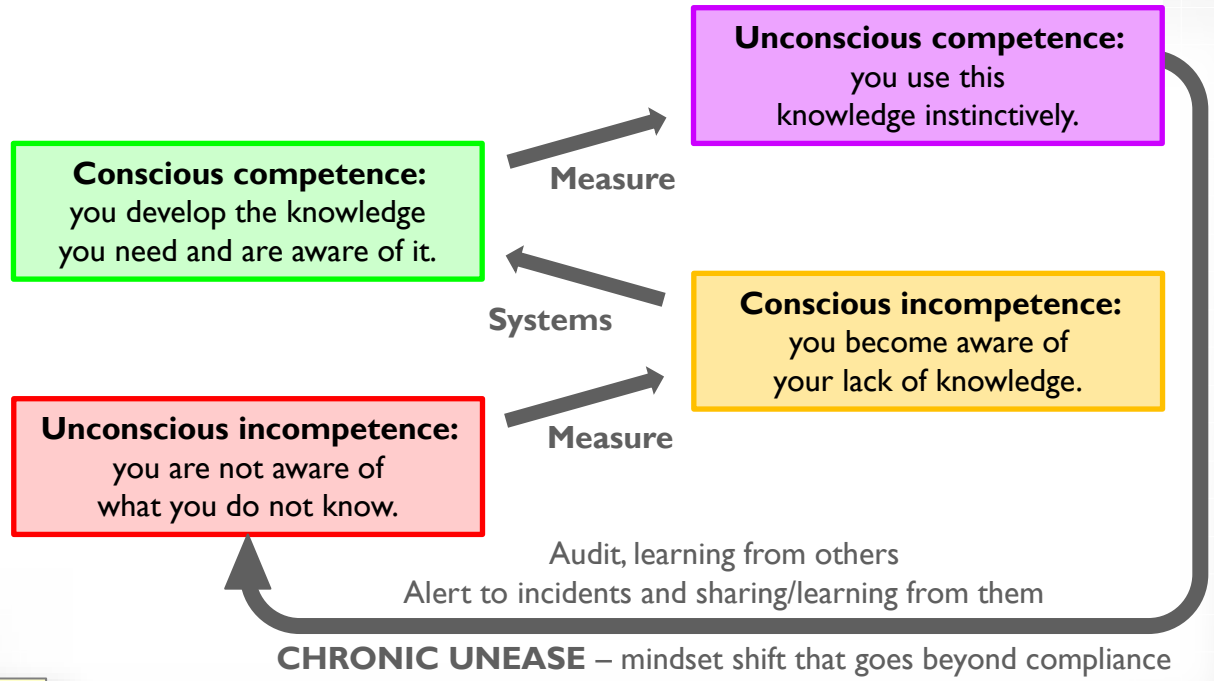

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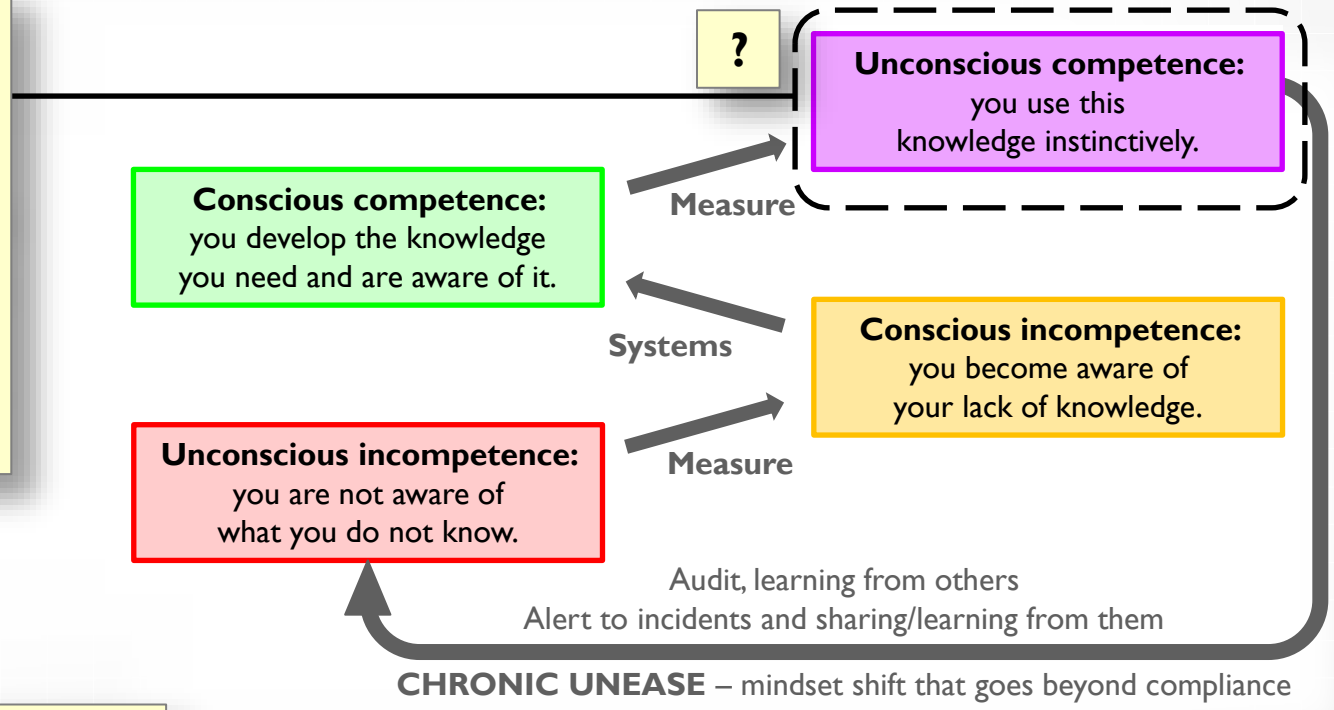

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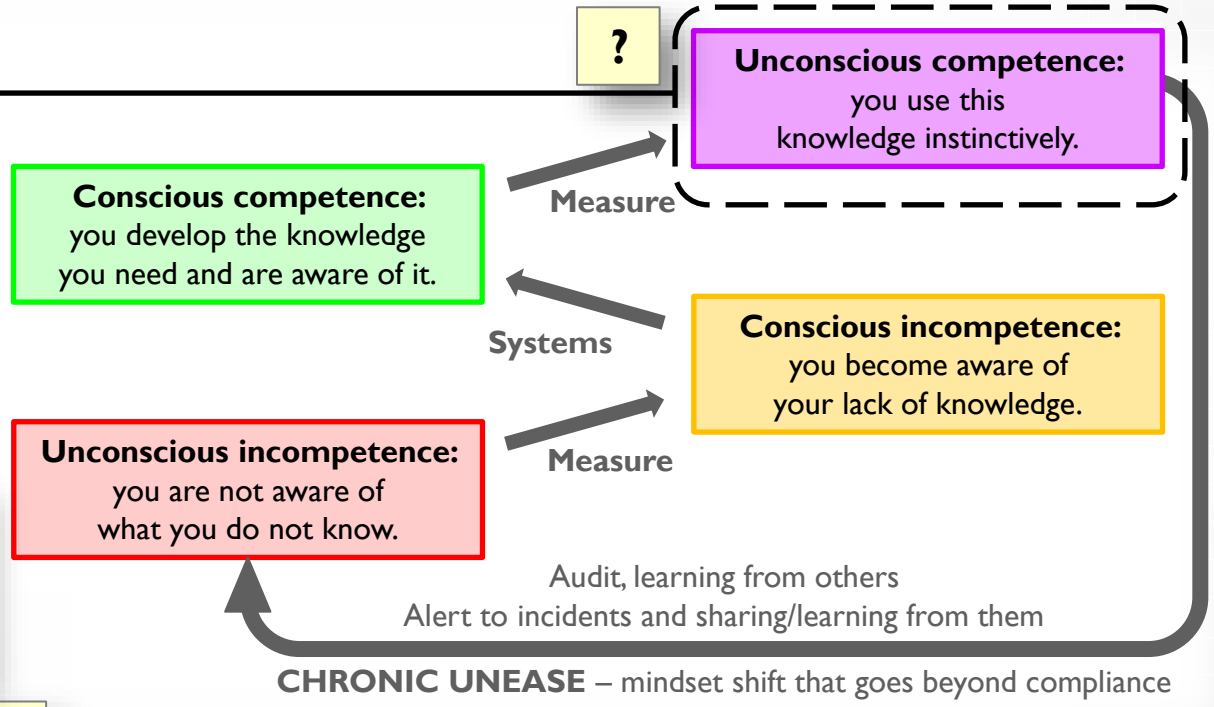

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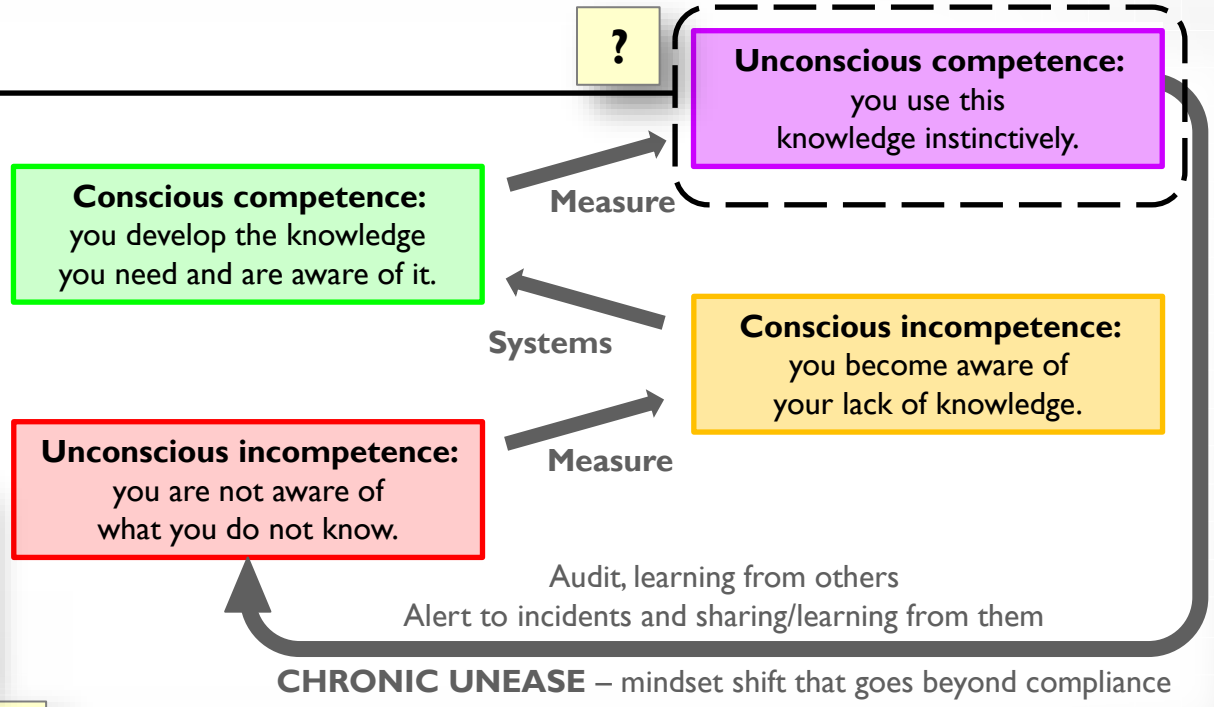

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VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- From the validation case of interest, a conceptual model is abstracted.
- From the conceptual model stem two branches:
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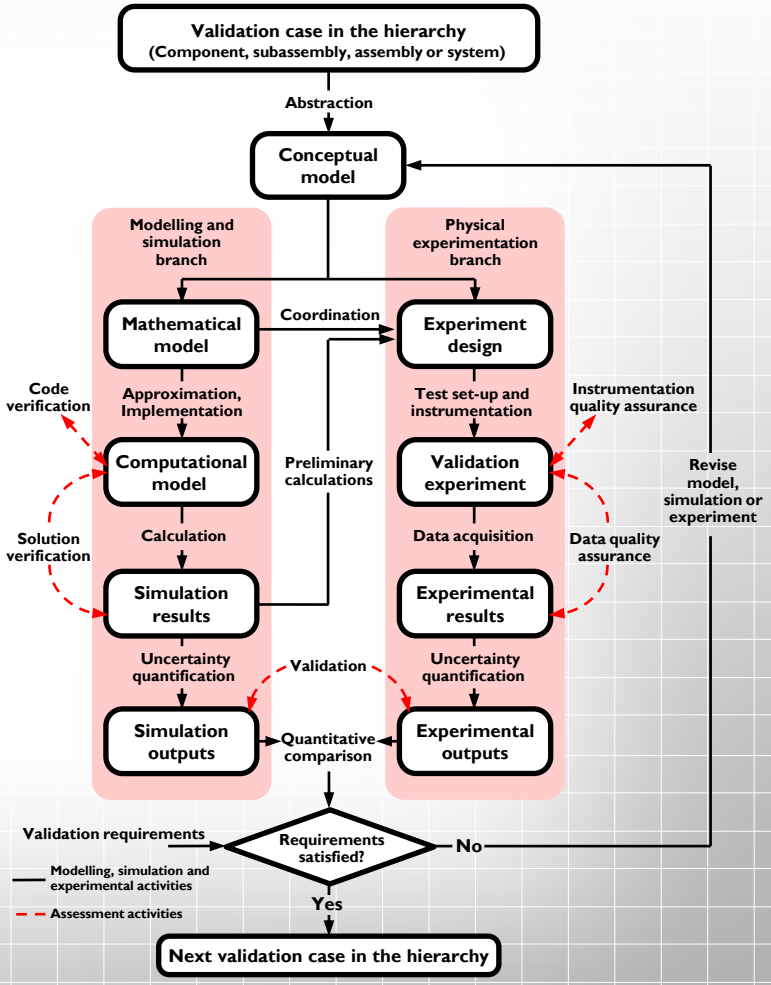
  - The physical experimentation branch comprises quality assurance and uncertainty quantification activities.
- At the bottom there is a quantitative comparison between the outputs from each branch – this is validation.



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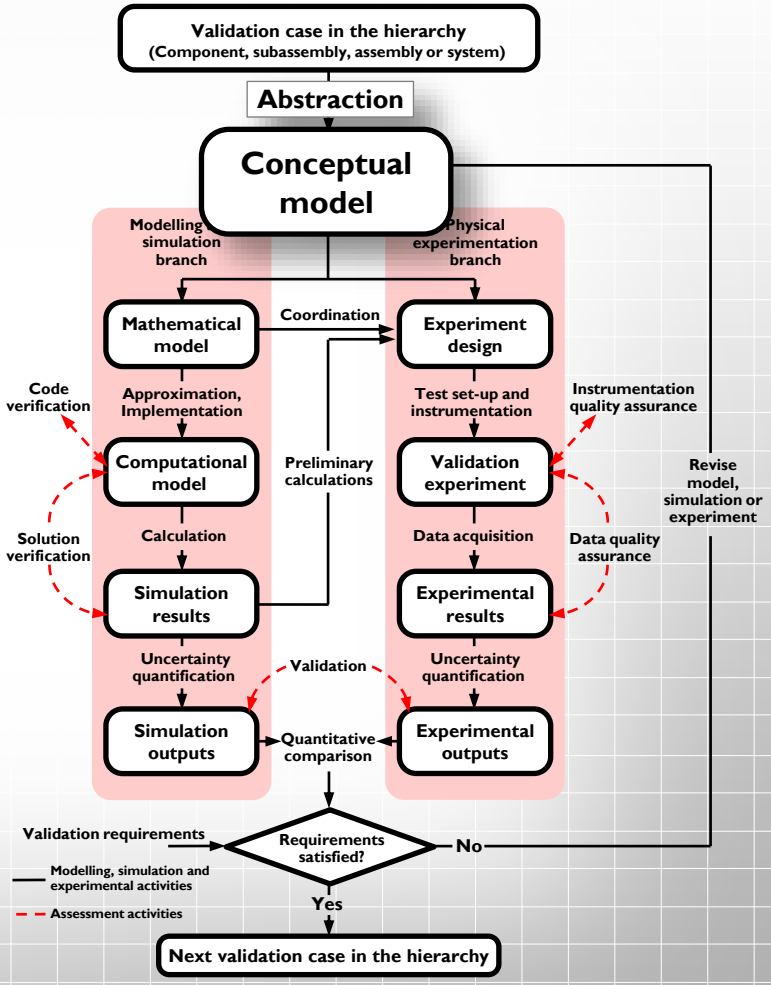

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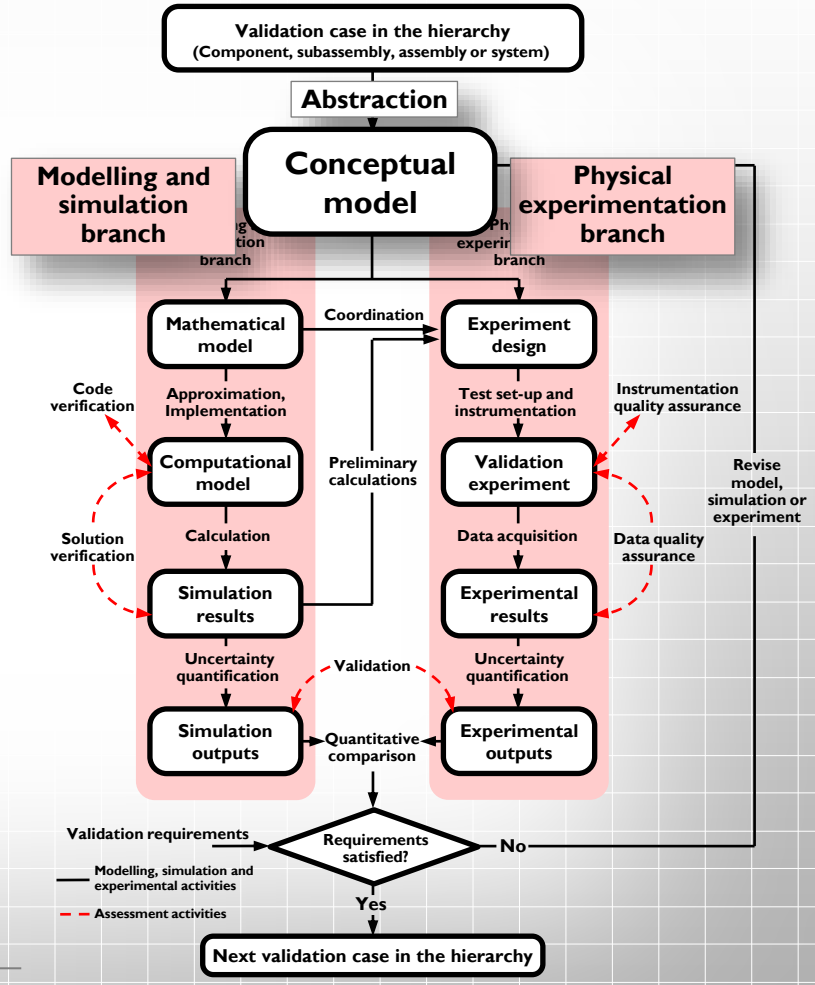

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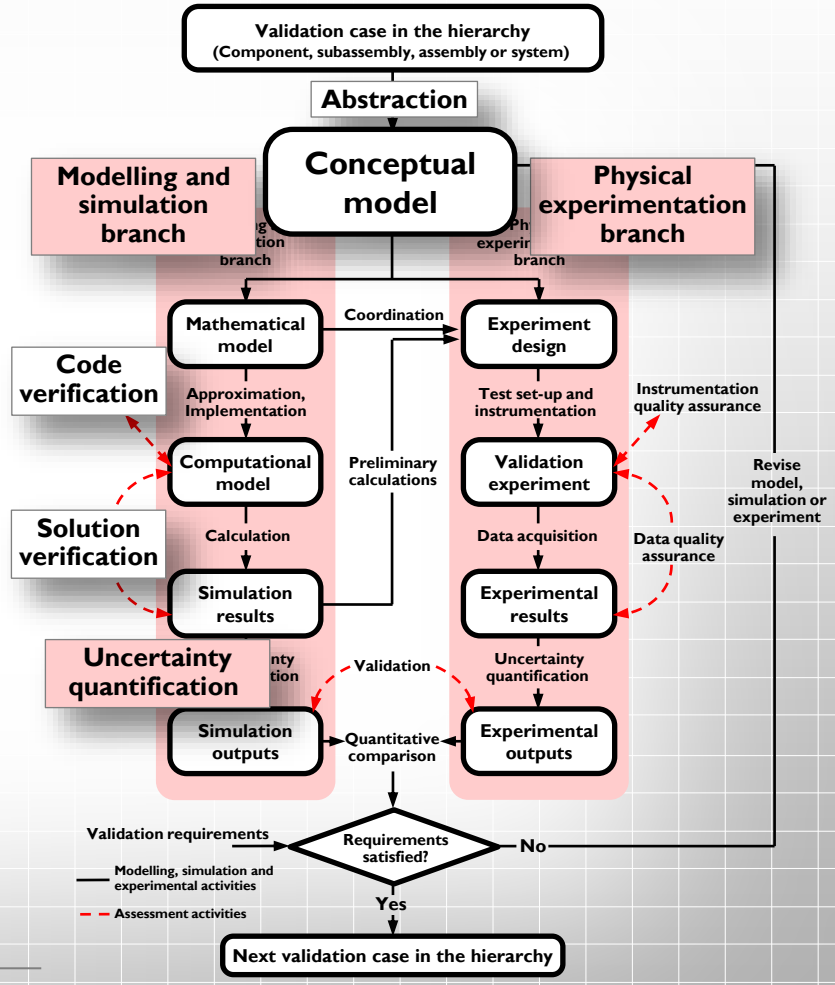

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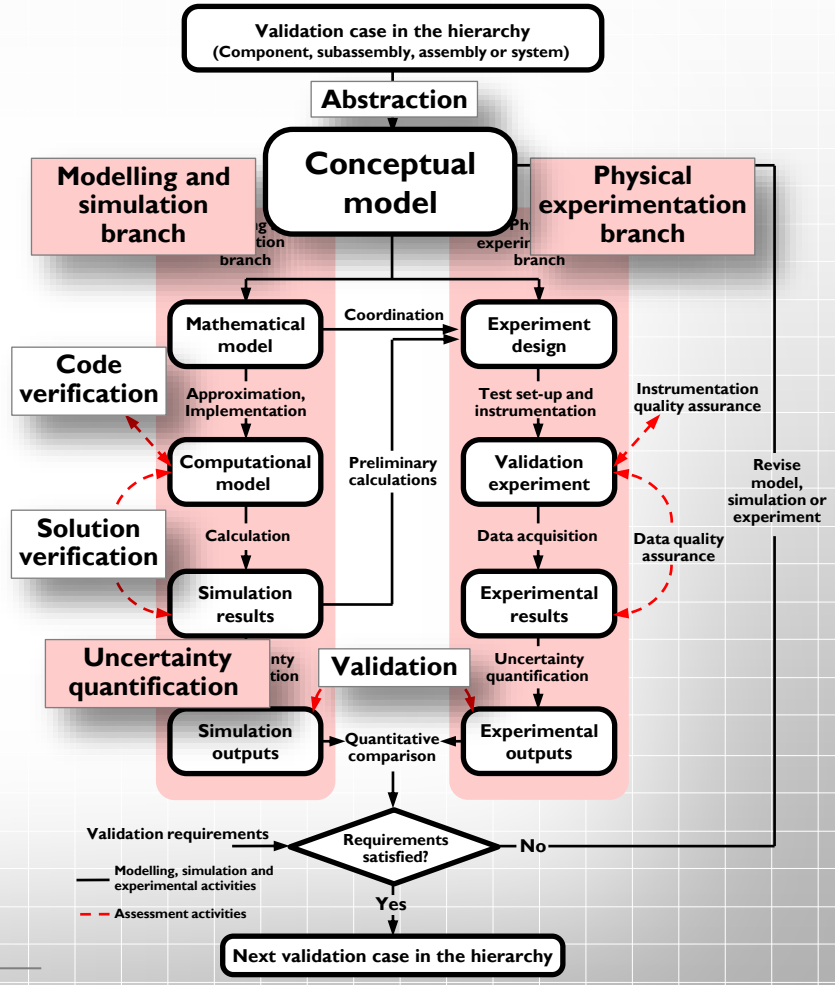

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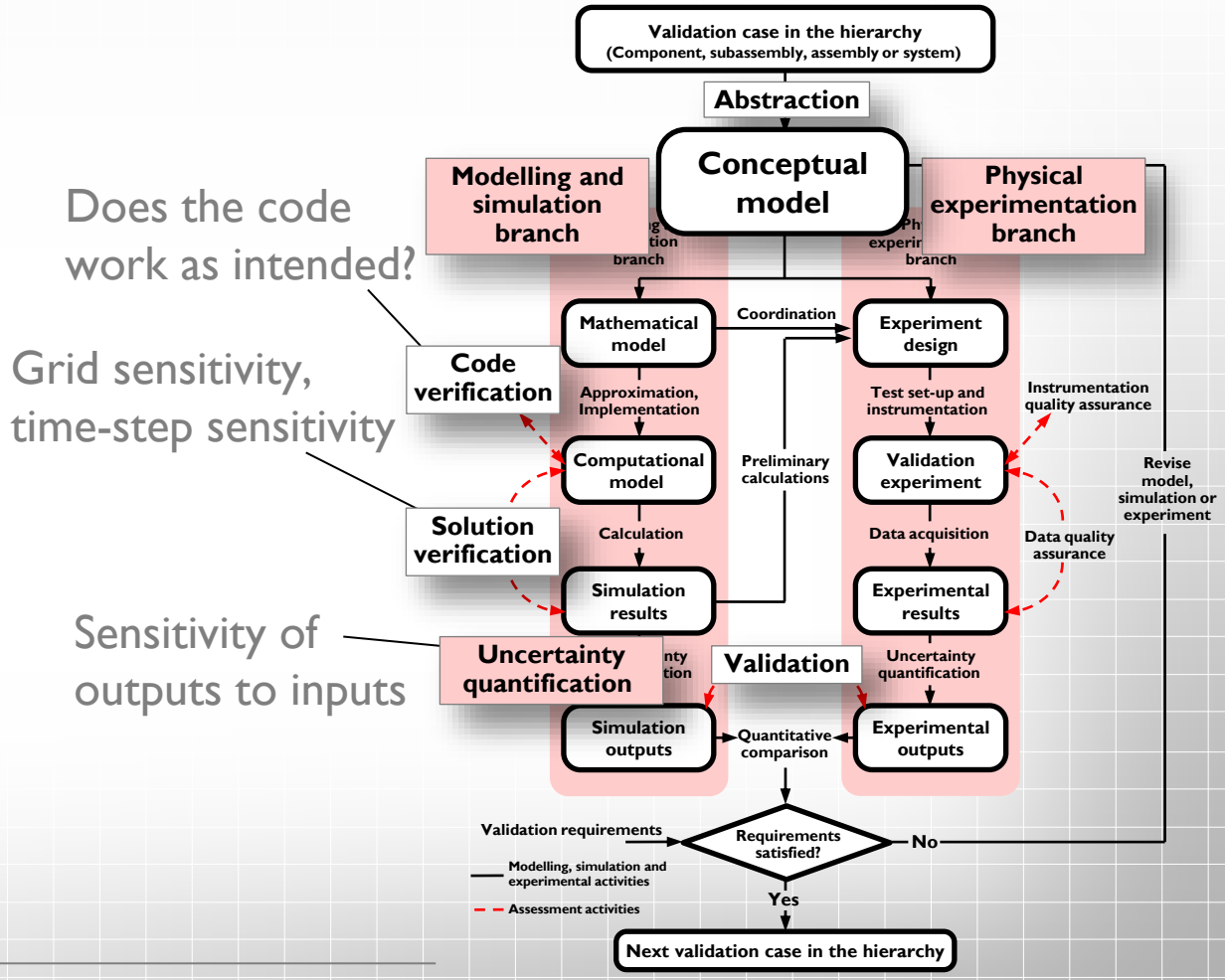

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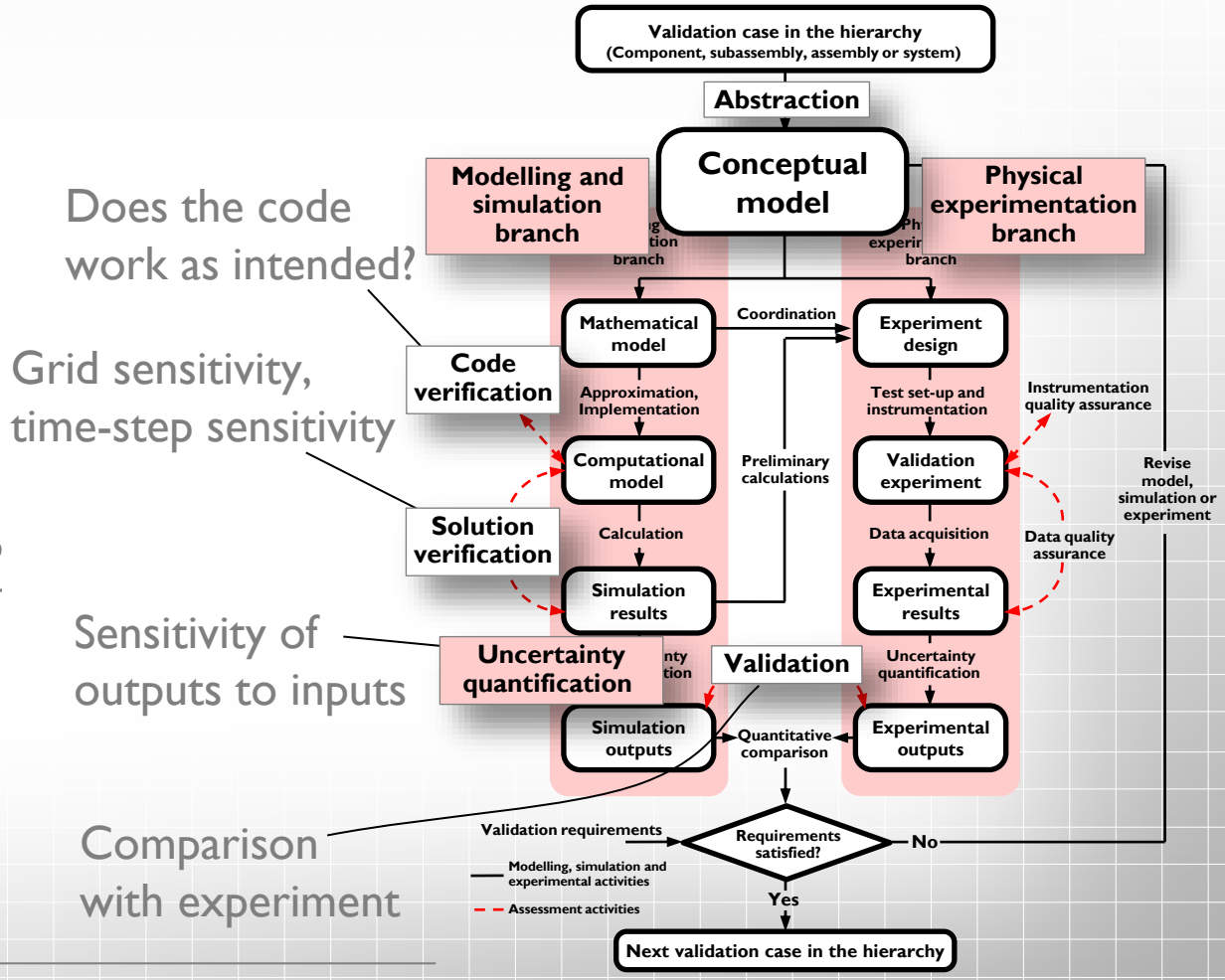
VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- **Verification** is the realm of mathematics and addresses the question: *are the underlying equations being solved correctly?*
- **Validation** is the realm of physics and addresses the question: *are the underlying equations being solved the correct equations?*



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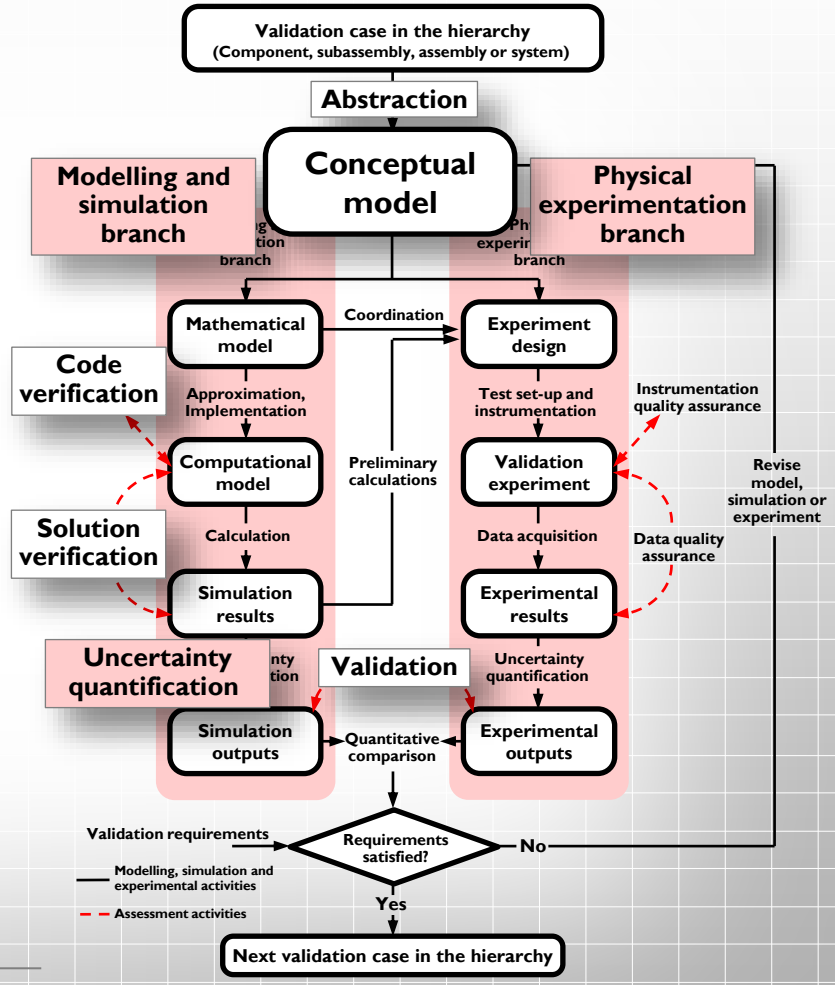
  - Solution verification?
  - Simulation UQ?
  - Validation?



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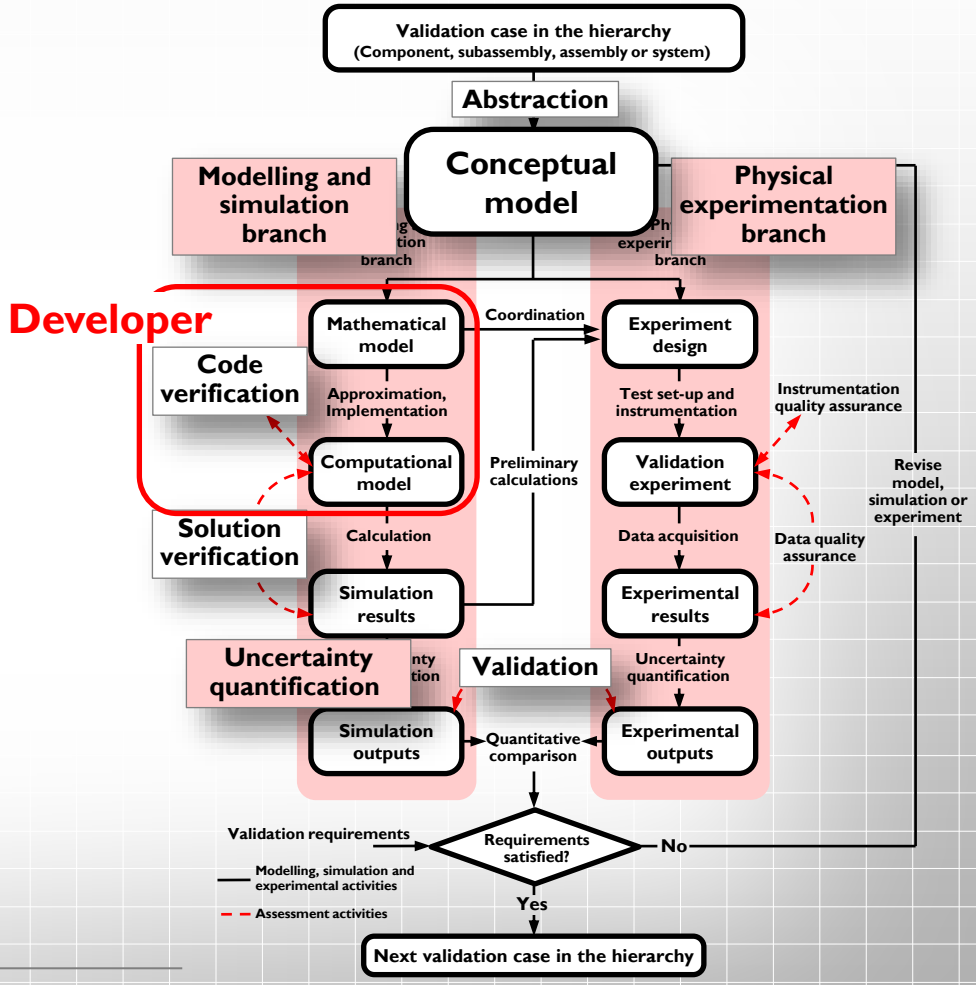

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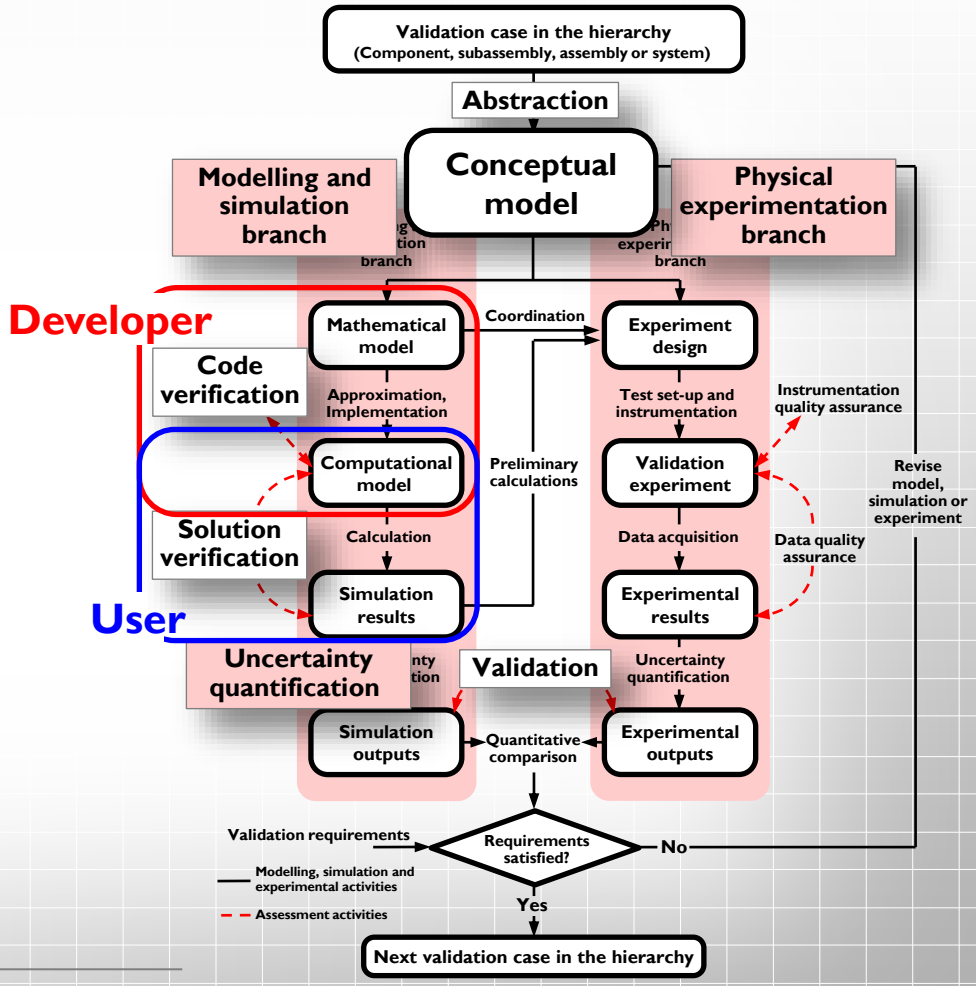
  - Simulation UQ?
  - Validation?

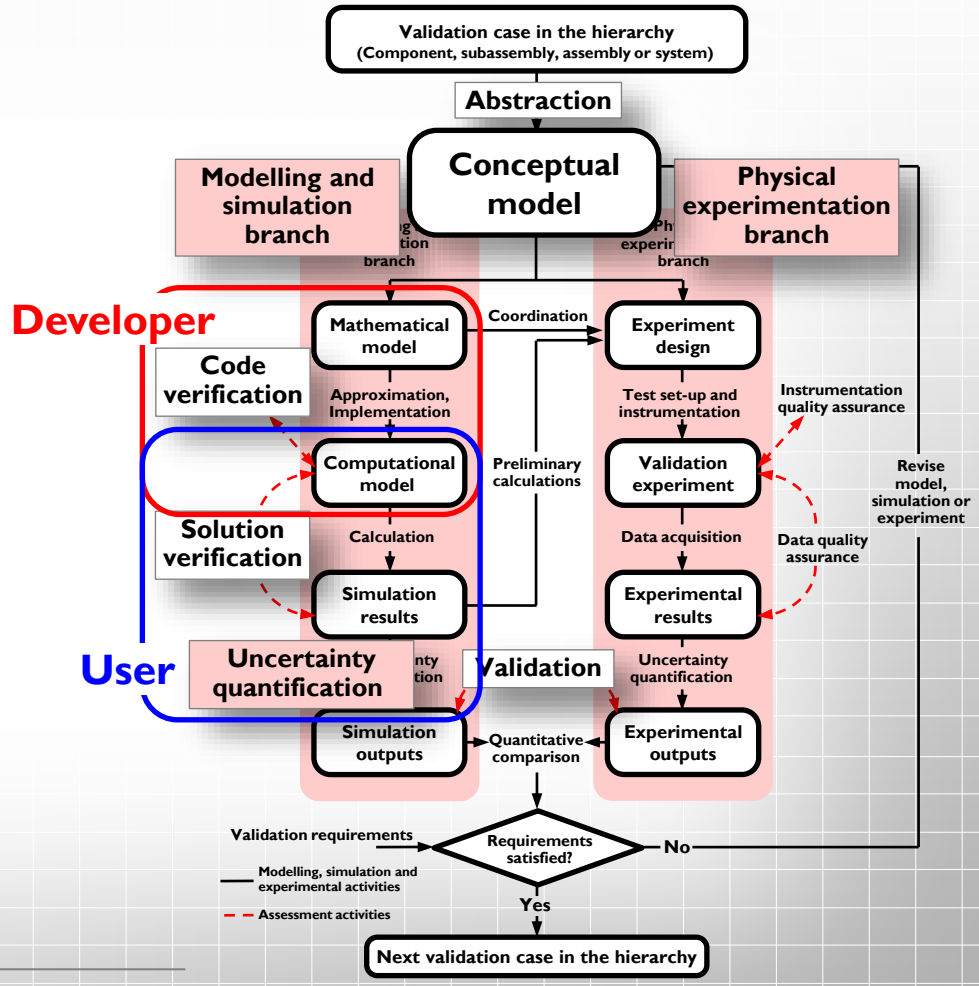


[Ref. 12]: Standard for Verification and Validation in Computational Solid Mechanics, ASME V&V 10:2019

VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- Who is responsible for VVUQ?
  - Code verification? _____ **Developer**
  - Solution verification? _____ **User**
  - Simulation UQ? _____ **User**
  - Validation?

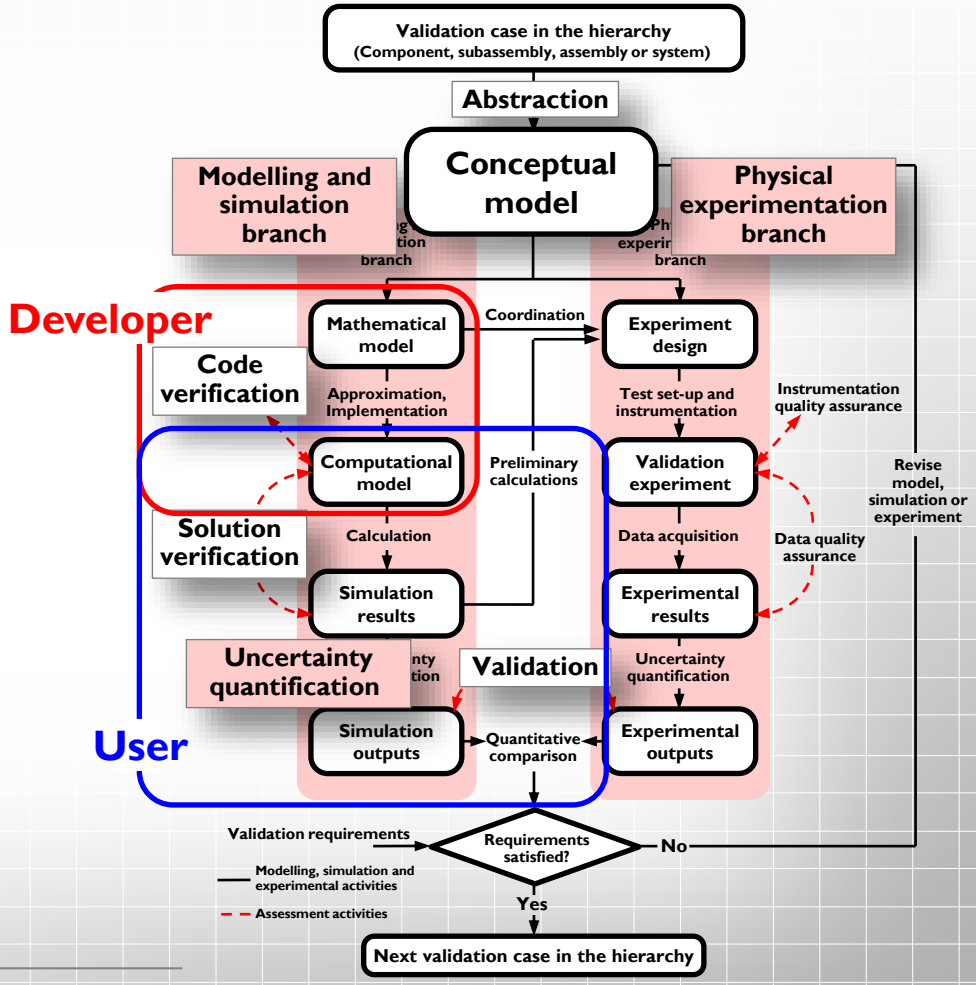


[Ref. 12]: Standard for Verification and Validation in Computational Solid Mechanics, ASME V&V 10:2019

VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- Who is responsible for VVUQ?
  - Code verification? _____ **Developer**
  - Solution verification? _____ **User**
  - Simulation UQ? _____ **User**
  - Validation? _____ **User**

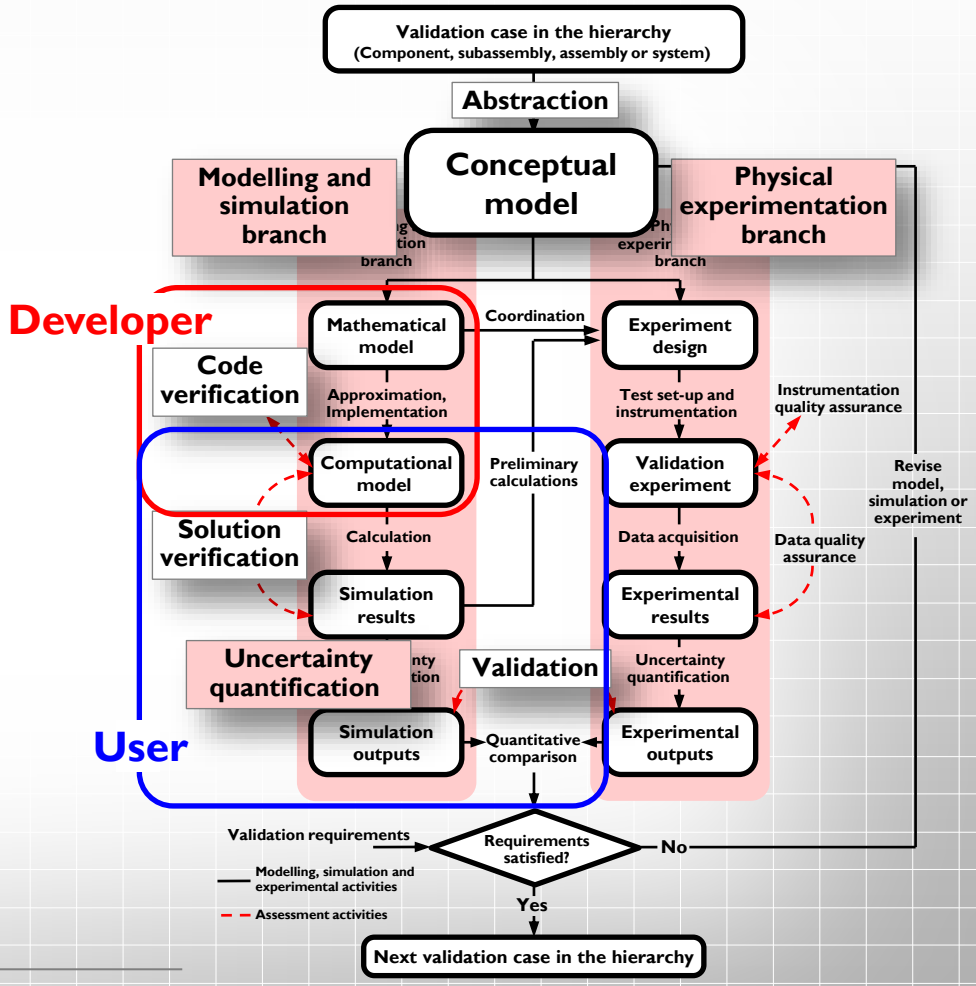


[Ref. 12]: Standard for Verification and Validation in Computational Solid Mechanics, ASME V&V 10:2019

VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- Who is responsible for VVUQ?
  - Code verification? _____ **Developer + User?**
  - Solution verification? _____ **User**
  - Simulation UQ? _____ **User**
  - Validation? _____ **User**

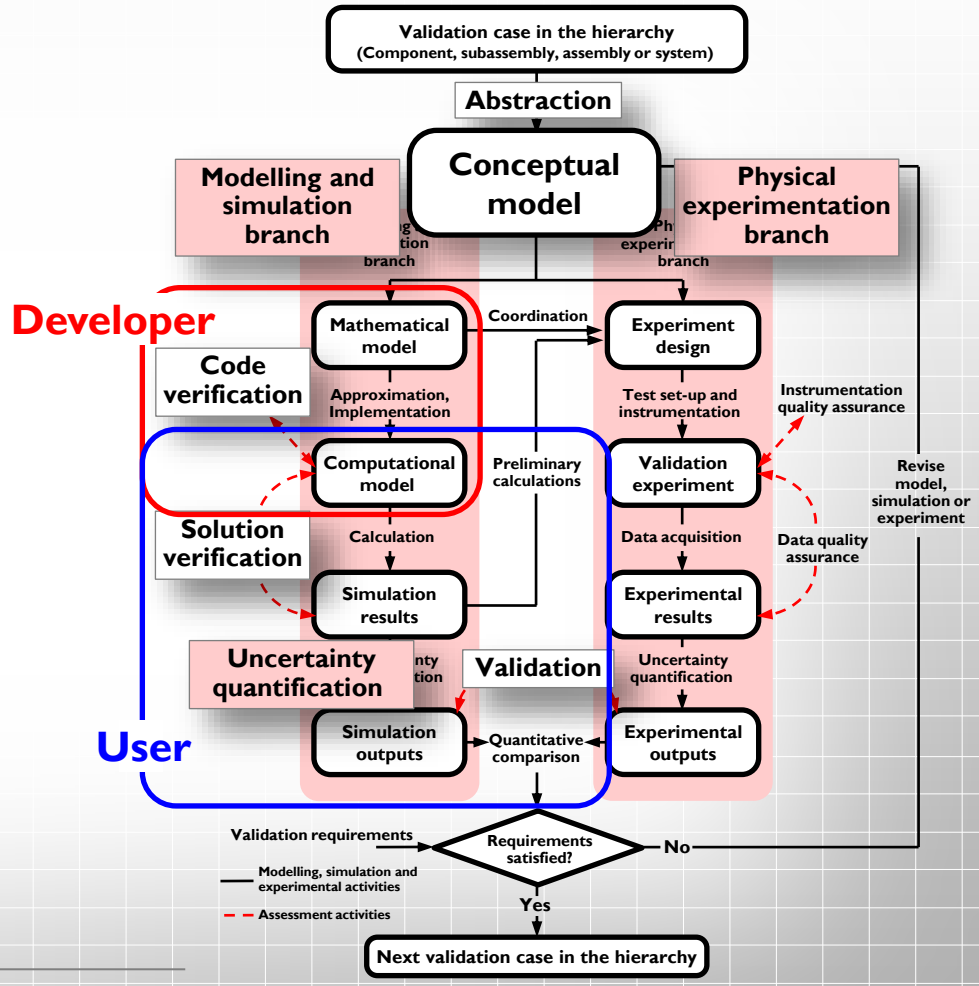


[Ref. 12]: Standard for Verification and Validation in Computational Solid Mechanics, ASME V&V 10:2019

VVUQ framework – NAFEMS/ASME

ASME V&V process diagram

- If a developer asserts that its PDR-CFD code is validated, this strictly refers to the validation of its own internal workflows.
- Unless the code *owns* the entire left-hand branch, such that a user cannot interfere with it, **validation is not of the code, but of the combination of code plus user/workflow.**
- Users should undertake validation for themselves, to understand how their own predictions compare to experiment…



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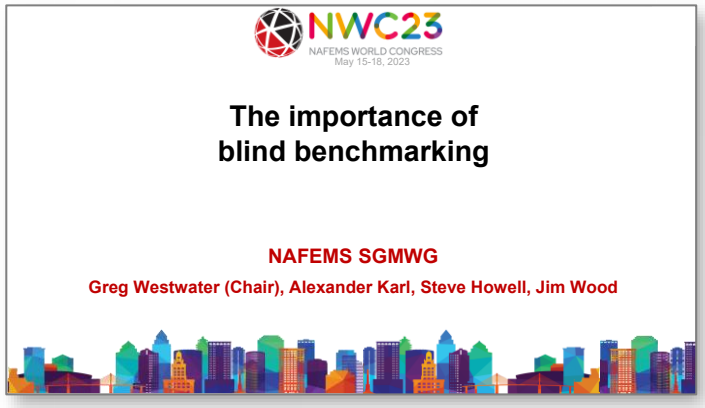
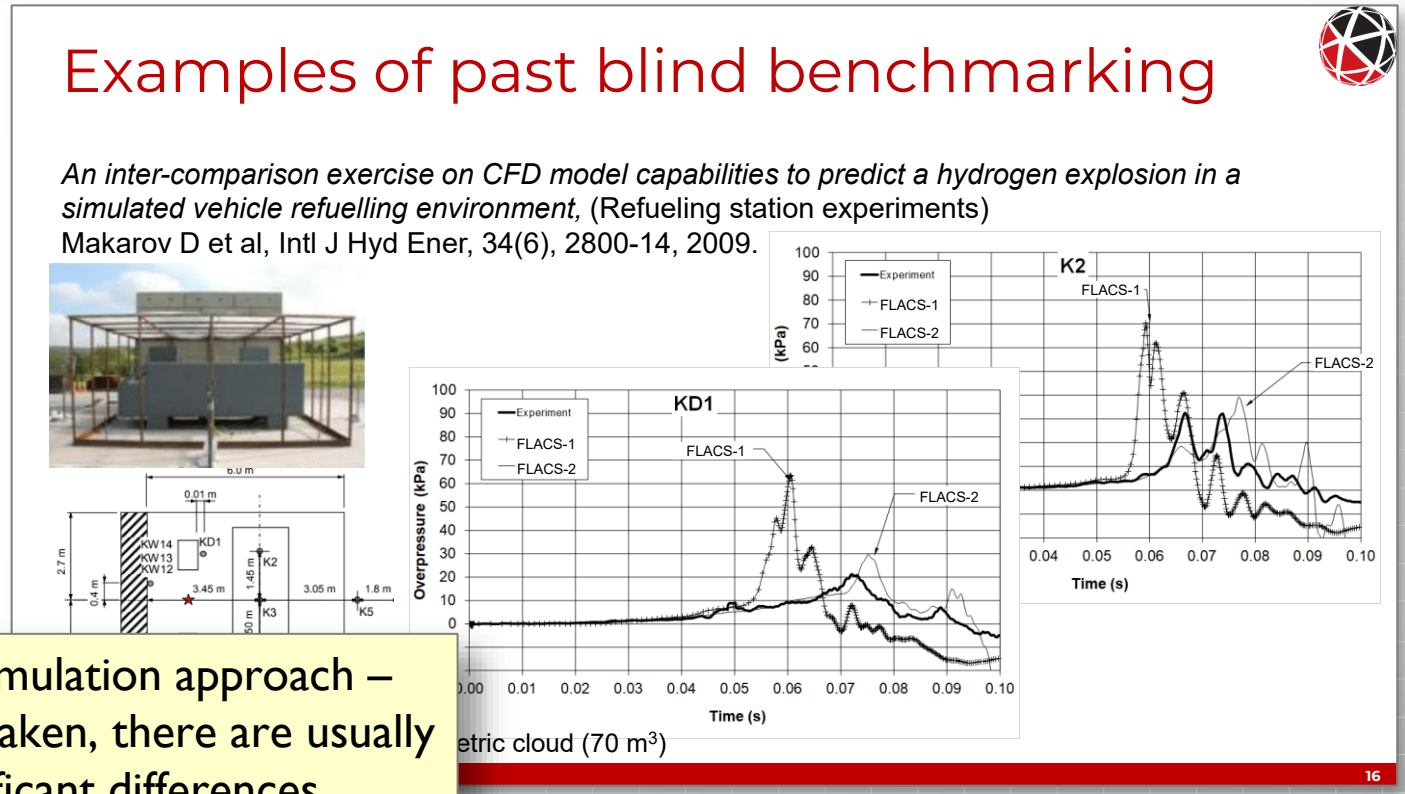
VVUQ framework – NAFEMS/ASME

Blind benchmarking





Blind benchmarking is the true test of any simulation approach – and whenever blind comparisons are undertaken, there are usually differences between participants, often significant differences.

[Ref. 13]: Westwater G, Karl A, Howell S and Wood J, "*The importance of blind benchmarking*", NAFEMS World Congress 2023.

VVUQ framework – NAFEMS/ASME

Blind benchmarking

NWC23
NAFEMS WORLD CONGRESS
May 15-18, 2023

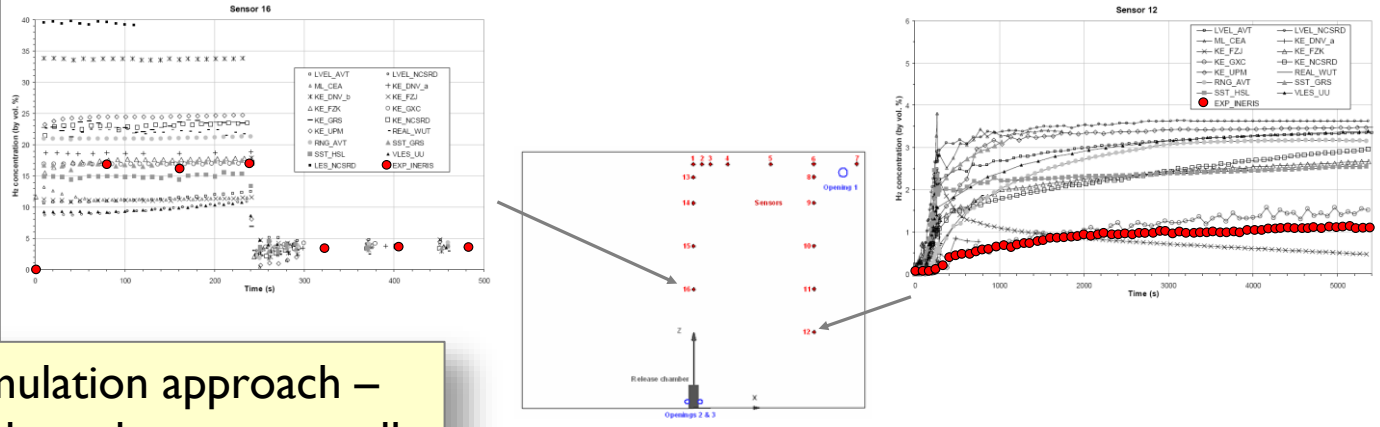
The importance of blind benchmarking

NAFEMS SGMWG

Greg Westwater (Chair), Alexander Karl, Steve Howell, Jim Wood

Examples of past blind benchmarking

An inter-comparison exercise on the capabilities of CFD models to predict the short and long term distribution and mixing of hydrogen in a garage, (INERIS Garage release experiments)
Venetsanos AG et al, Intl J Hyd Ener, 34(14), 5912-23, 2009.



s) in a 80 m³ room

15

Blind benchmarking is the true test of any simulation approach – and whenever blind comparisons are undertaken, there are usually differences between participants, often significant differences.

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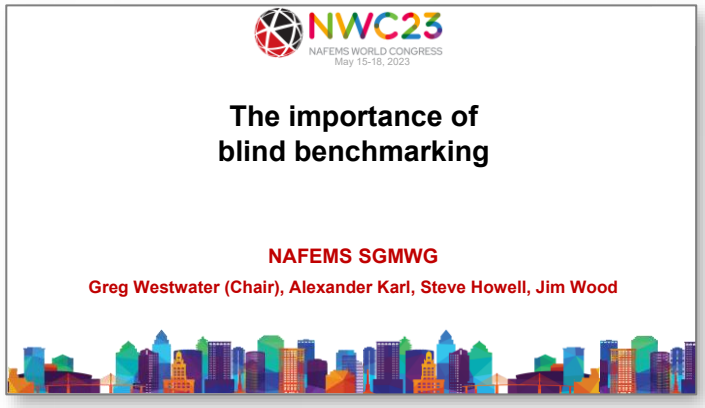
VVUQ framework – NAFEMS/ASME

Blind benchmarking



Examples of past blind benchmarking

[Jimwd-25] *Round-Robin Study of a-priori Modelling Prediction of the Dalmarnock Fire Test One*, G. Rein et al, Fire Safety Journal 44 (4), 590-602, 2009.

(Presentation to SGMWG/CFDWG, 27 February 2023)

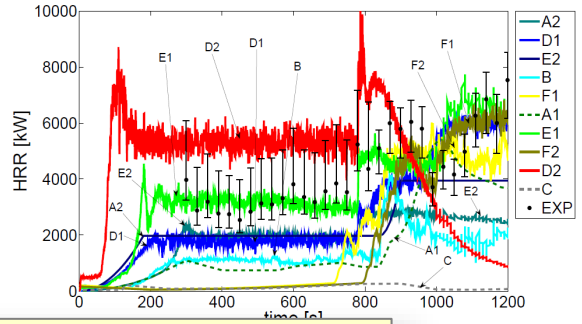


Table 2: Comparison of simulated time to flashover and maximum average temperature in the smoke layer of the main compartment with experimental data.

Simulation	Time to Flashover[s]	Maximum Average Smoke Layer Temperature [°C]
A1	850	790
A2	290	500
B	840	690
C	no flashover	200
D1	200	720
D2	80	1150
E1	180	900
E2	180	610
F1	720	590
F2	850	720
Experimental	300	750

https://era.ed.ac.uk/bitstream/handle/1842/2704/Rein_RoundRobinModelling_FSJ09_preprint.pdf;sequence=1

13

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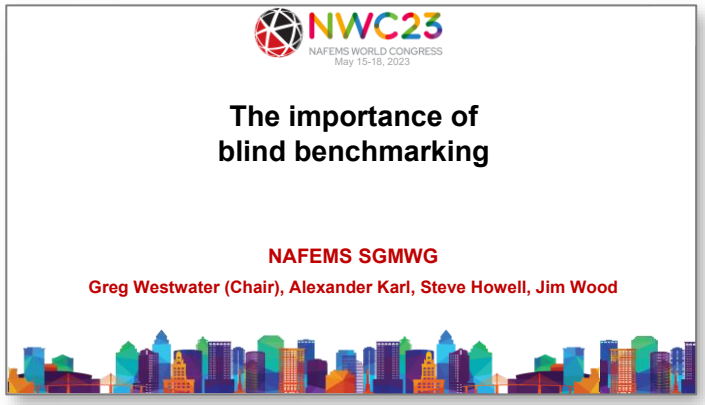
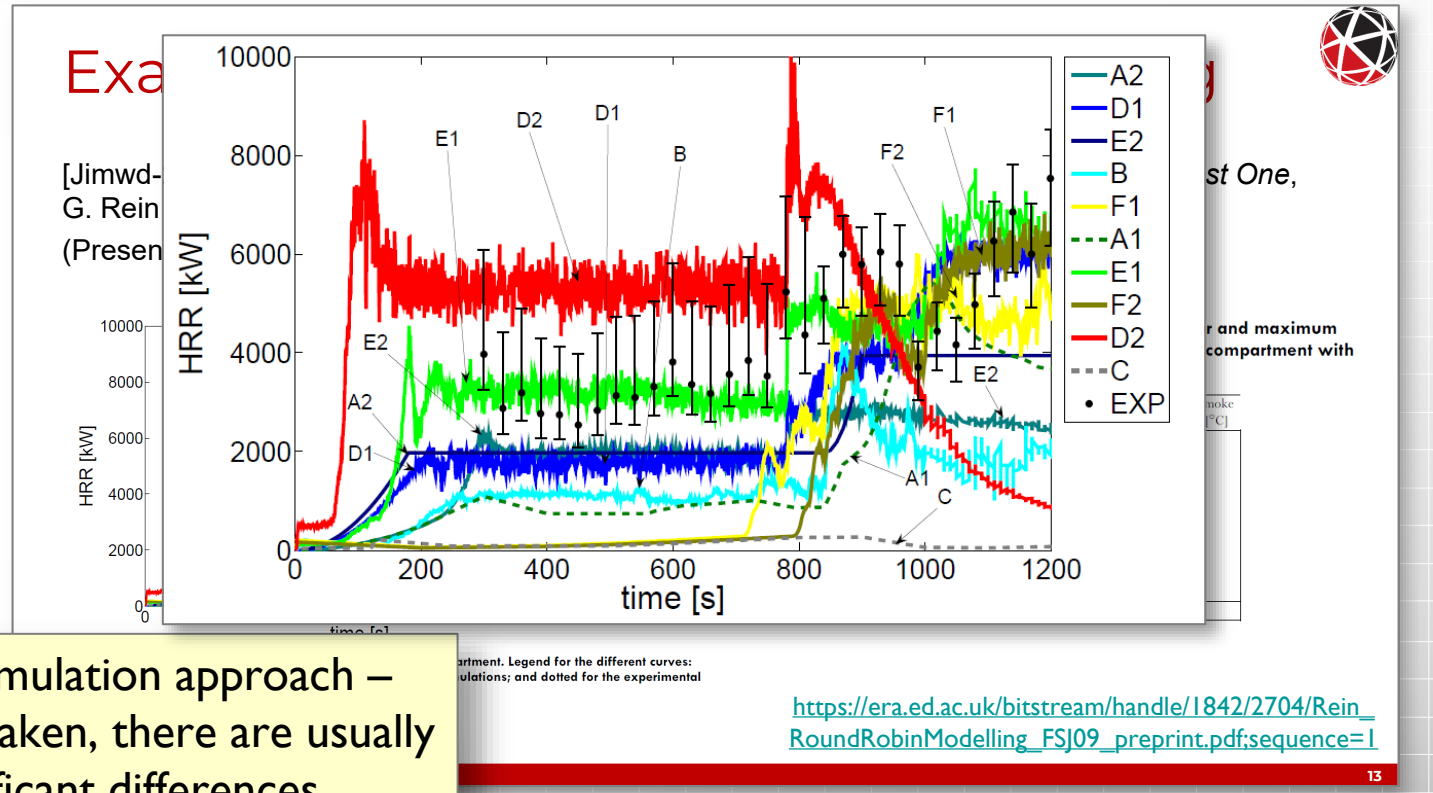
VVUQ framework – NAFEMS/ASME

Blind benchmarking





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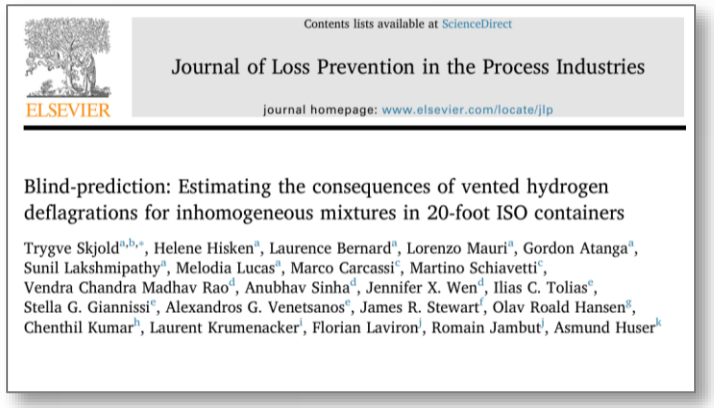
VVUQ framework – NAFEMS/ASME

Blind benchmarking



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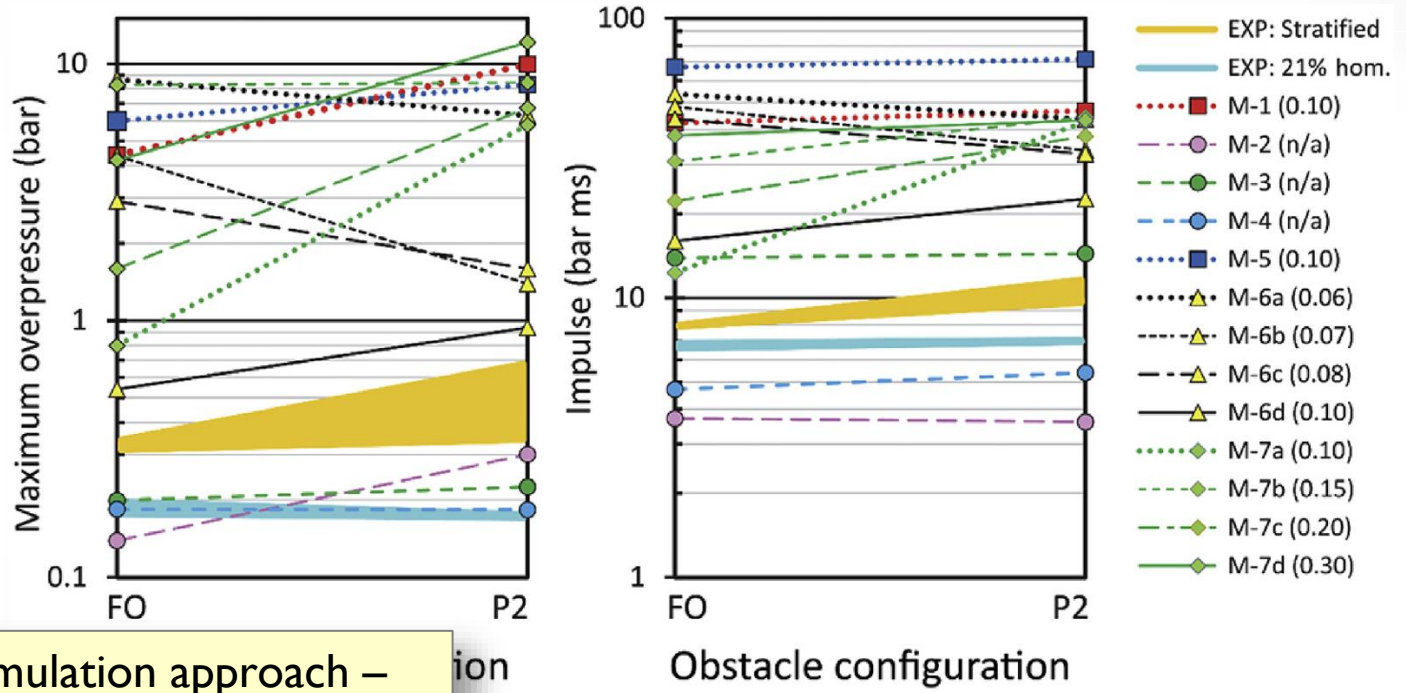
Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for inhomogeneous mixtures in 20-foot ISO containers

Trygve Skjold[a,b,*], Helene Hisken[a], Laurence Bernard[a], Lorenzo Mauri[a], Gordon Atanga[a], Sunil Lakshmipathy[a], Melodia Lucas[a], Marco Carcassi[c], Martino Schiavetti[c], Vendra Chandra Madhav Rao[d], Anubhav Sinha[d], Jennifer X. Wen[d], Ilias C. Tolias[e], Stella G. Giannissi[e], Alexandros G. Venetsanos[e], James R. Stewart[f], Olav Roald Hansen[g], Chenthil Kumar[h], Laurent Krumenacker[i], Florian Laviron[j], Romain Jambut[j], Asmund Huser[k]



Blind benchmarking is the true test of any simulation approach – and whenever blind comparisons are undertaken, there are usually differences between participants, often significant differences.

[Ref. 14]: Skjold T et al, "*Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for inhomogeneous mixtures in 20-foot ISO containers*", J. Loss Prev. Proc. Ind. 61 pp 220-236. 2019.

VVUQ framework – NAFEMS/ASME

Validation domain

- PDR-CFD may now have a 40-year track record, but the core experience is perhaps largely focussed within the offshore sector considering hydrocarbon vapour cloud explosions within large platforms.
- There is now increasing interest in new applications – hydrogen, renewables, battery energy storage, etc – which may differ from offshore platforms in terms of geometry length scales, congestion densities, and fuels, so how do we know that we can move into these new application domains with confidence?

VVUQ framework – NAFEMS/ASME

Validation domain

- PDR-CFD may now have a 40-year track record, but the core experience is perhaps largely focussed within the offshore sector considering hydrocarbon vapour cloud explosions within large platforms.
- There is now increasing interest in new applications – hydrogen, renewables, battery energy storage, etc – which may differ from offshore platforms in terms of geometry length scales, congestion densities, and fuels, so how do we know that we can move into these new application domains with confidence?
- What does a 40-year track record really mean anyway?
  - Are the people who developed the PDR-CFD code during those 40 years still there and involved?
  - Is the knowledge from those people still woven into day-to-day practice within the organisation?
  - Did we manage to resolve all of the key knowledge gaps during those 40 years in the first place?

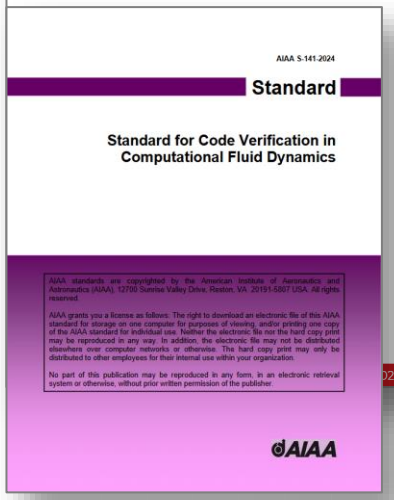
User VVUQ – code verification

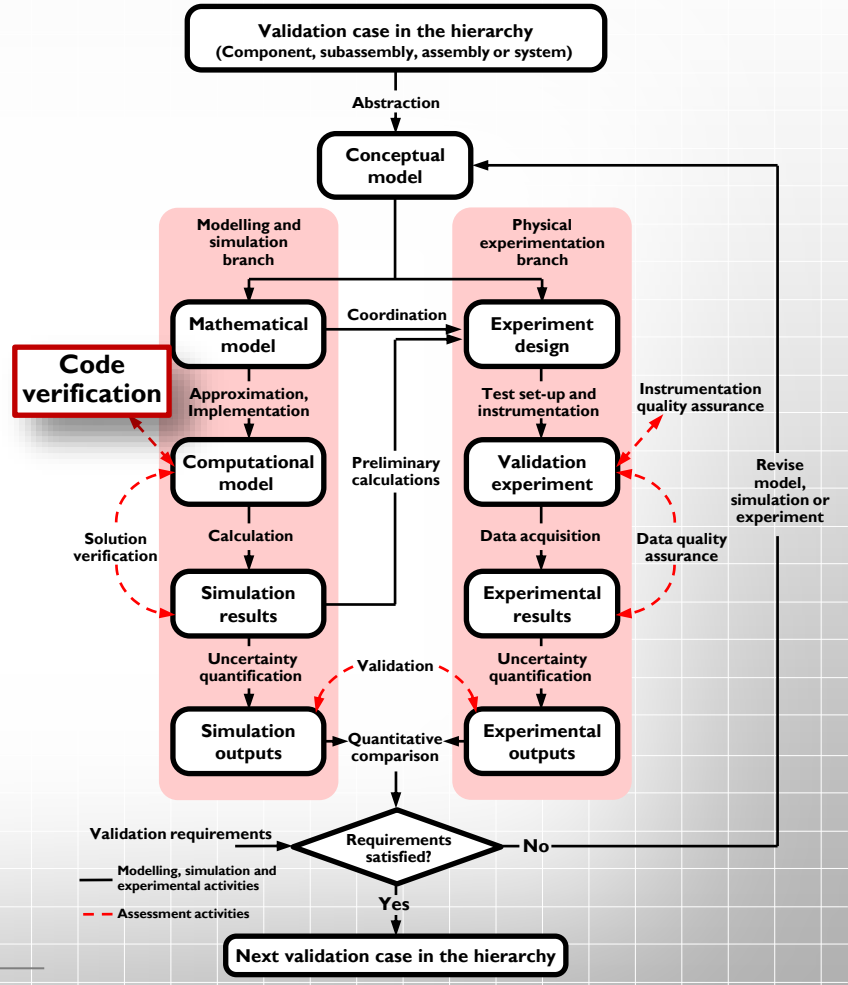
NWC25
NAFEMS WORLD CONGRESS

The New AIAA Standard for Code Verification of CFD

The importance of the observed order of accuracy, and exemplars to show the process

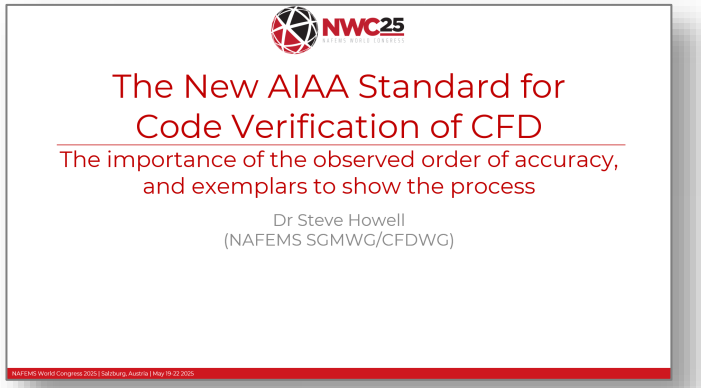
Dr Steve Howell
(NAFEMS SGMWG/CFDWG)

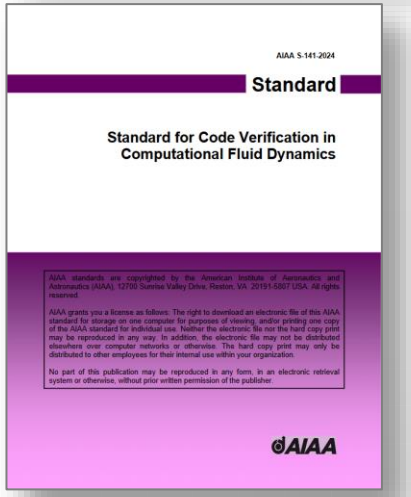




[Ref. 15]: Standard for Code Verification in Computational Fluid Dynamics, AIAA S-141:2024

User VVUQ – code verification

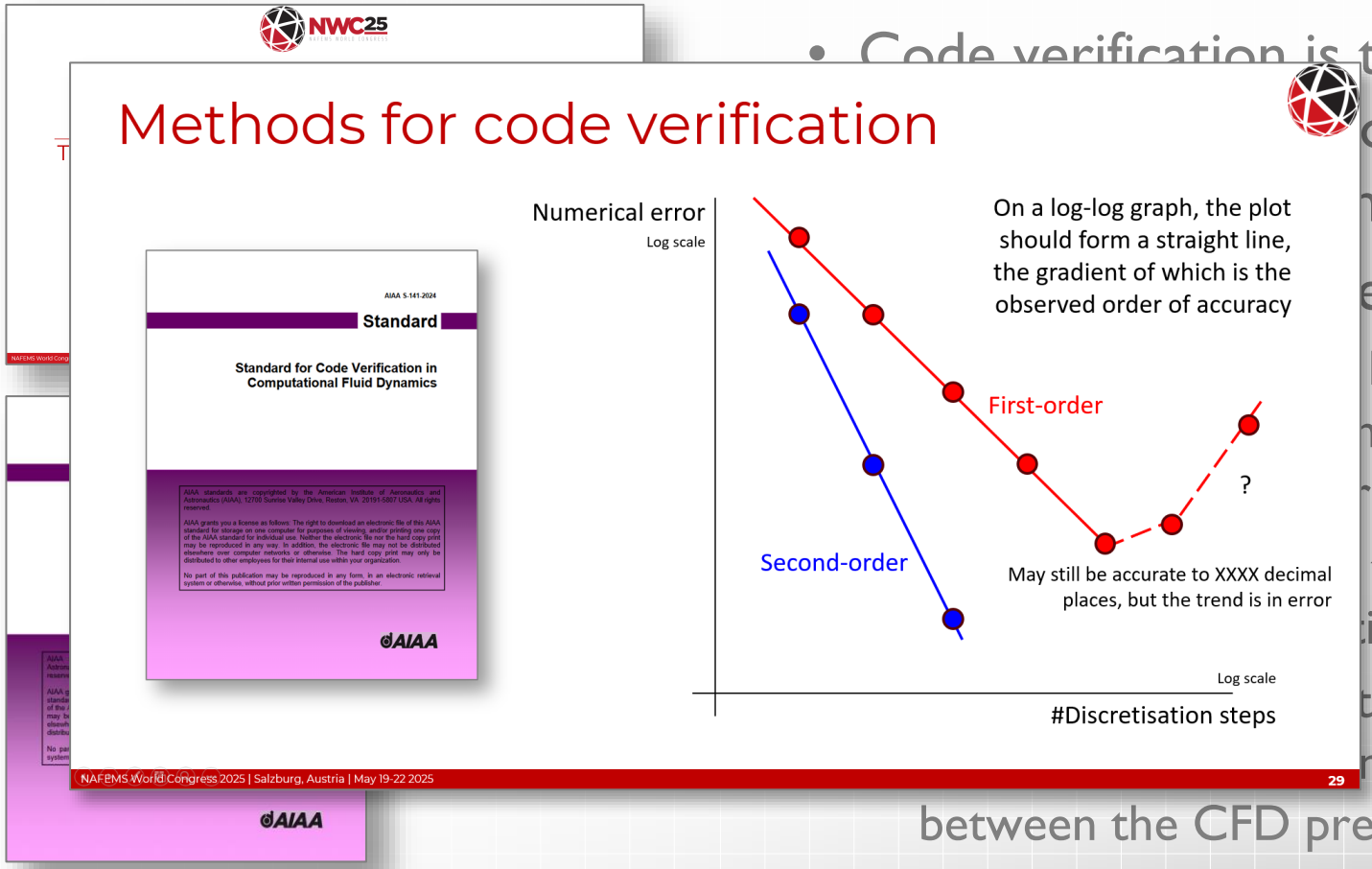




- Code verification is the process of establishing the correctness of the computational algorithms and their implementation in a CFD code.
- The standard requires:
  - Establish correctness by comparing the observed order of accuracy of the computational solutions from the code with the formal order of accuracy of the code.
  - This involves plotting the trend of the discretization error against the discretization step on a log-log graph.
  - In order to calculate the discretization error, an exact reference solution is needed – this error is the difference between the CFD prediction and the reference solution.

[Ref. 15]: Standard for Code Verification in Computational Fluid Dynamics, AIAA S-141:2024

User VVUQ – code verification



- Code verification is the process of establishing the
  omputational algorithms and
  n in a CFD code.
  es:
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  the trend of the discretization error
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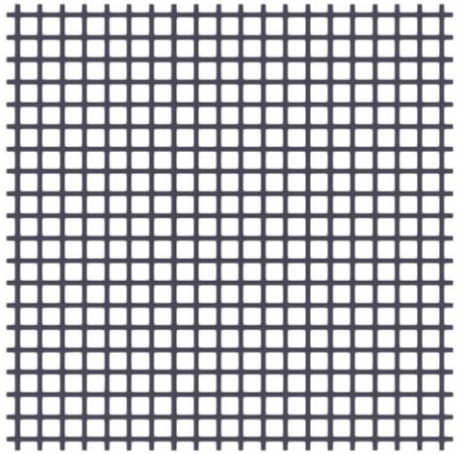
User VVUQ – code verification

- Commercially available PDR-CFD codes are generally black-box tools, so users don't have the full functionality needed to apply this standard for themselves.
- Just because a user cannot apply the AIAA standard in full, doesn't mean the user can't do anything. There are some simple checks that all users of PDR-CFD codes can do for themselves:
  - Symmetry checks.
  - Rotational checks.
- **Users should focus on what they can do, rather than what they can't do.**

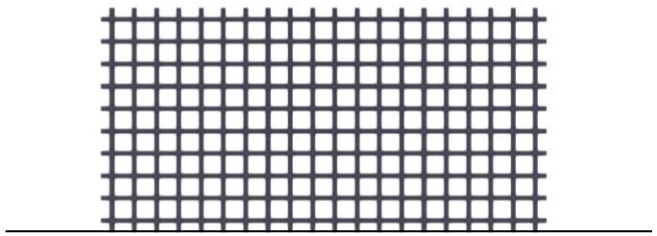
User VVUQ – code verification

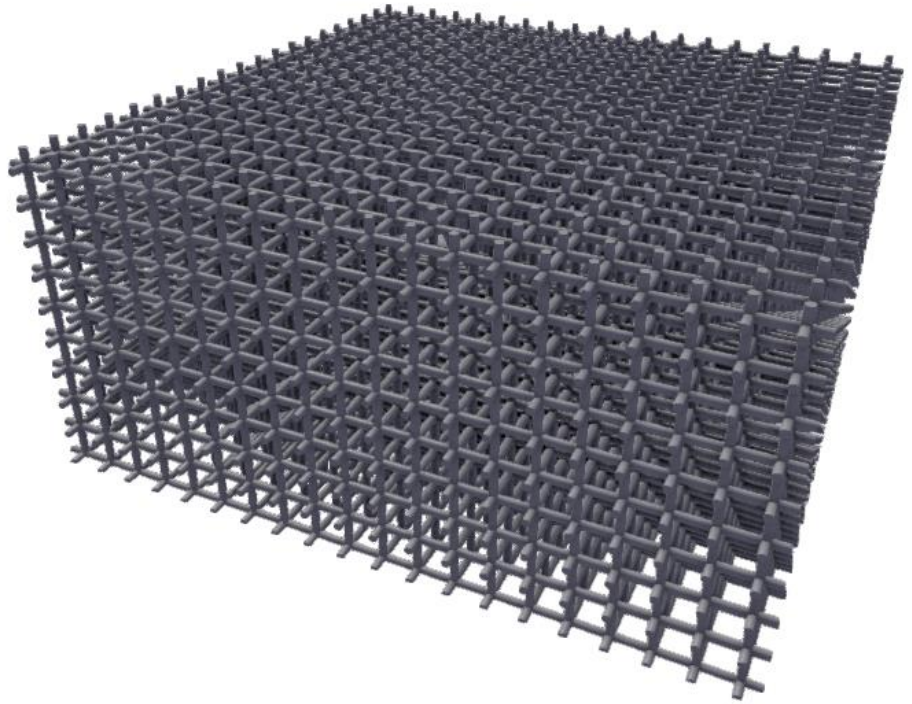
Symmetry checks

Looking downward



Looking horizontally

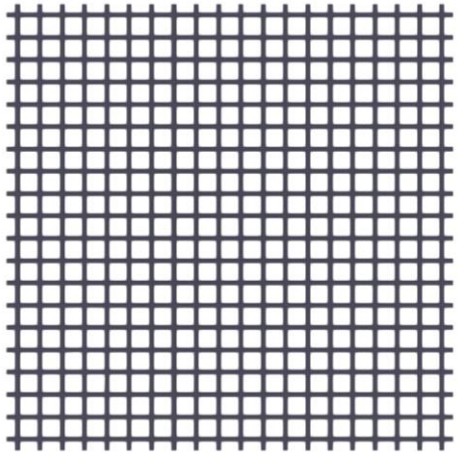




User VVUQ – code verification

Symmetry checks

Looking downward



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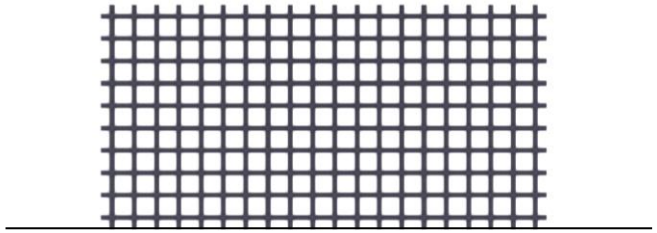
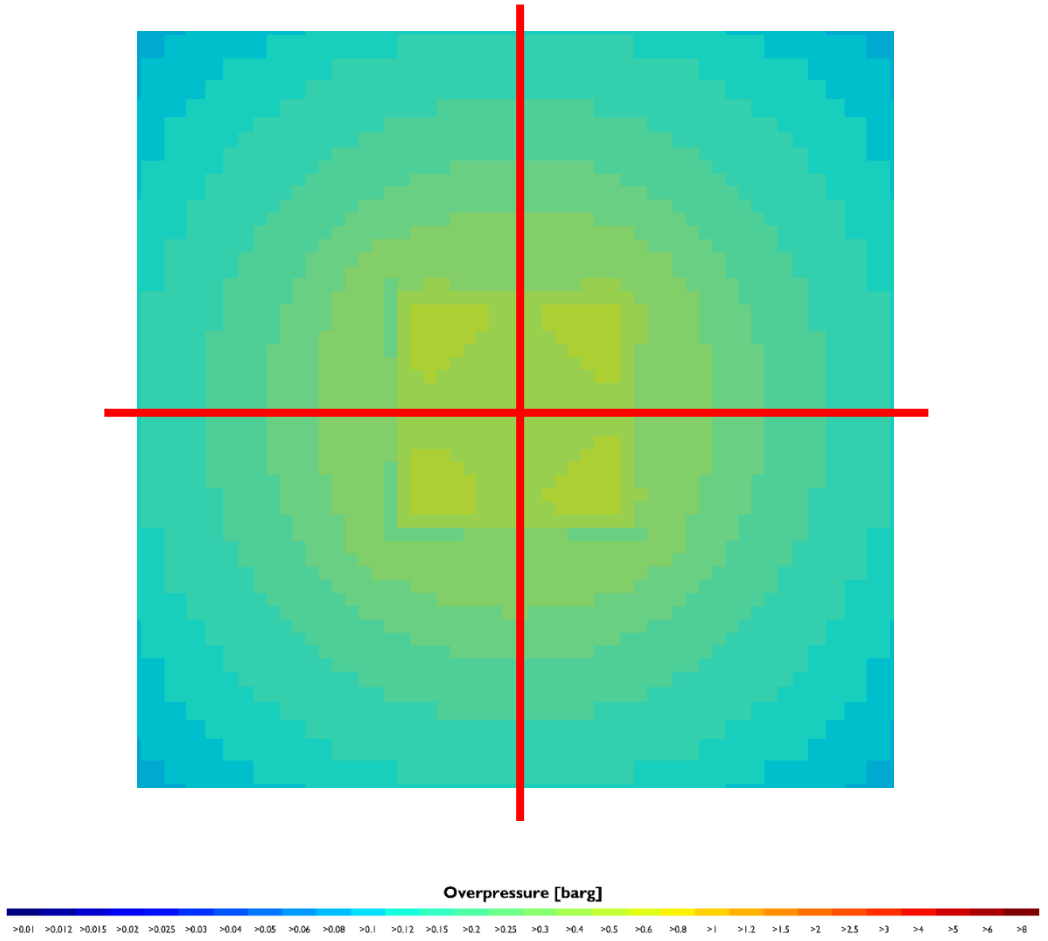
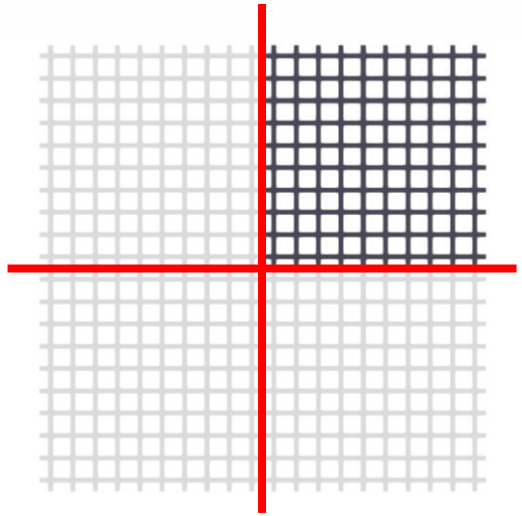




User VVUQ – code verification

Symmetry checks

Looking downward



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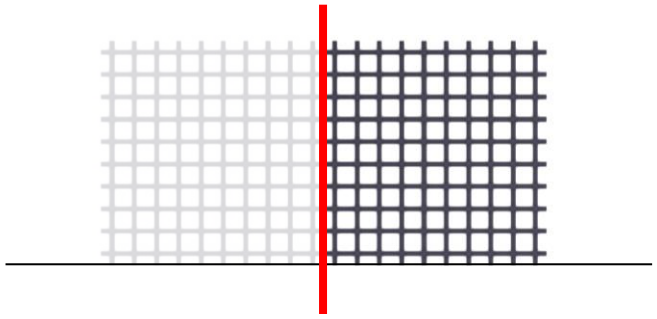

User VVUQ – code verification

Symmetry checks

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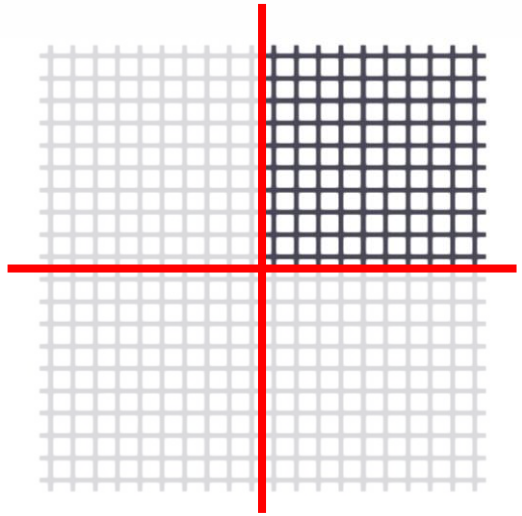

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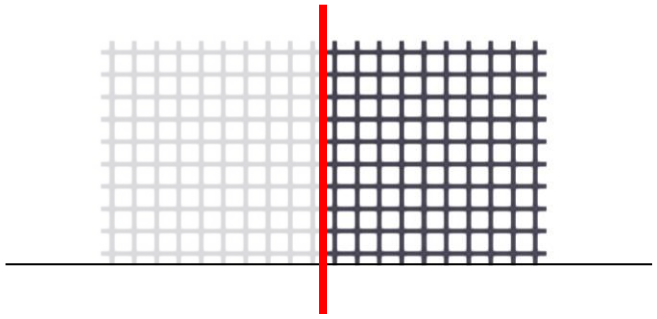
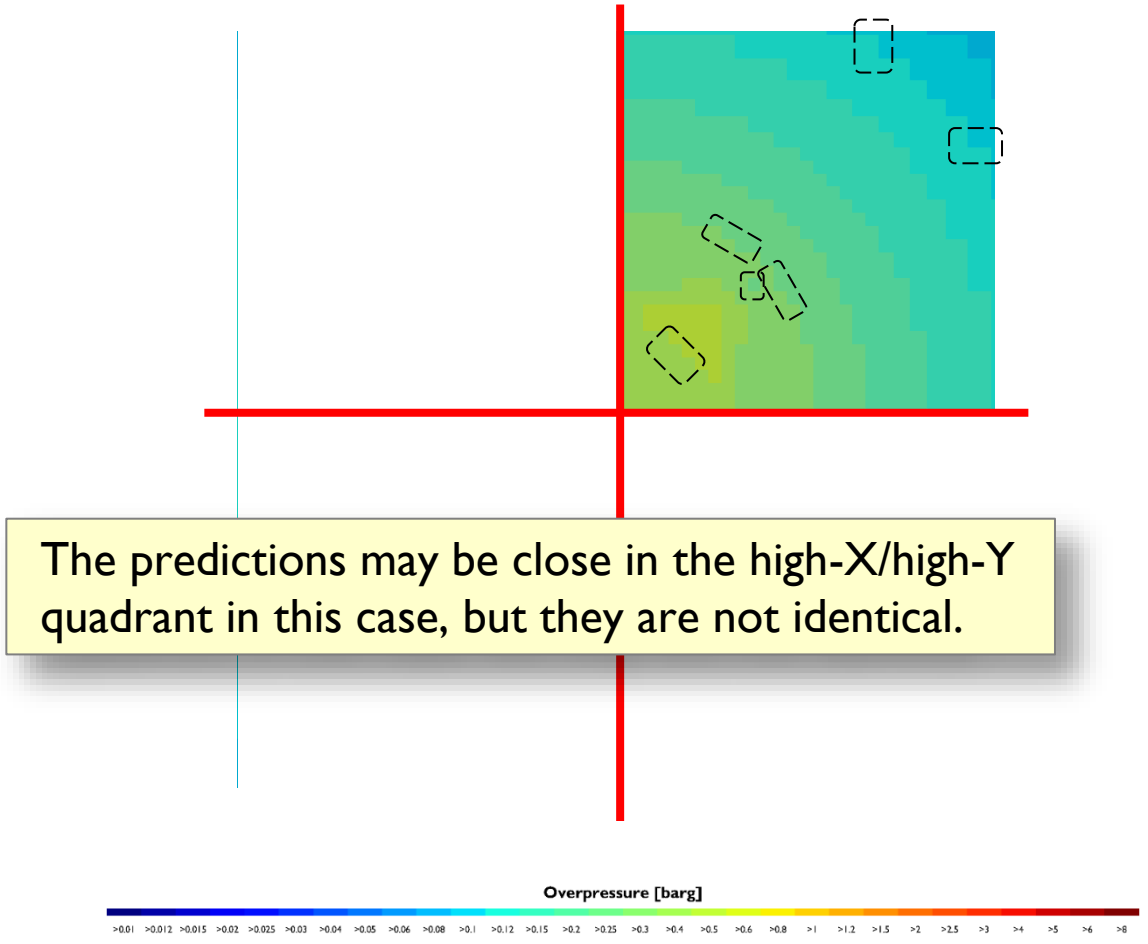


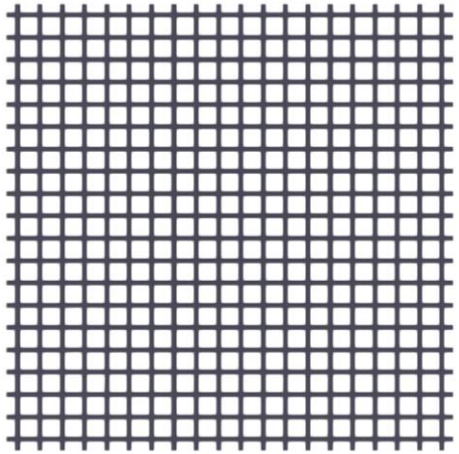


The predictions may be close in the high-X/high-Y quadrant in this case, but they are not identical.

User VVUQ – code verification

Symmetry checks

Looking downward



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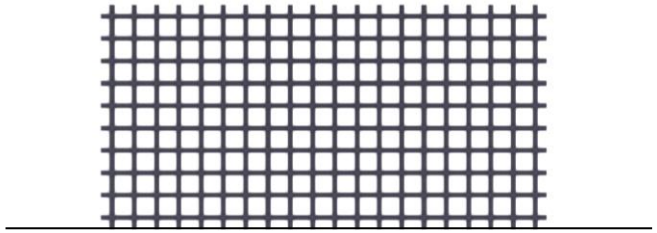

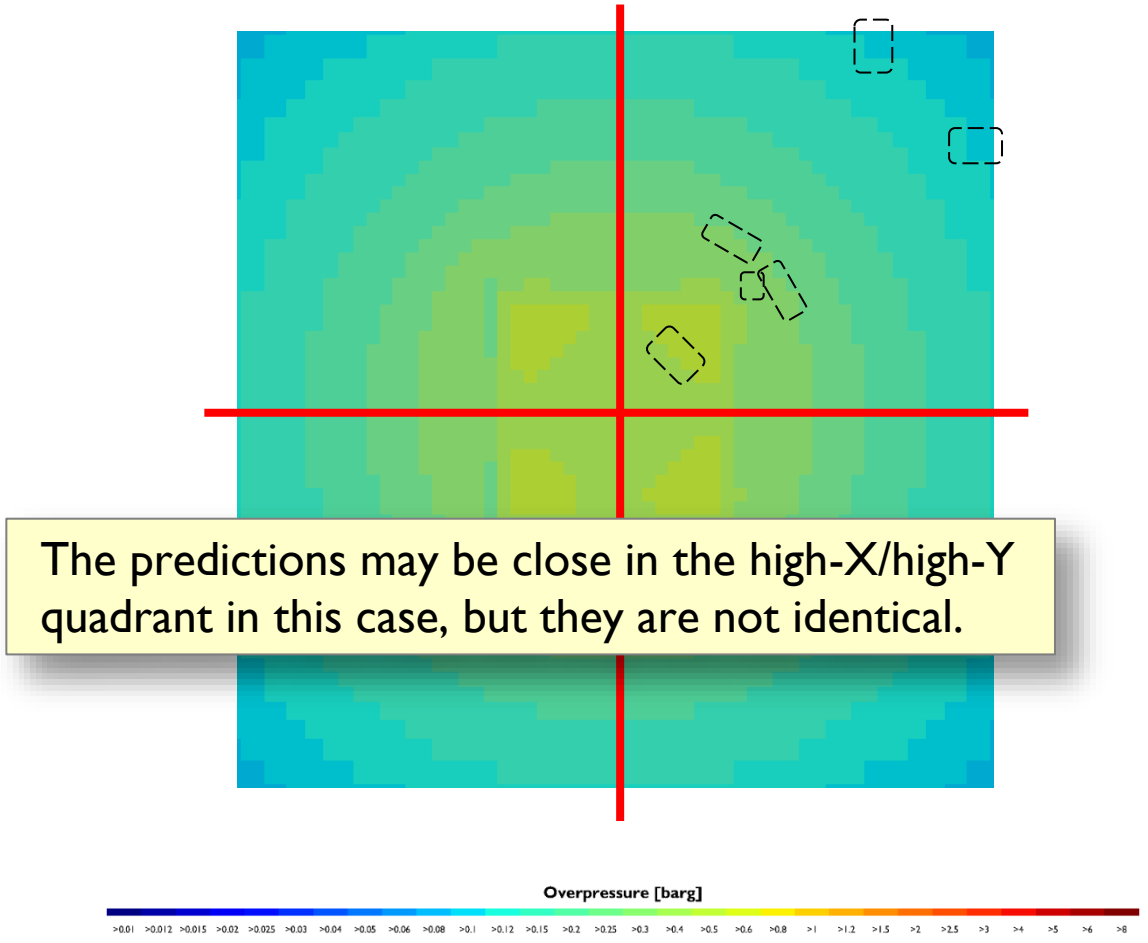

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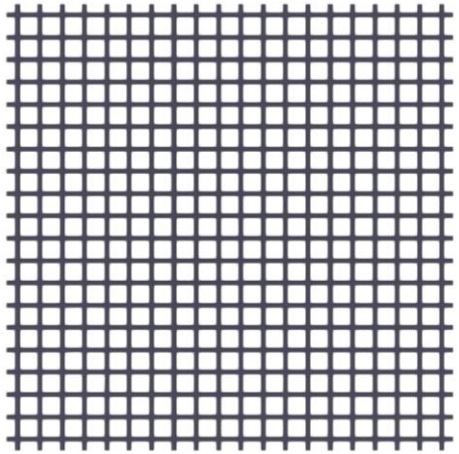

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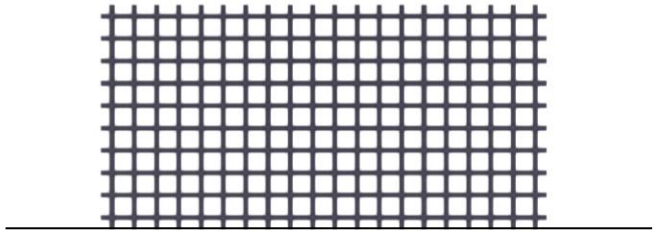

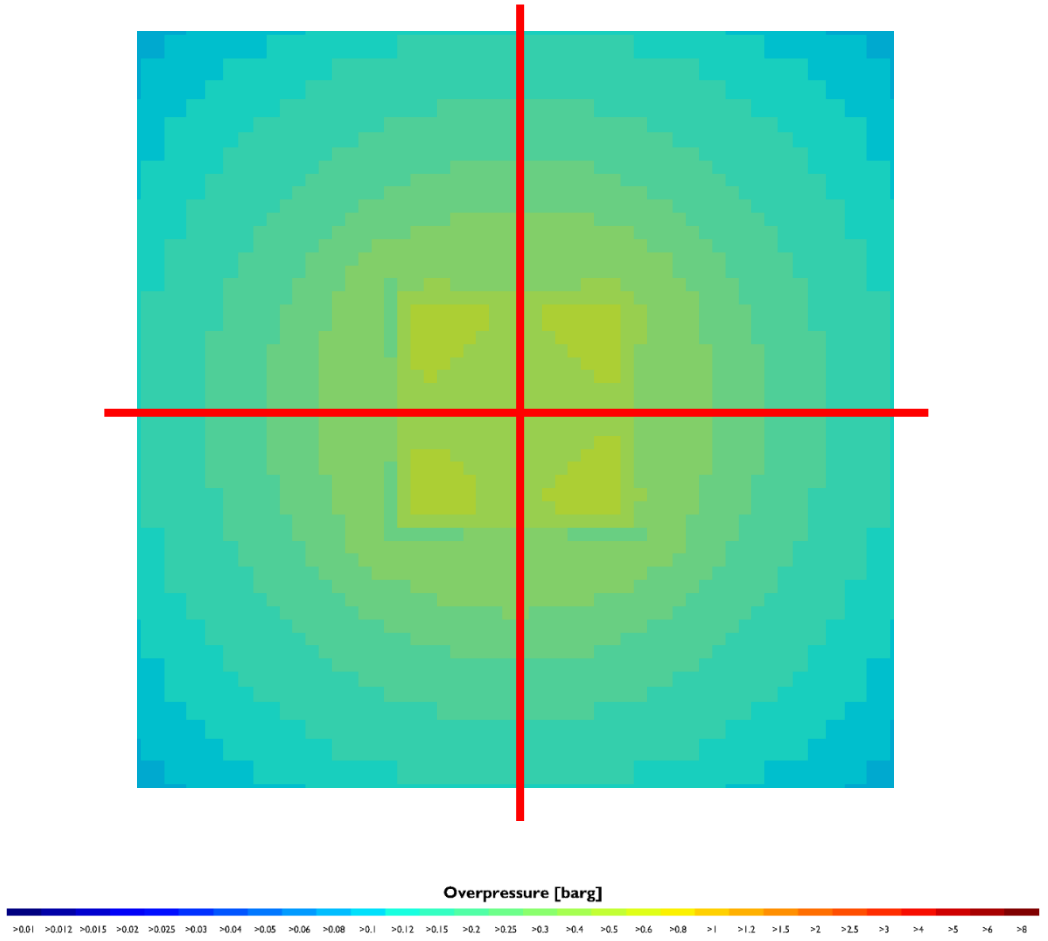

User VVUQ – code verification

Symmetry checks

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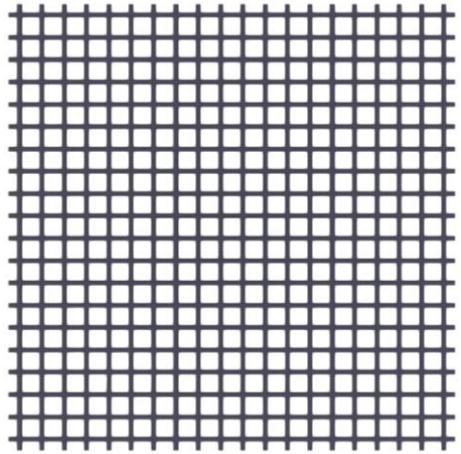

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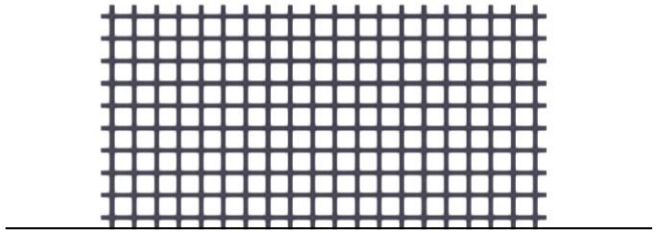

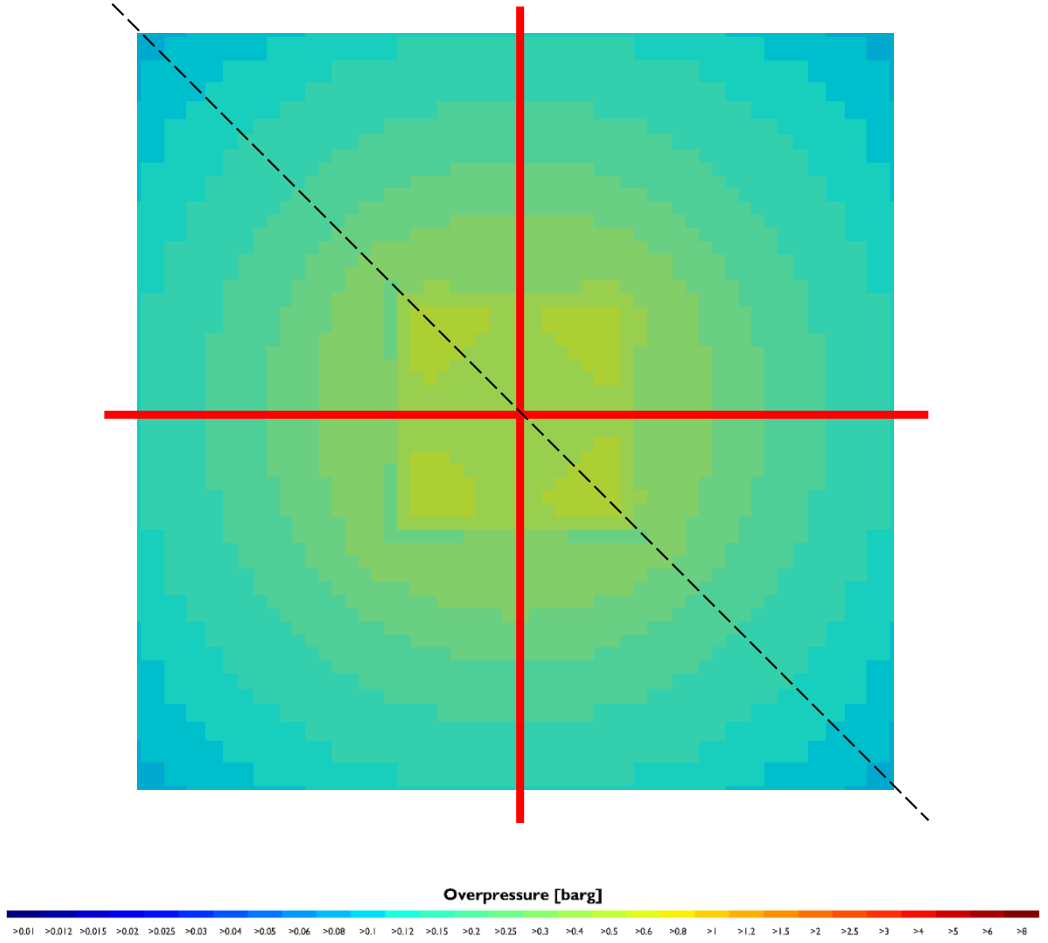

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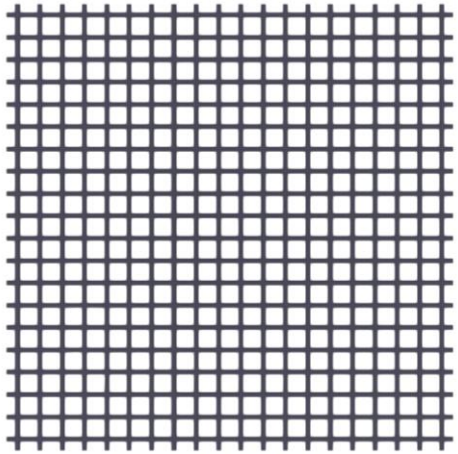
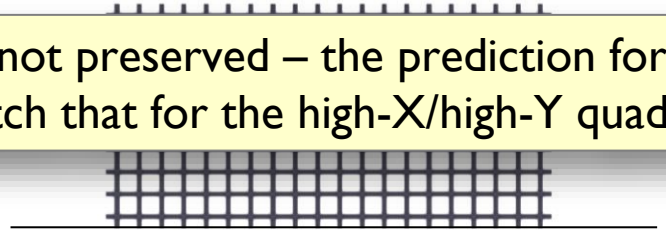
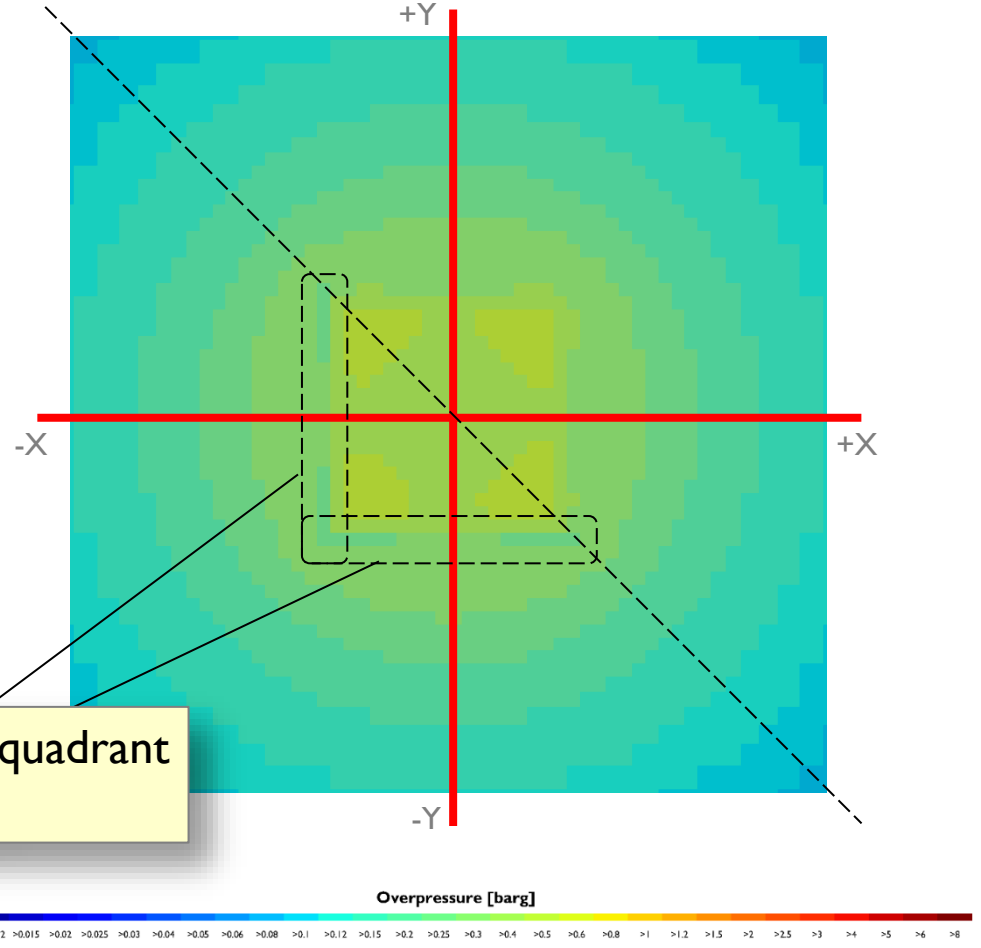


Looking horizontally



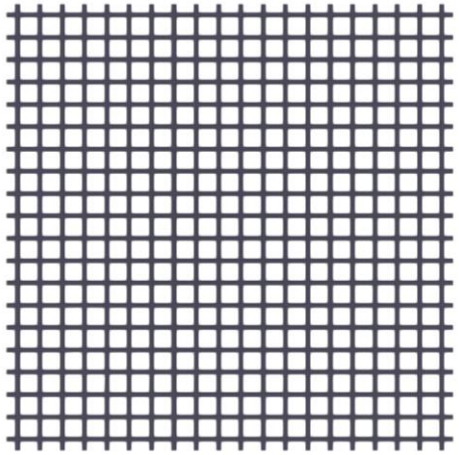


Symmetry is not preserved – the prediction for the low-X/low-Y quadrant does not match that for the high-X/high-Y quadrant in this case…

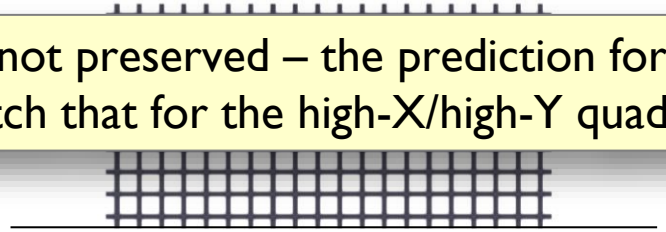
User VVUQ – code verification

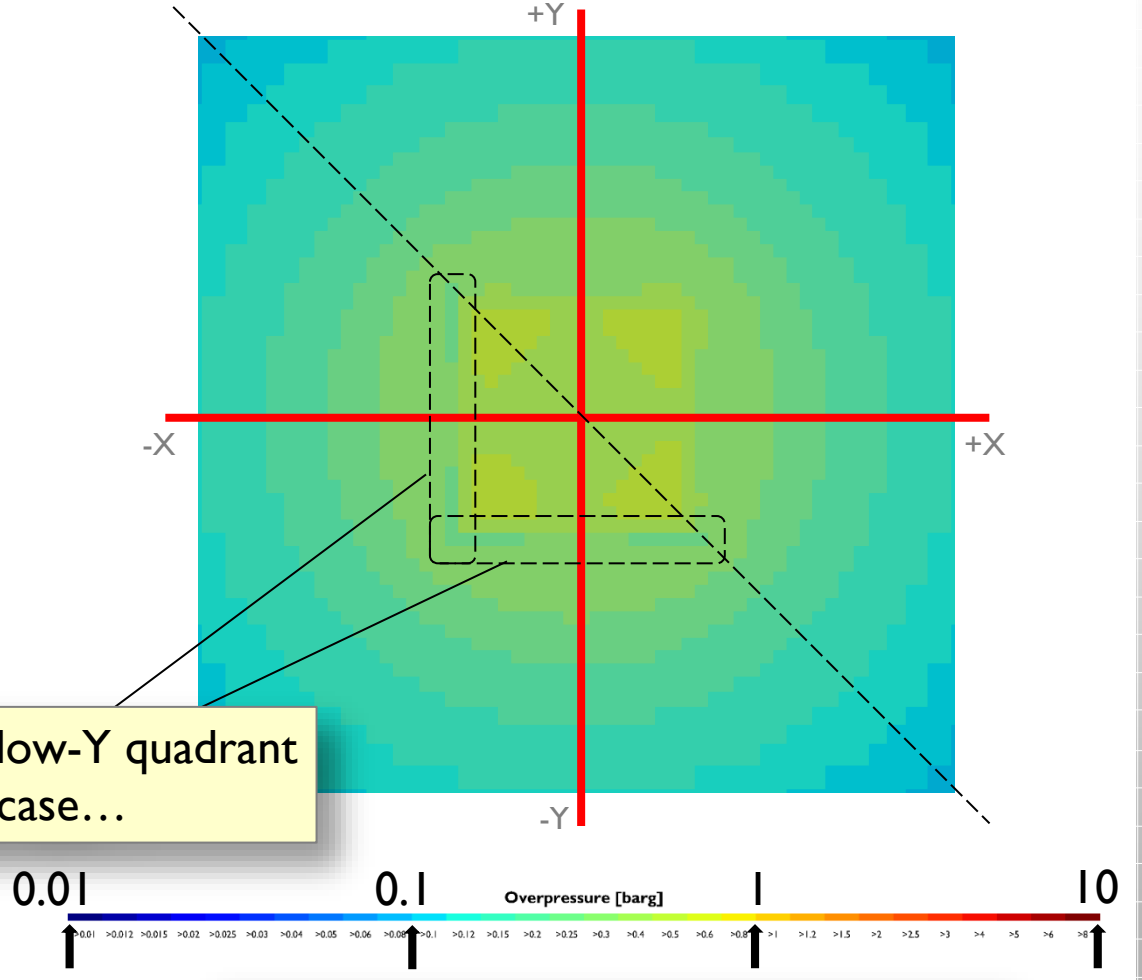
Symmetry checks

Looking downward



Looking horizontally





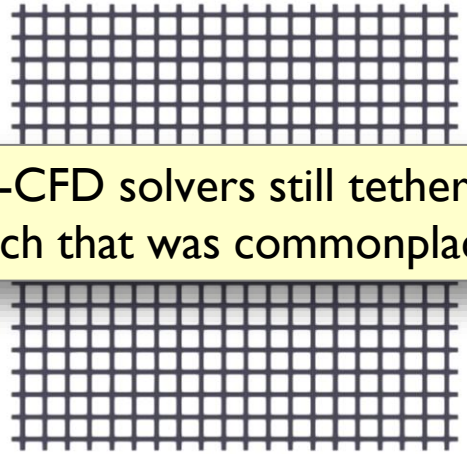
Symmetry is not preserved – the prediction for the low-X/low-Y quadrant does not match that for the high-X/high-Y quadrant in this case…

Note the colour scale is logarithmic and covers three orders of magnitude!

User VVUQ – code verification

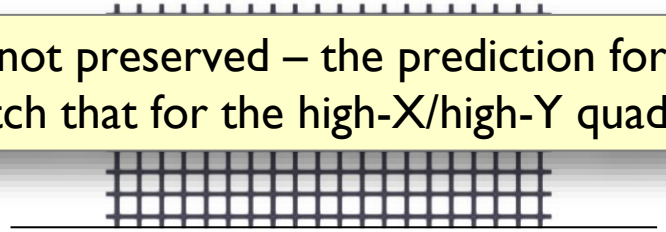
Symmetry checks

Looking downward



… are the PDR-CFD solvers still tethered to the staggered meshing approach that was commonplace 40 years ago?

Looking horizontally



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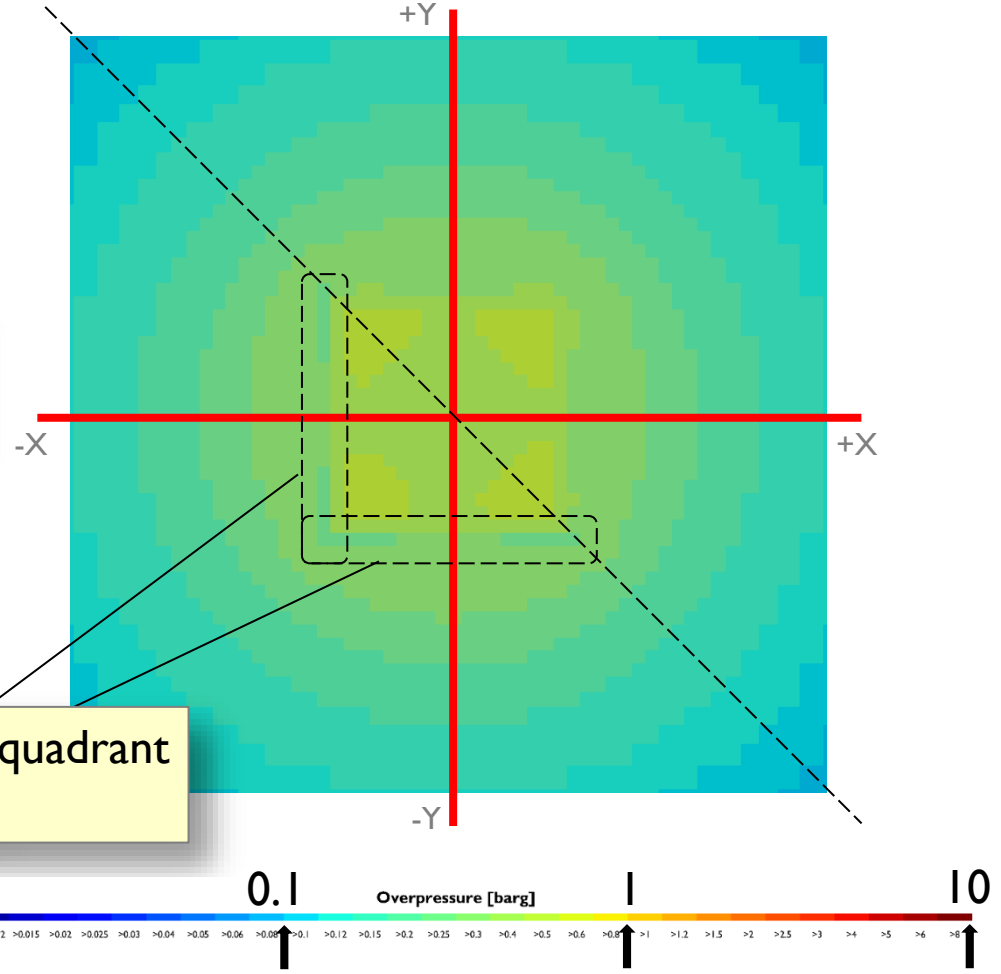
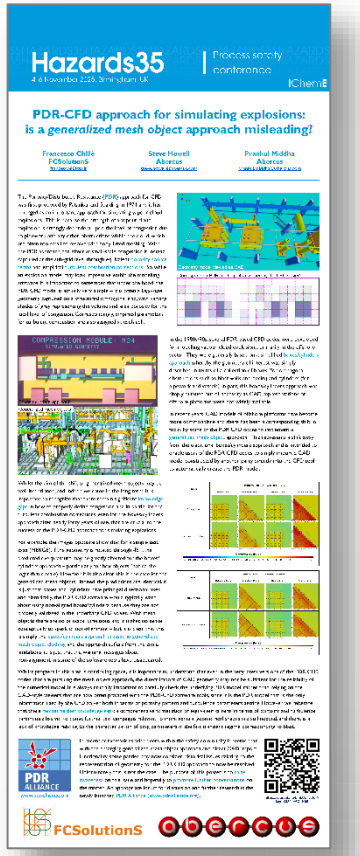


User VVUQ – code verification

Rotational checks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IChemE

PDR-CFD approach for simulating explosions: is a *generalized mesh object* approach misleading?

Francesco Chitti FCSolutionS

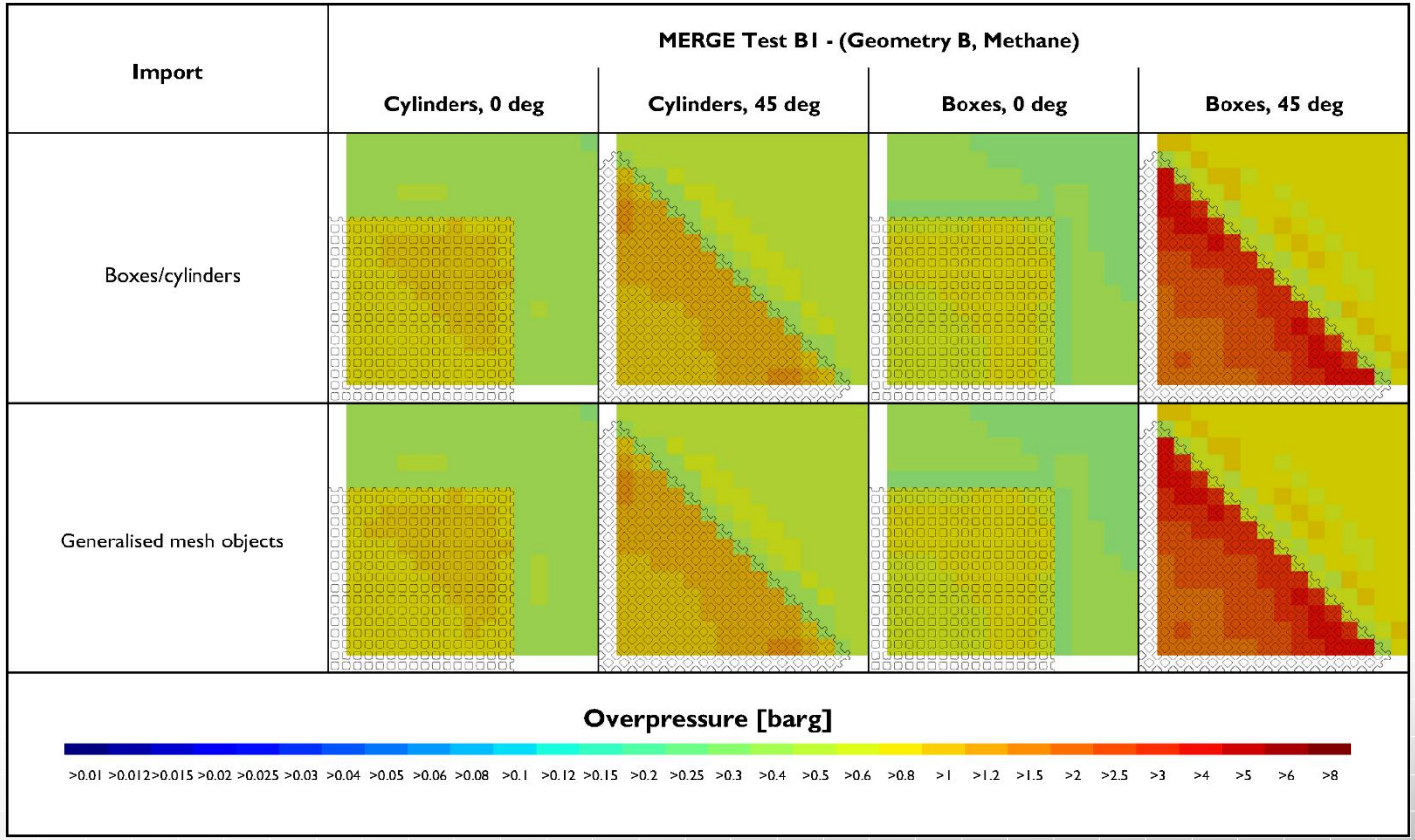
Steve Hovell Abercus

Prashul Middha Abercus

PDR ALLIANCE

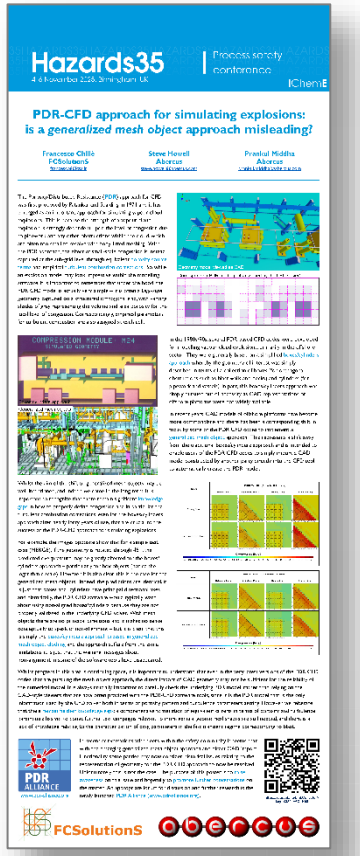
FCSolutionS

abercus



User VVUQ – code verification

Rotational checks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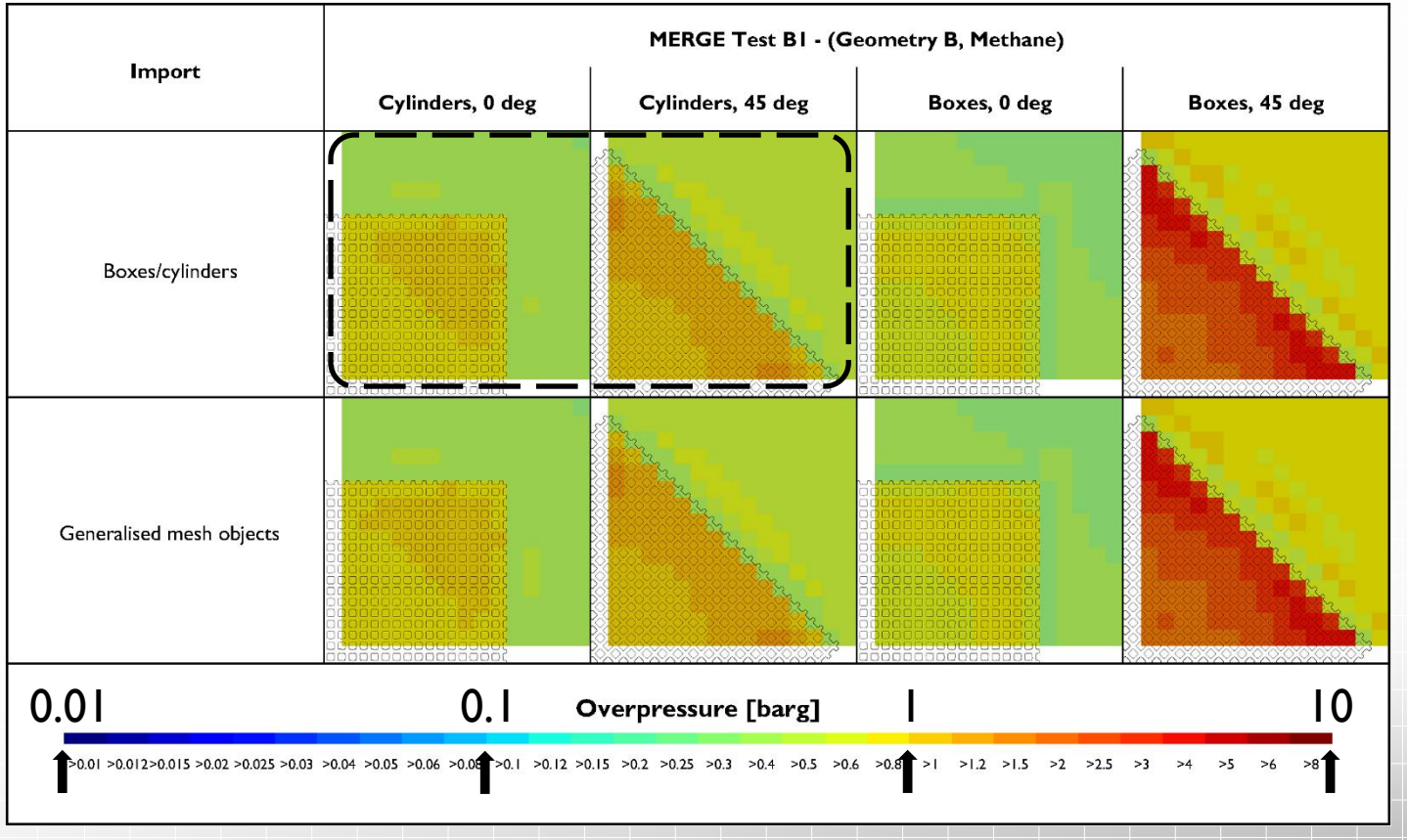
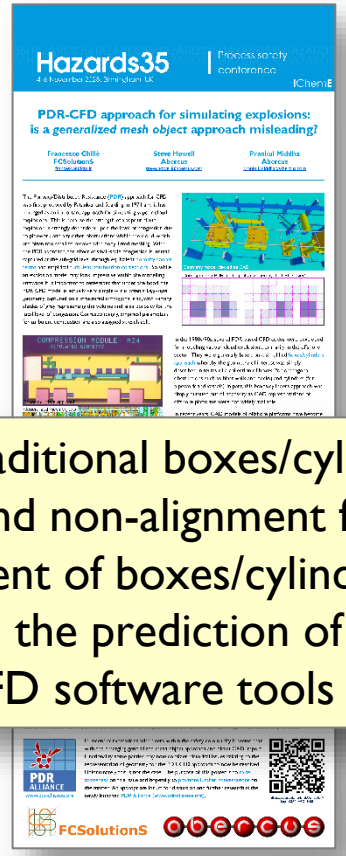
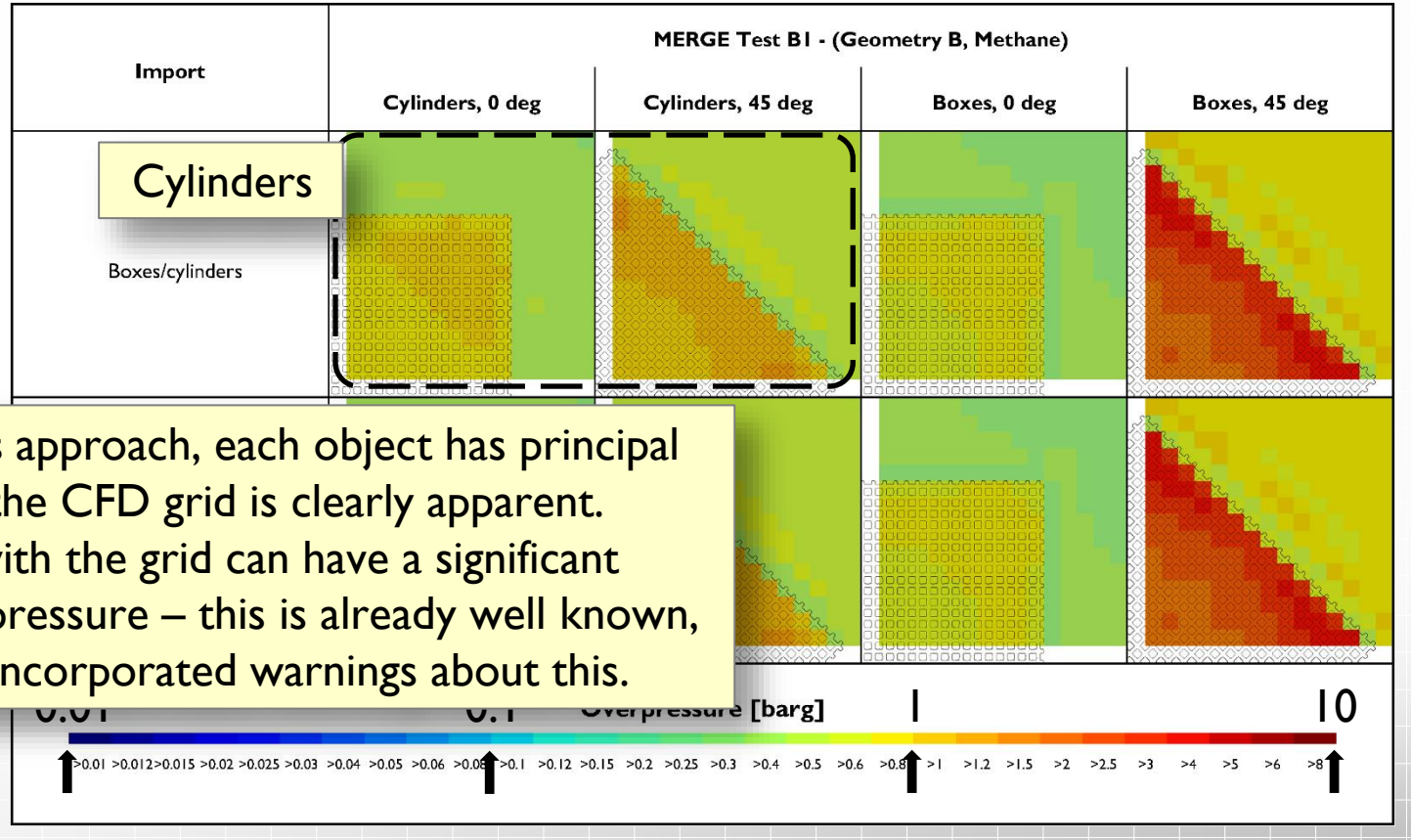


User VVUQ – code verification

Rotational checks

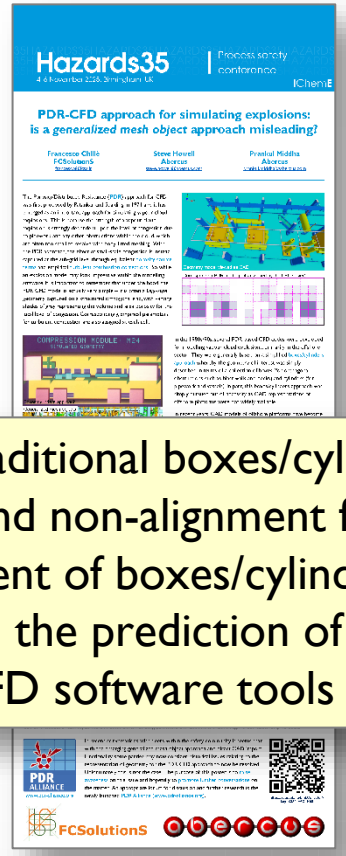


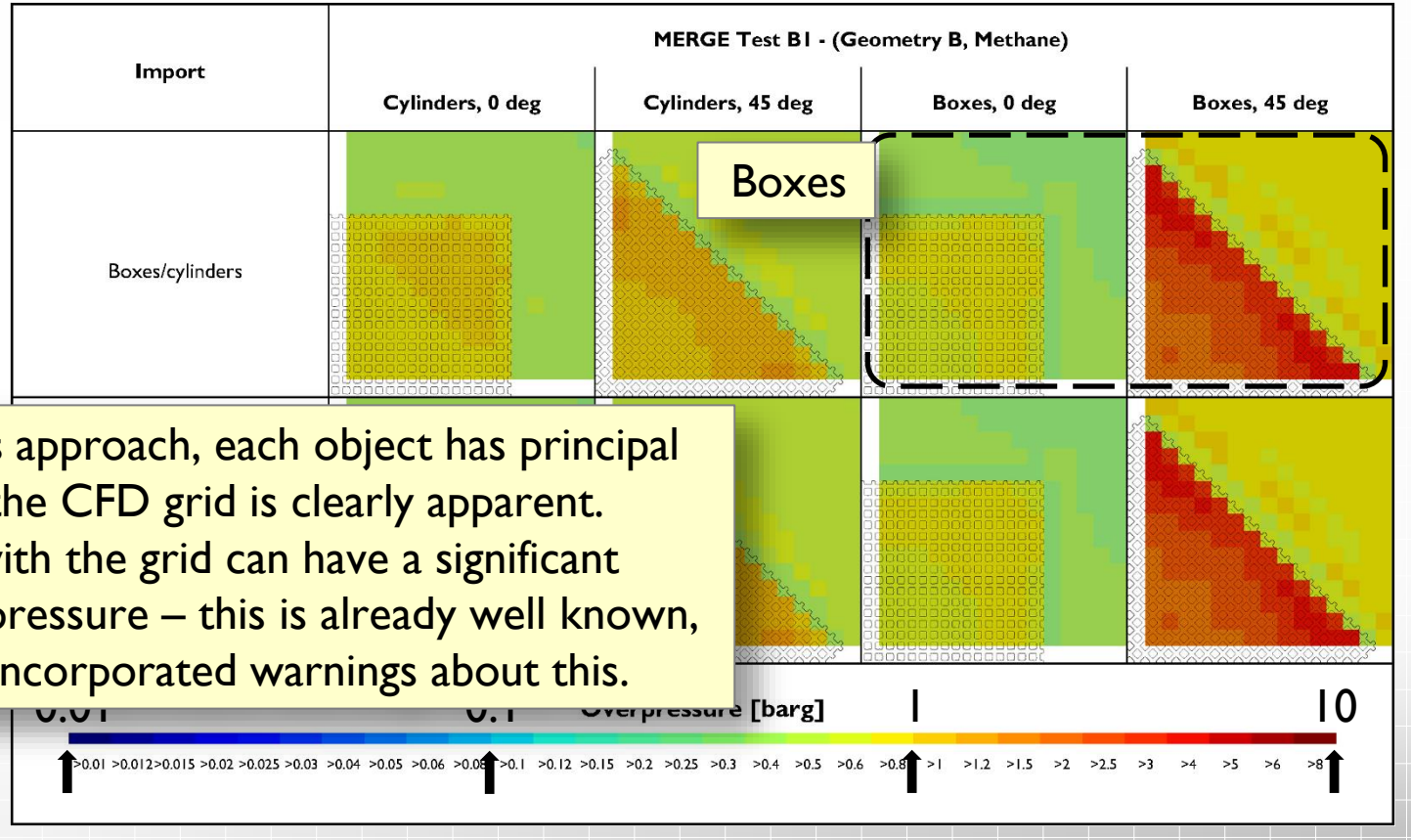


With the traditional boxes/cylinders approach, each object has principal directions and non-alignment from the CFD grid is clearly apparent. Non-alignment of boxes/cylinders with the grid can have a significant impact upon the prediction of overpressure – this is already well known, and PDR-CFD software tools have incorporated warnings about this.

User VVUQ – code verification

Rotational checks





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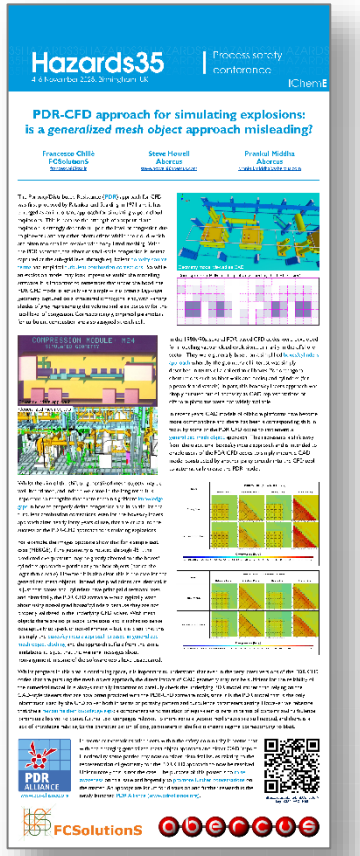
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IChemE

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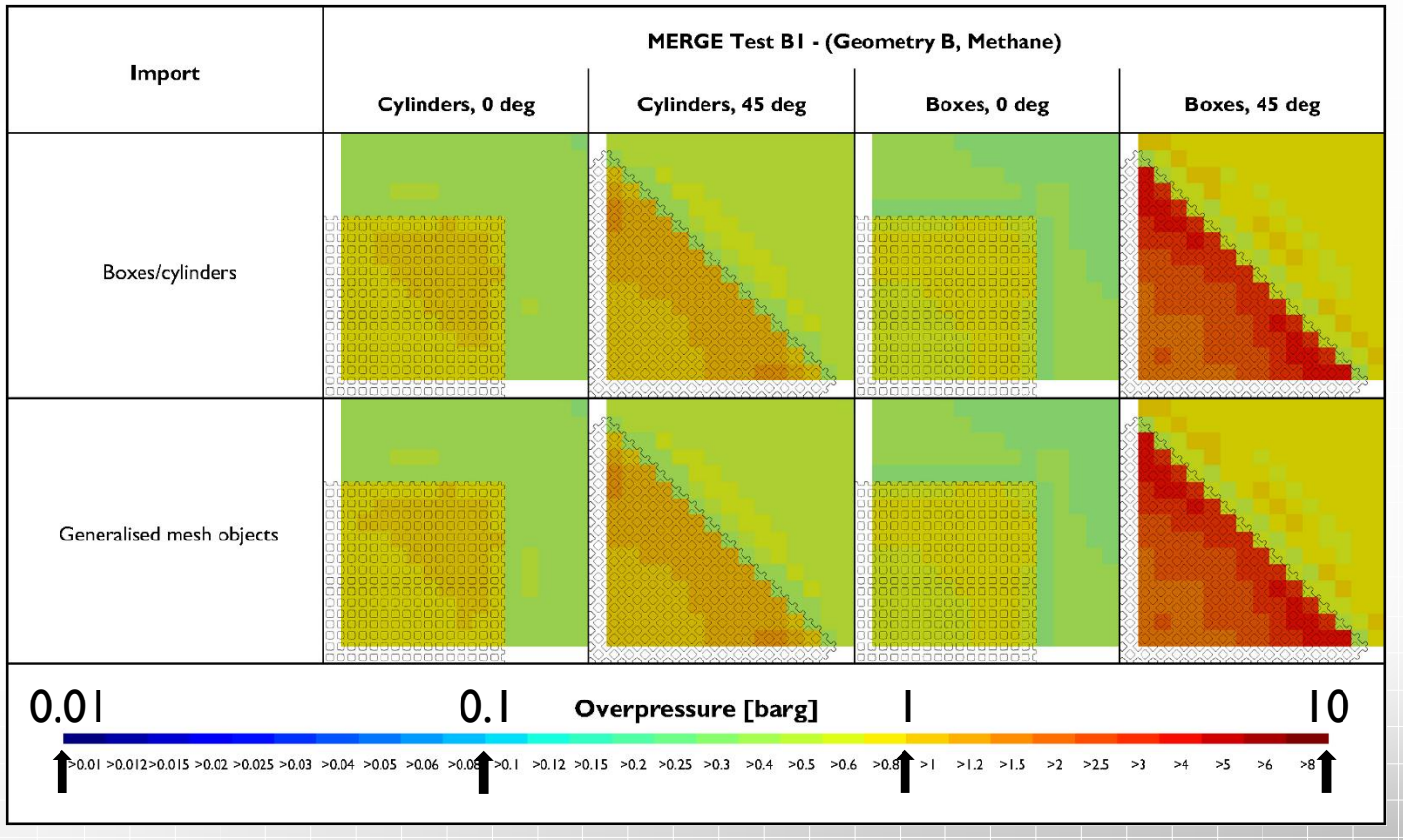
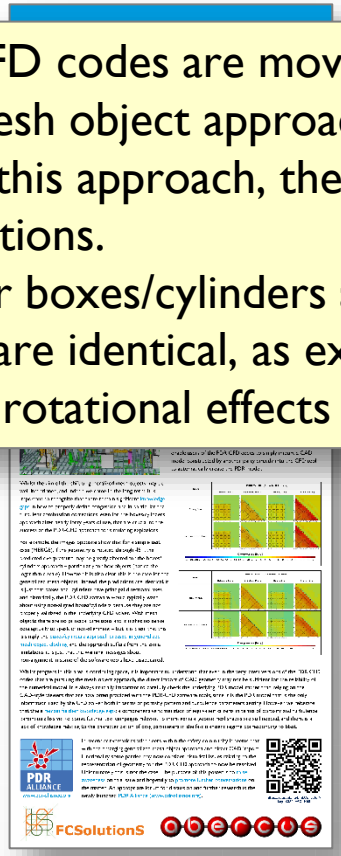
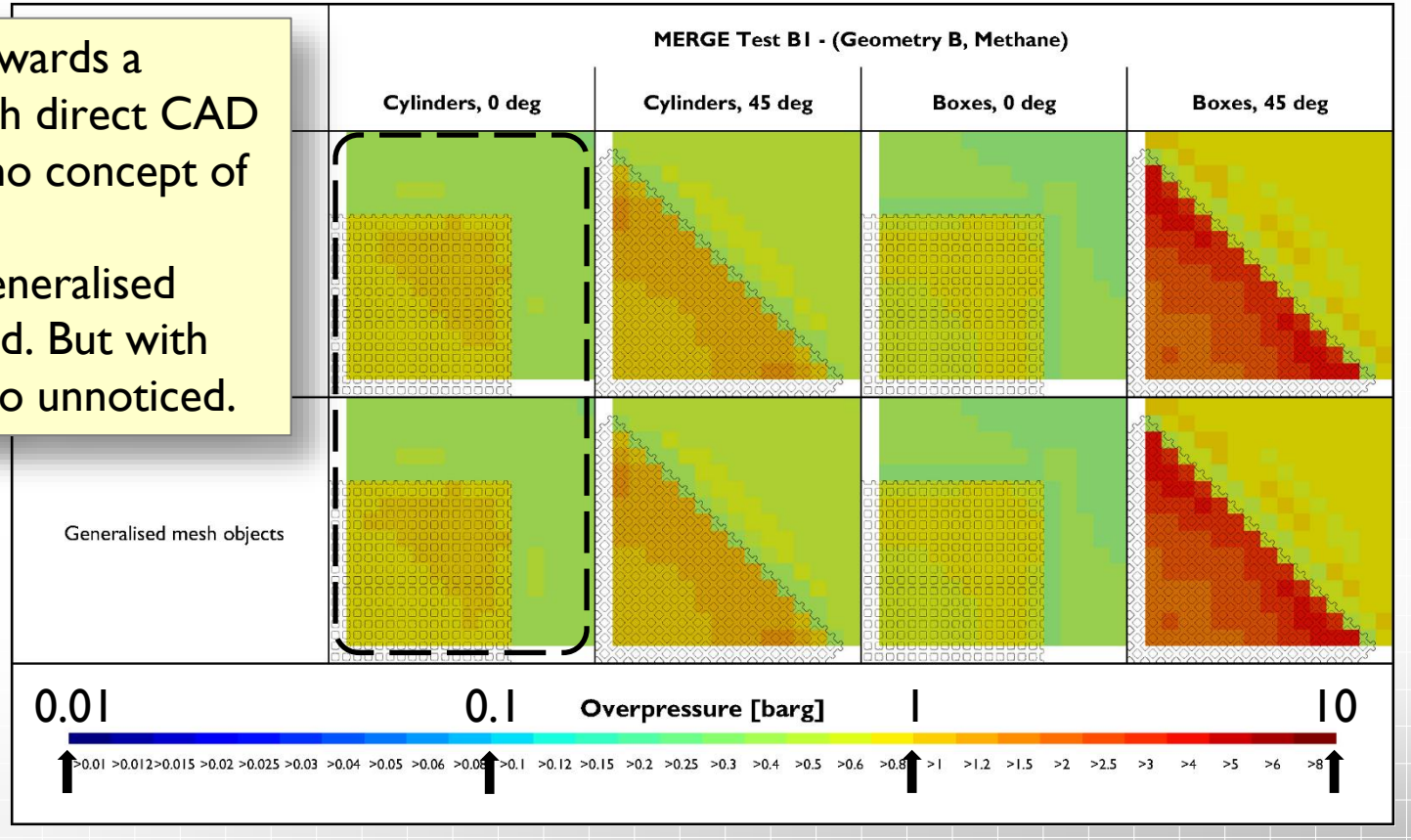


User VVUQ – code verification

Rotational checks

Some PDR-CFD codes are moving towards a generalised mesh object approach with direct CAD import. With this approach, there is no concept of principal directions.
Predictions for boxes/cylinders and generalised mesh objects are identical, as expected. But with mesh objects, rotational effects may go unnoticed.





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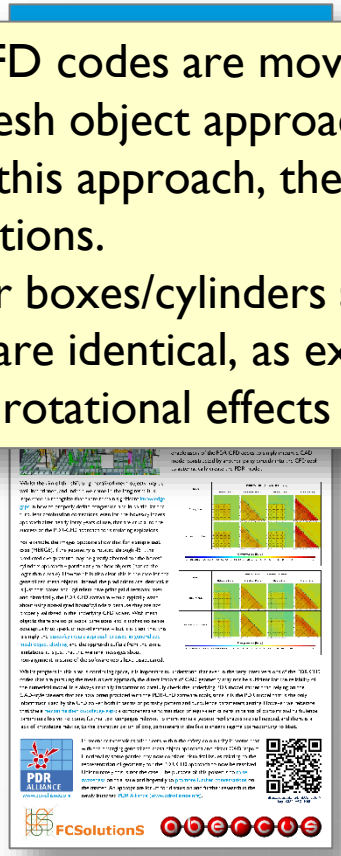

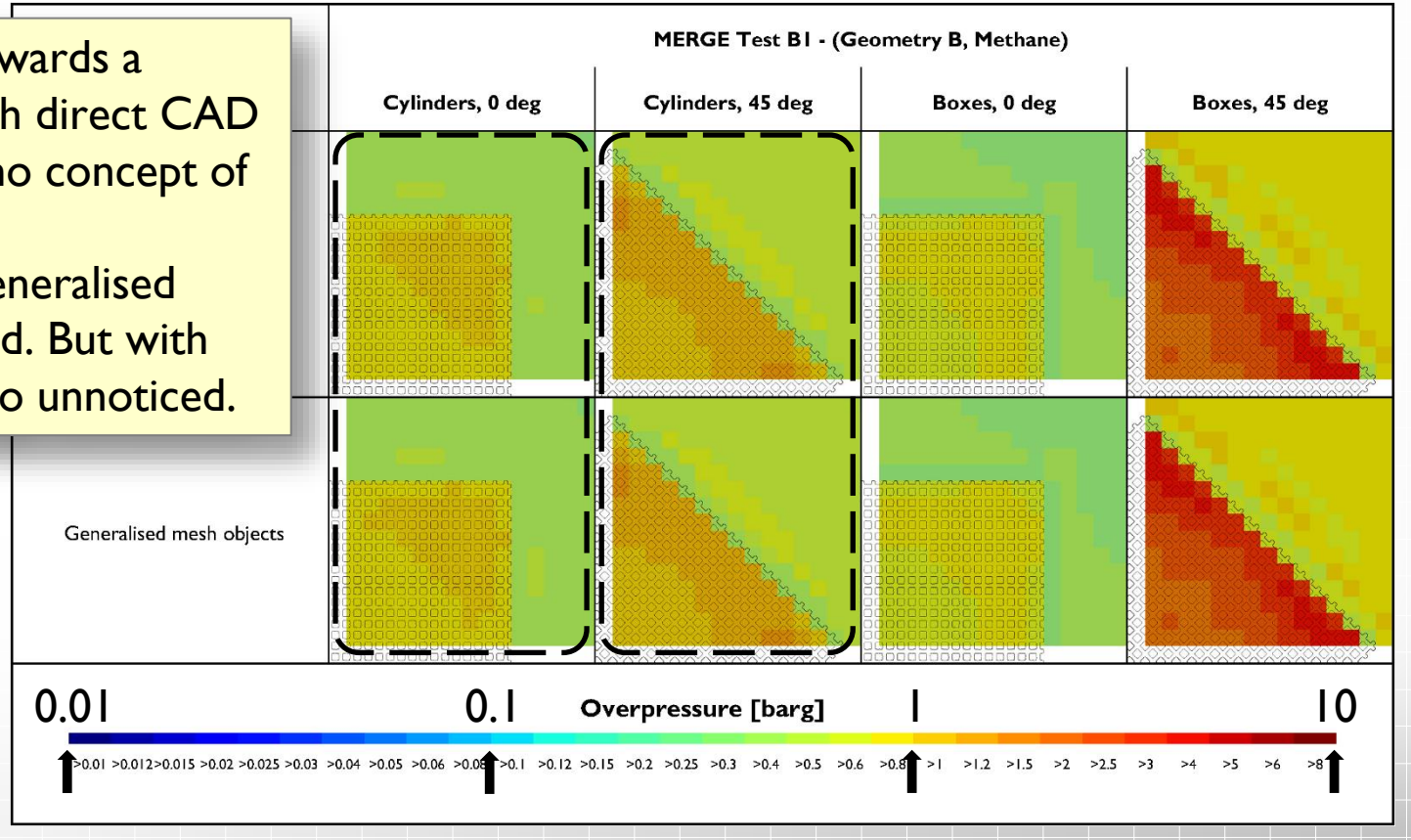

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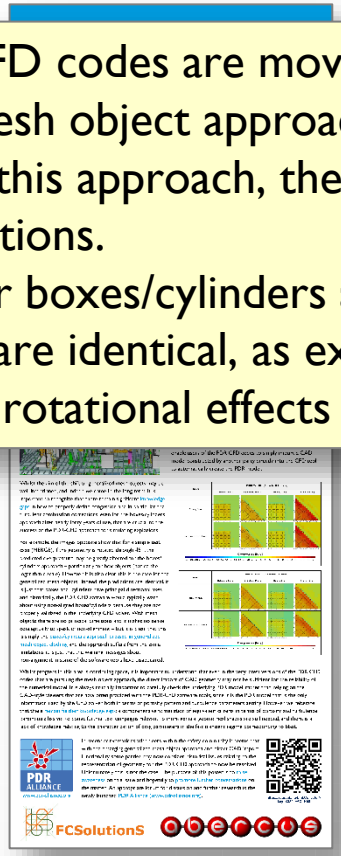

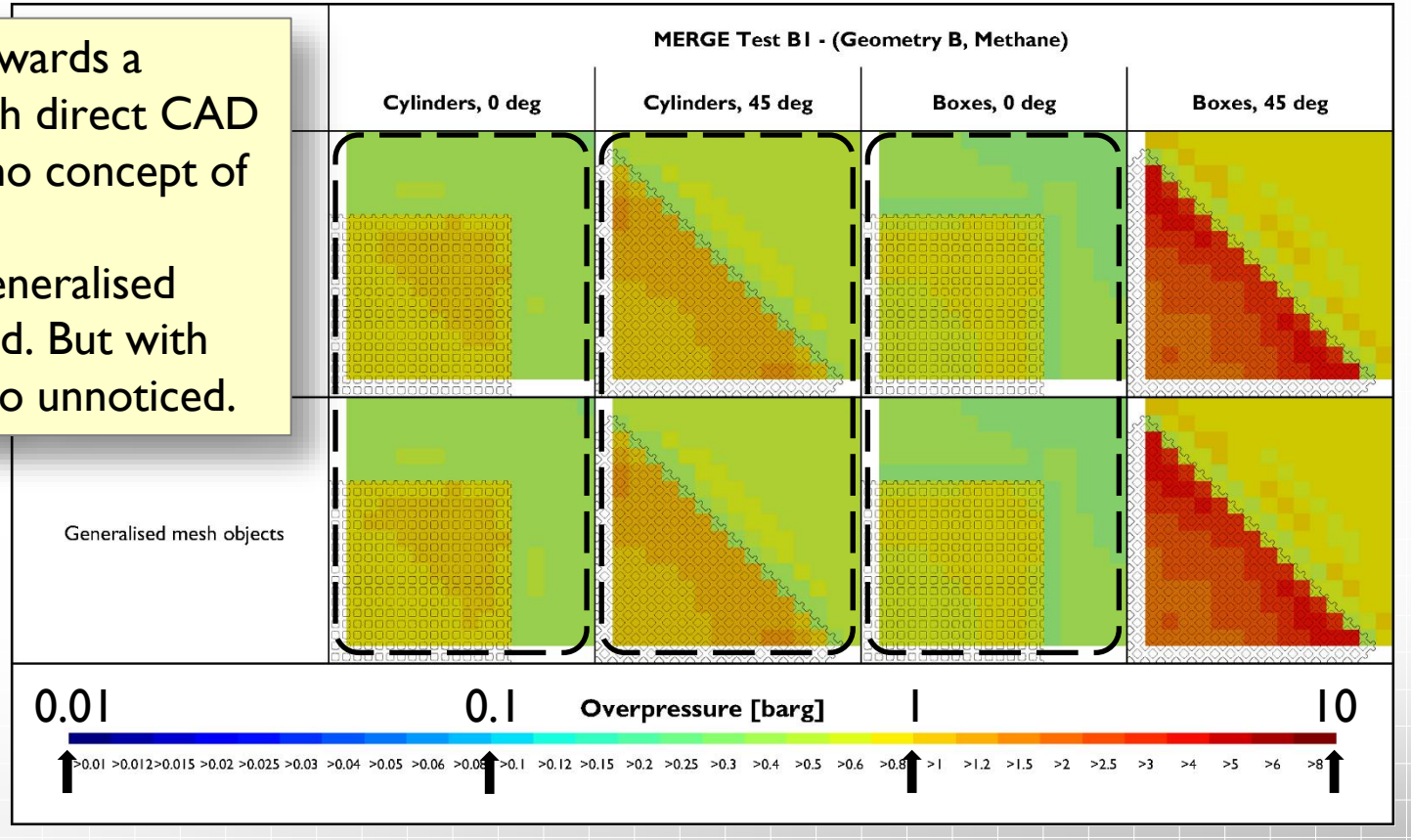

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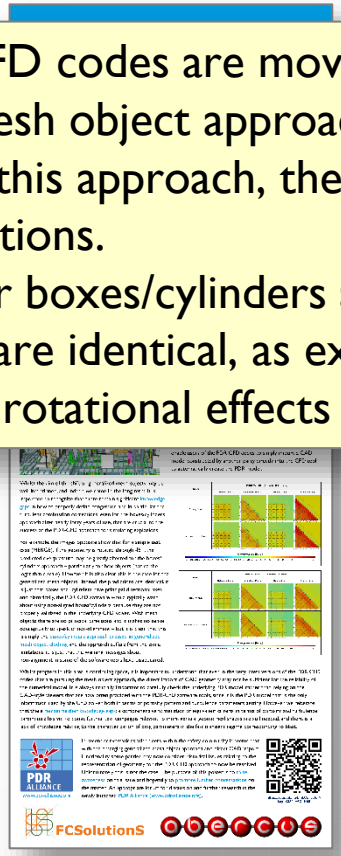

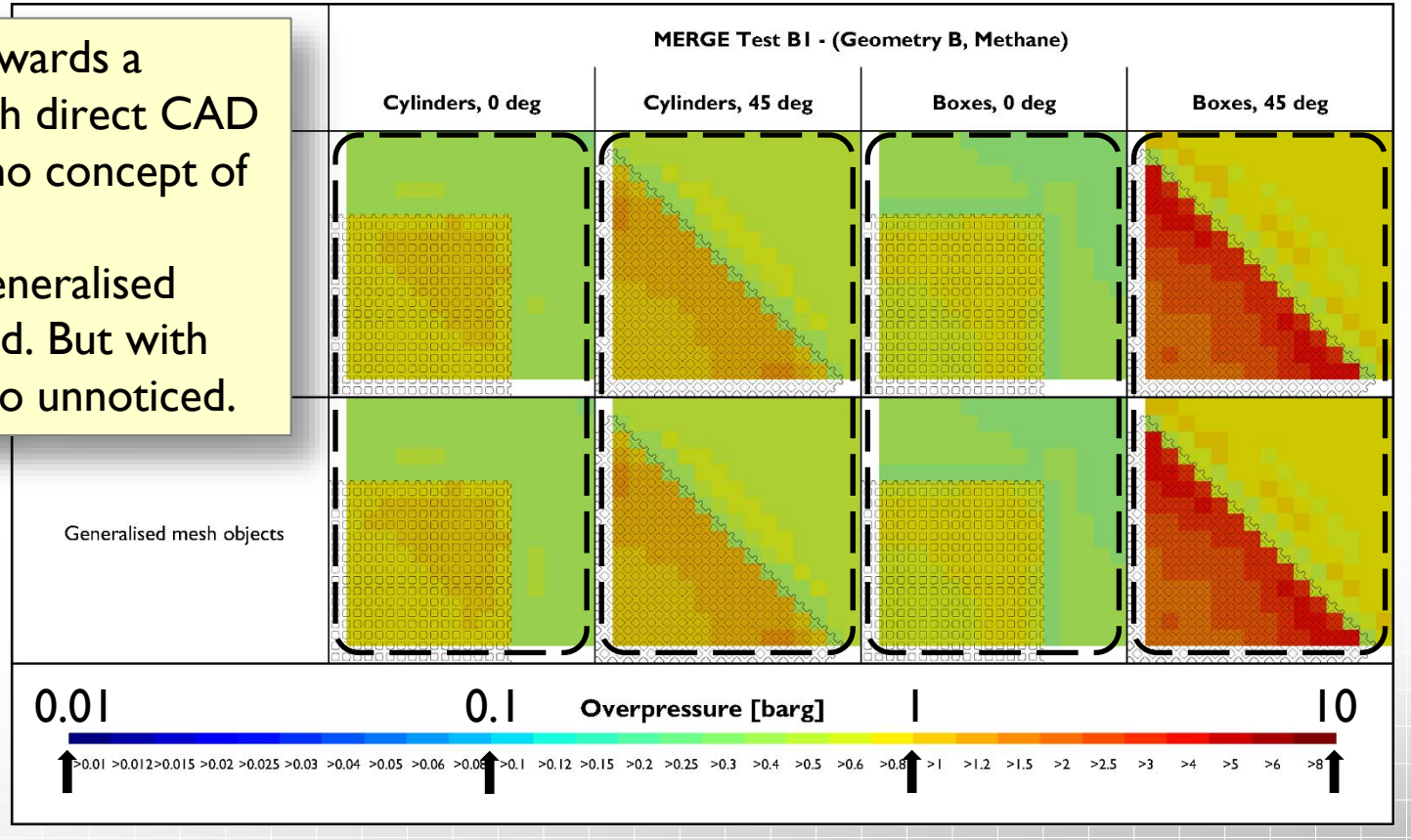

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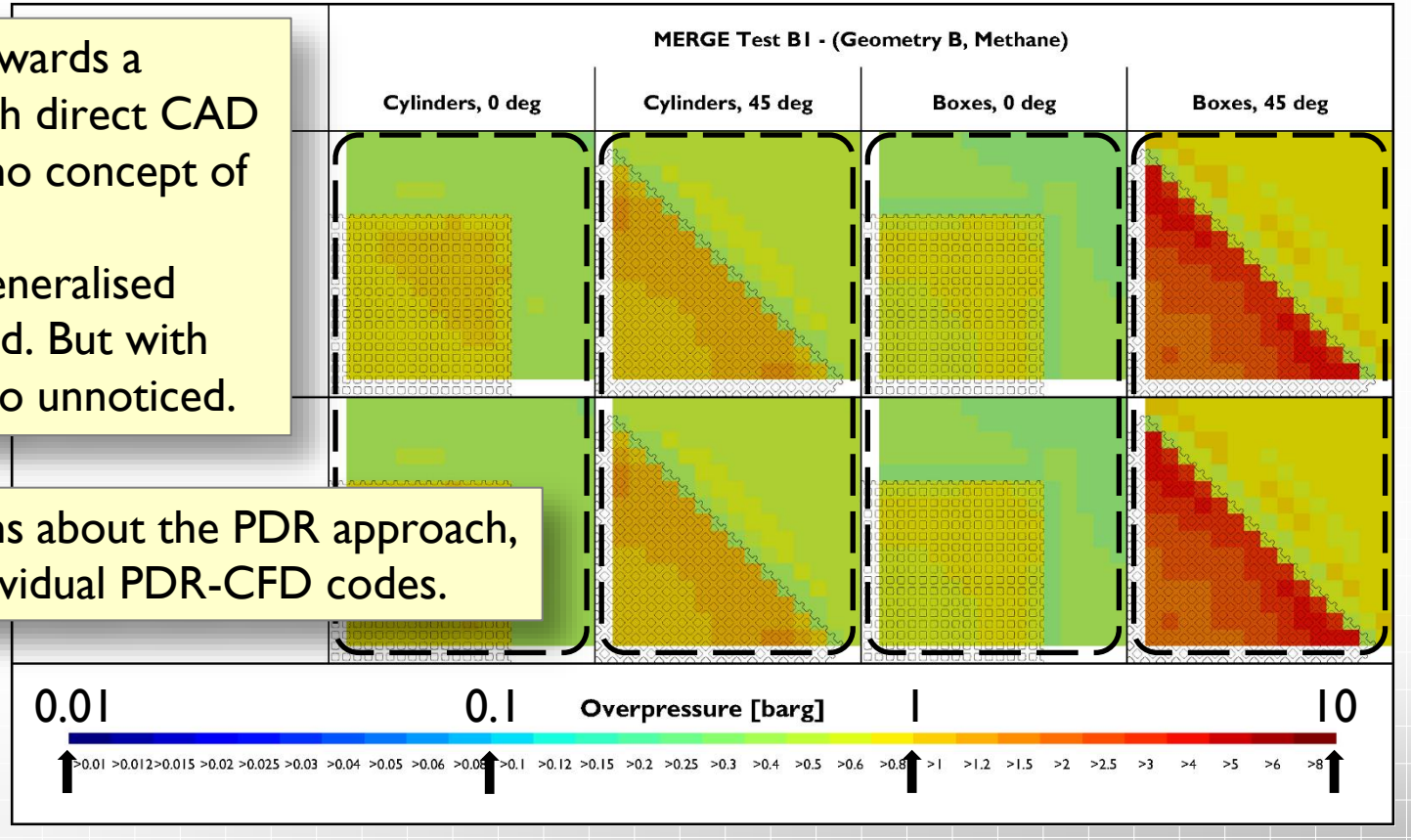
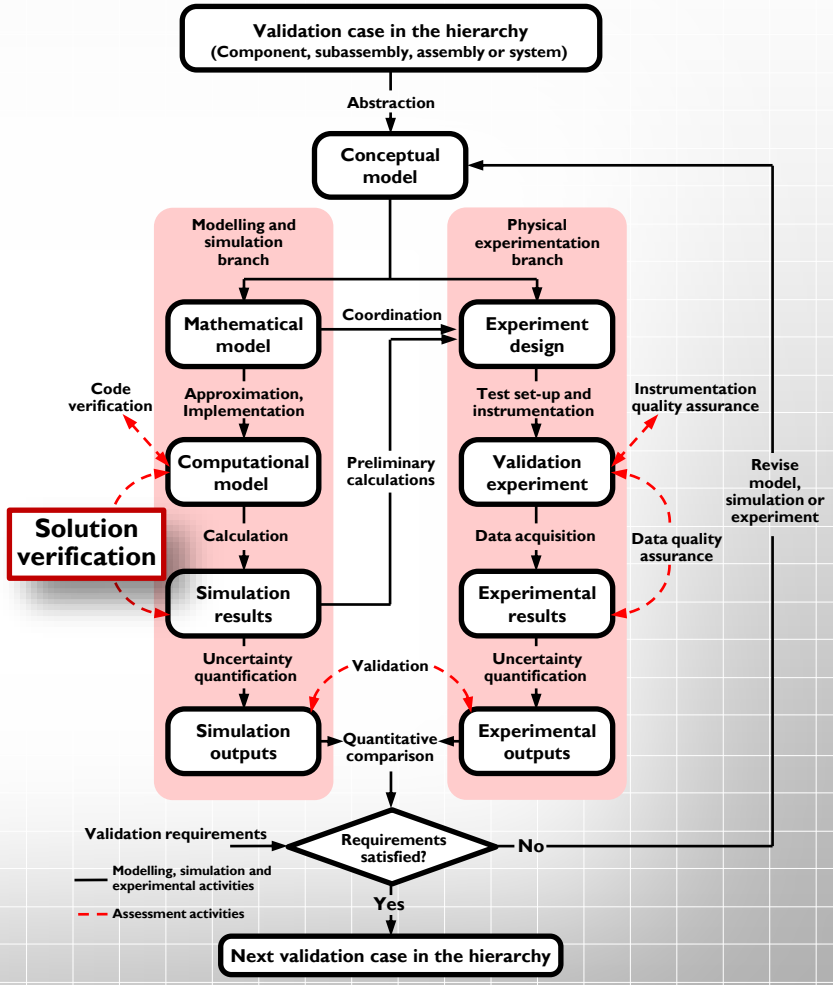
There remain plenty of open questions about the PDR approach, and how it is implemented within individual PDR-CFD codes.



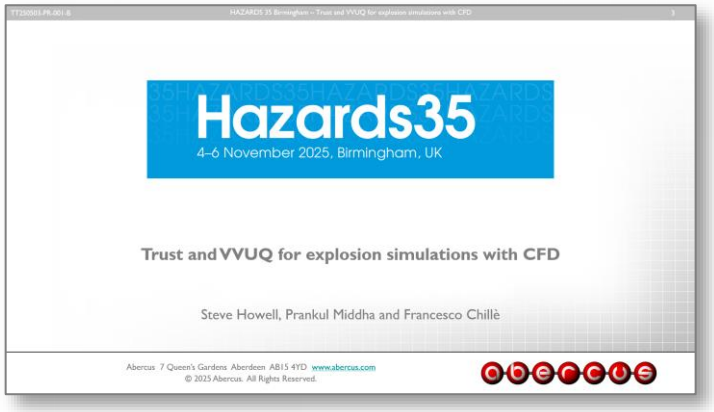
User VVUQ – solution verification

- Solution verification is the process of determining the accuracy of a particular numerical solution relative to an estimate of the exact solution of the computational model.
- It is a user activity relating to convergence and estimating the error in the computational solution:
  - The mesh/time-step resolution.
  - Iterative convergence.
- Code verification is an error evaluation process, whereas solution verification is an error estimation process – no exact solutions are available.



User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – PDR-CFD training (1994 report)



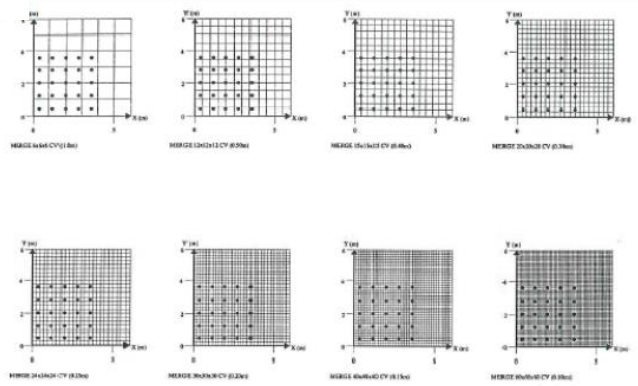


Figure 2.35 Grid resolutions MERGE type E geometry with domain extended 50% outside the geometry in each direction.

Resolution	CPU-time (HP735)	Max. pressure	Time of max. press.	Press. impulse
6x6x6	5.2 s	5 mbar	0.72 s	58 Pas
12x12x12	74.8 s (1 min)	61 mbar	0.43 s	239 Pas
15x15x15	222 s (4 min)	153 mbar	0.42 s	375 Pas
20x20x20	902 s (15 min)	184 mbar	0.44 s	405 Pas
24x24x24	1.576 s (25 min)	187 mbar	0.34 s	508 Pas
30x30x30	4.173 s (1 h)	217 mbar	0.37 s	508 Pas
40x40x40	12.800 s (4 h)	205 mbar	0.33 s	535 Pas
60x60x60	68.588 s (19 h)	100 mbar	0.41 s	318 Pas

User VVUQ – solution verification

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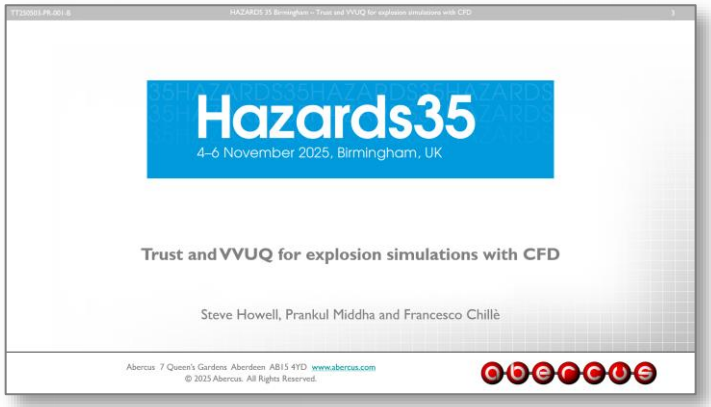

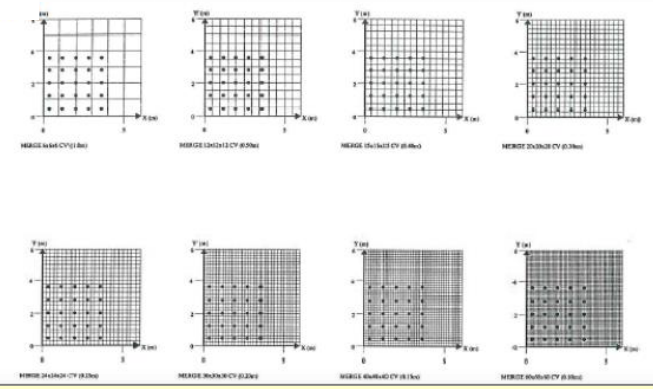

MERGE Case 23: Geometry E, methane.

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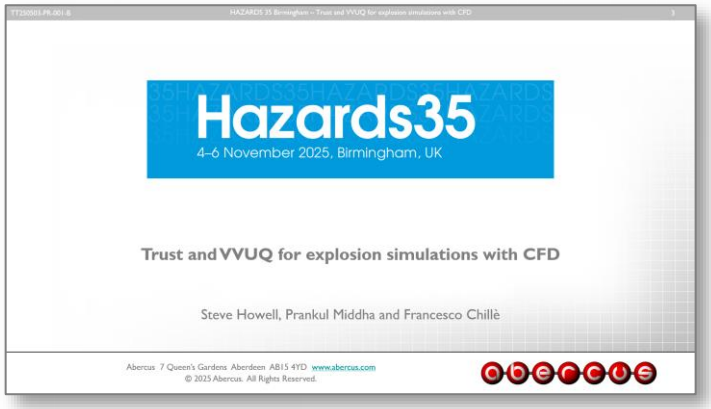

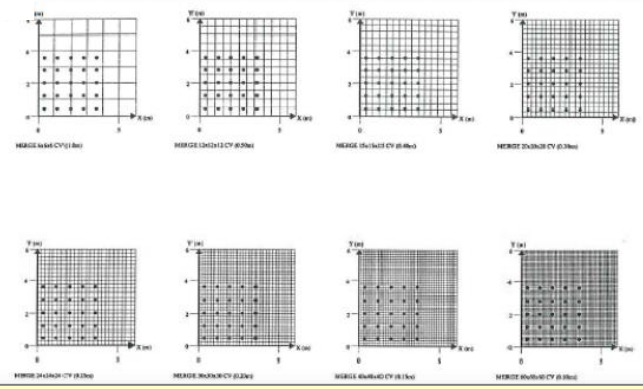

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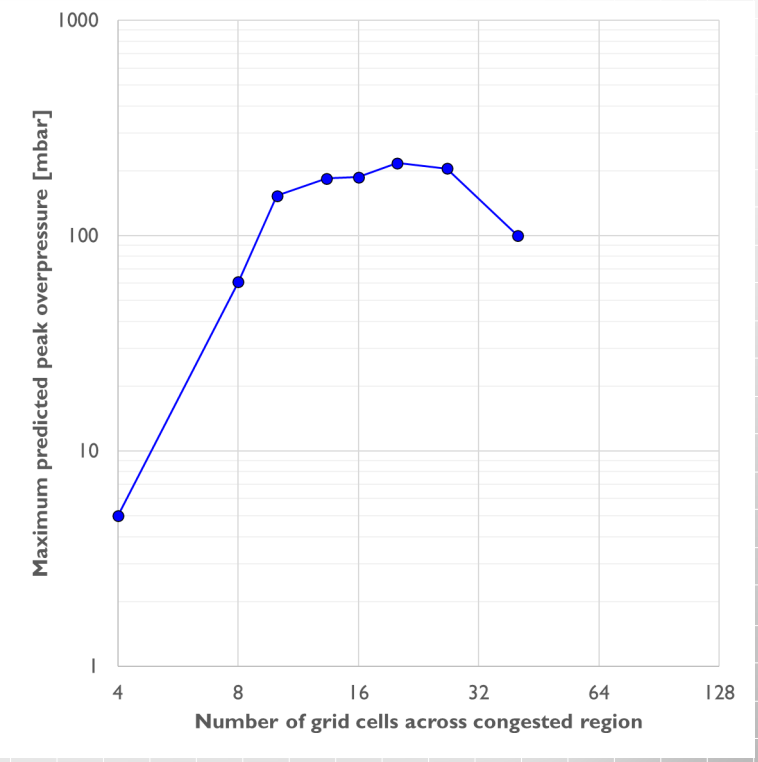
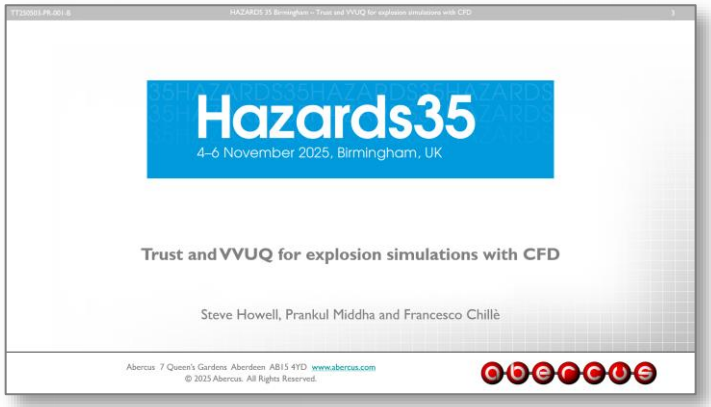
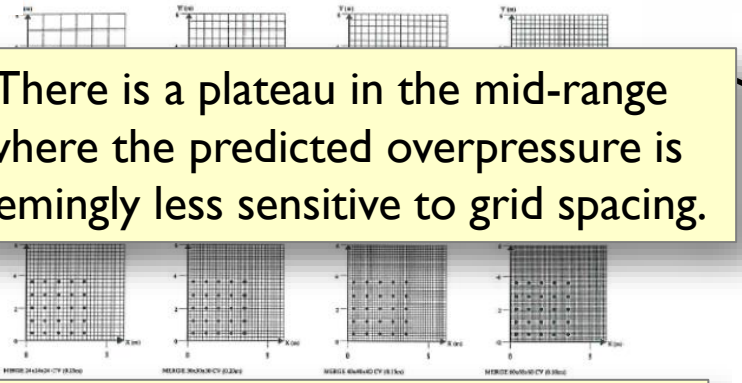


User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – PDR-CFD training (1994 report)





There is a plateau in the mid-range where the predicted overpressure is seemingly less sensitive to grid spacing.

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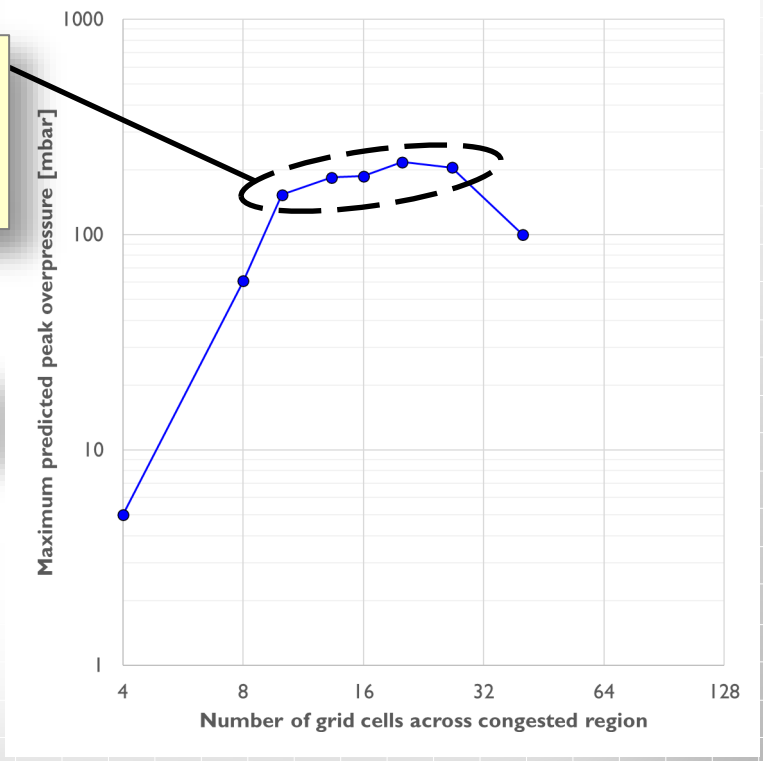
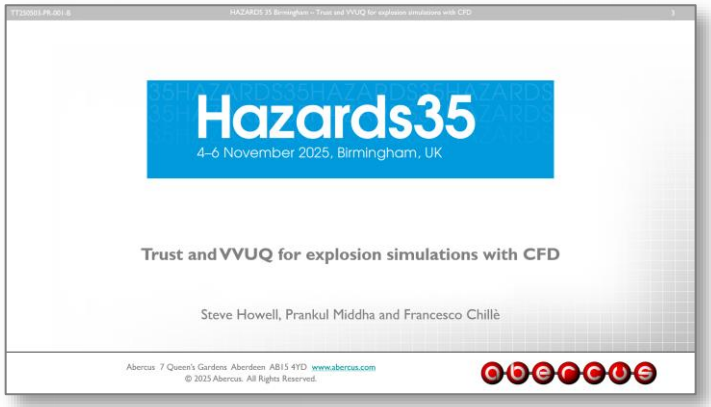
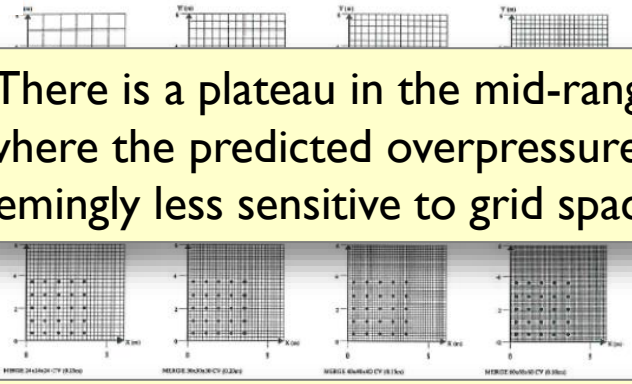


User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – PDR-CFD training (1994 report)





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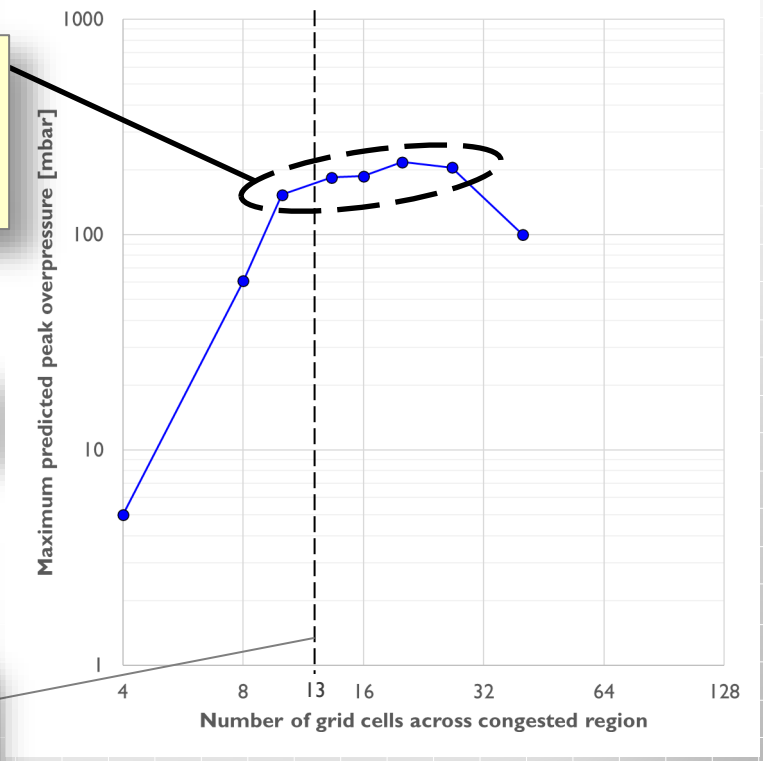
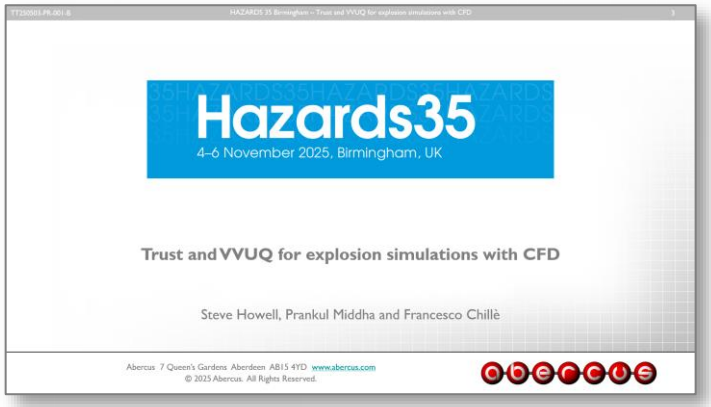
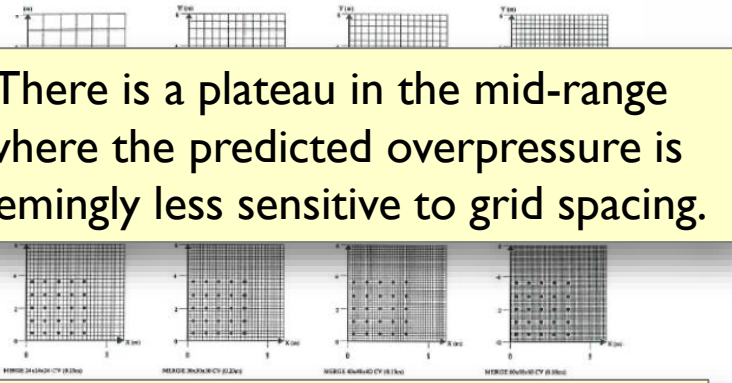
Grid recommendations at the time were for 13 cells across the cloud.
(This could be reduced if bounded by a solid surface).



User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – PDR-CFD training (1994 report)



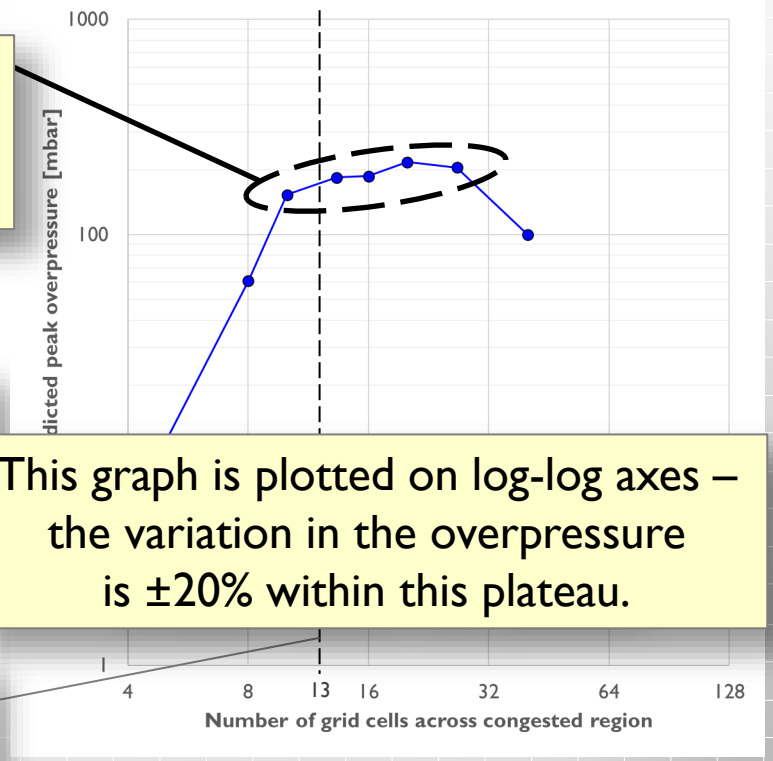


There is a plateau in the mid-range where the predicted overpressure is seemingly less sensitive to grid spacing.

MERGE Case 23: Geometry E, methane.

Resolution	CPU-time (HP735)	Max. pressure	Time of max. press.	Press. impulse
6x6x6	5.2 s	5 mbar	0.72 s	58 Pas
12x12x12	74.8 s (1 min)	61 mbar	0.43 s	239 Pas
15x15x15	222 s (4 min)	153 mbar	0.42 s	375 Pas
20x20x20	902 s (15 min)	184 mbar	0.44 s	405 Pas
24x24x24	1.576 s (25 min)	187 mbar	0.34 s	508 Pas

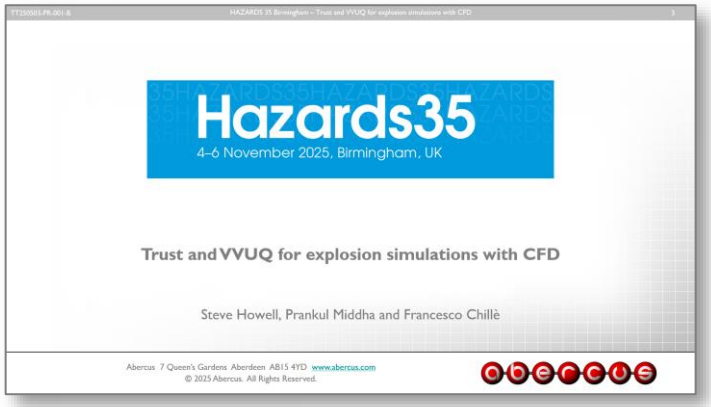
Grid recommendations at the time were for 13 cells across the cloud.
(This could be reduced if bounded by a solid surface).

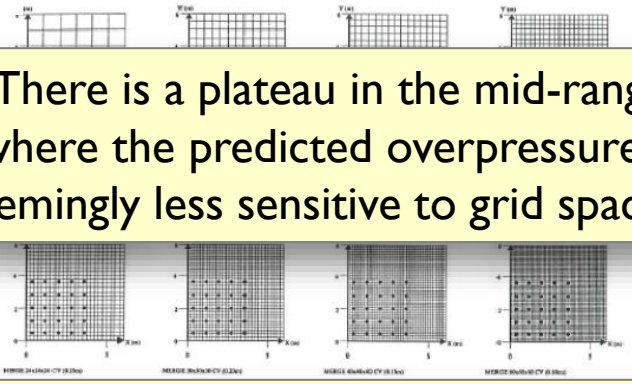


This graph is plotted on log-log axes – the variation in the overpressure is ±20% within this plateau.

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – PDR-CFD training (1994 report)





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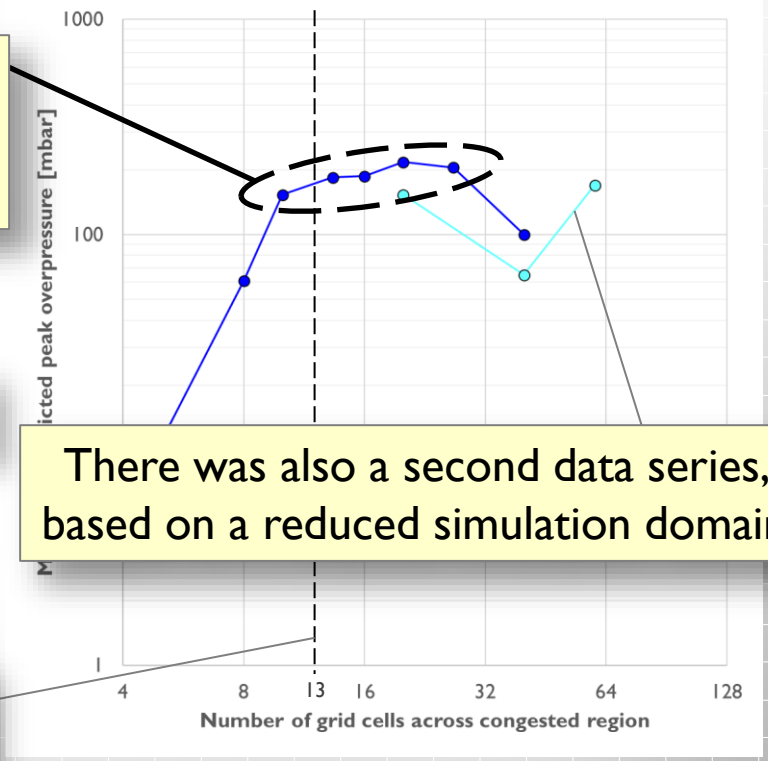
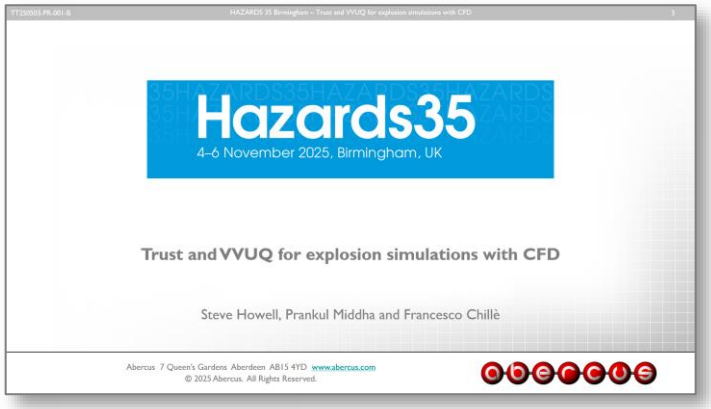


There was also a second data series, based on a reduced simulation domain

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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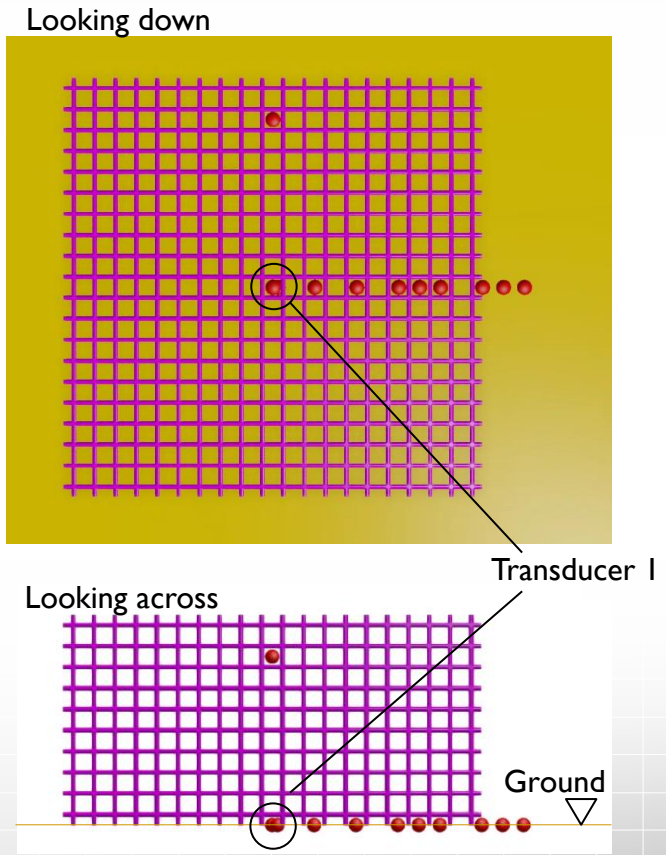
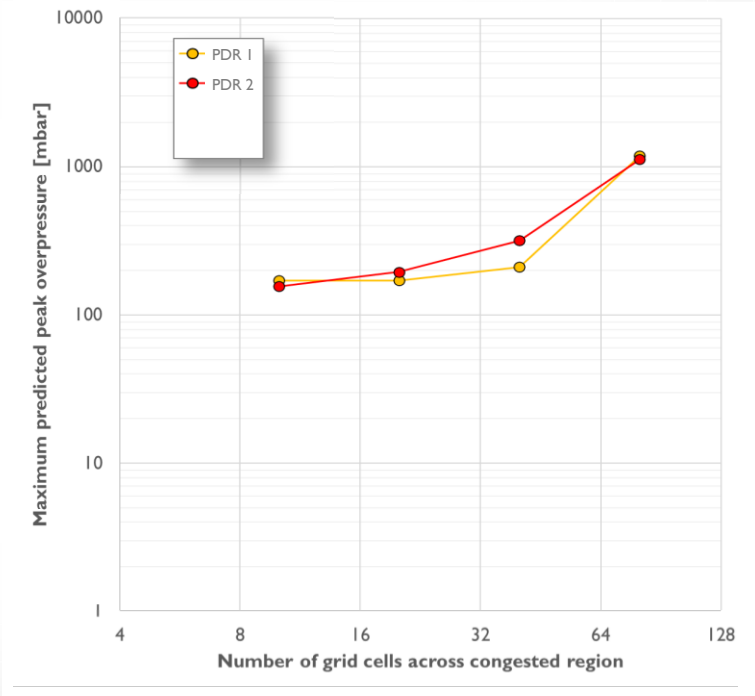
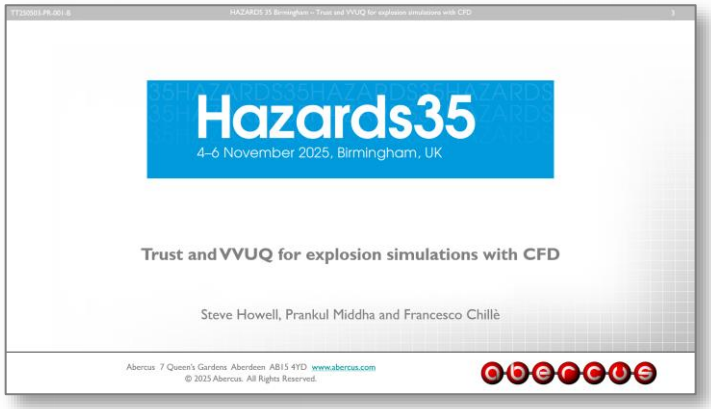




User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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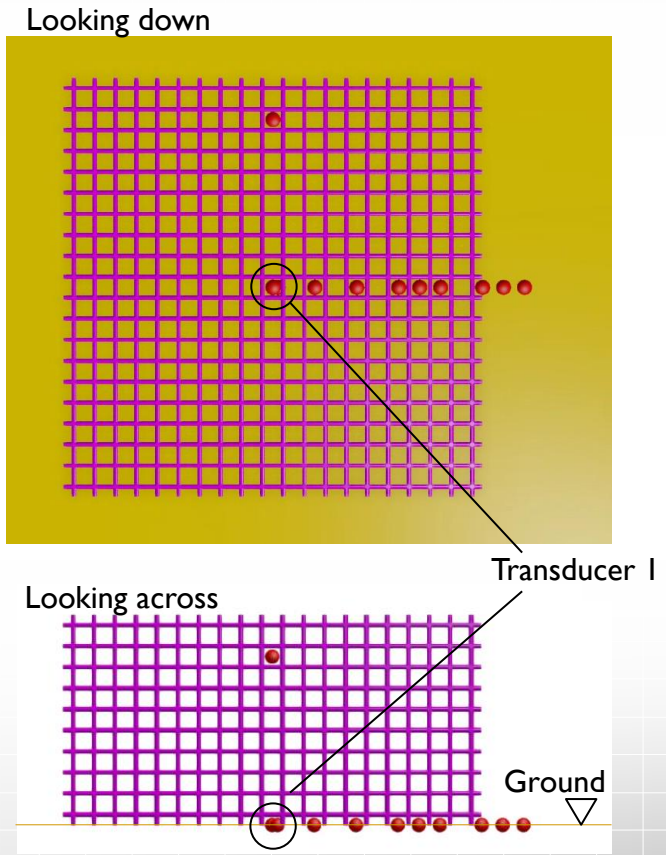
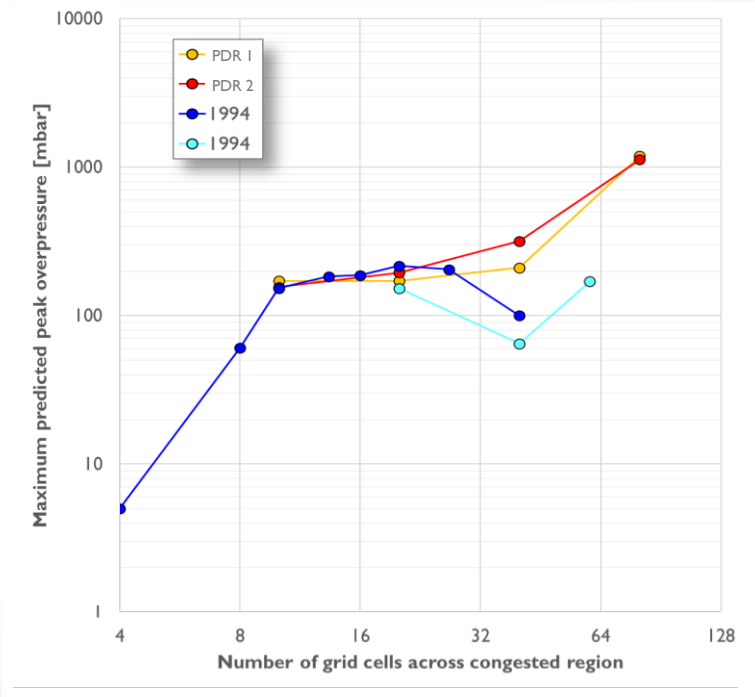
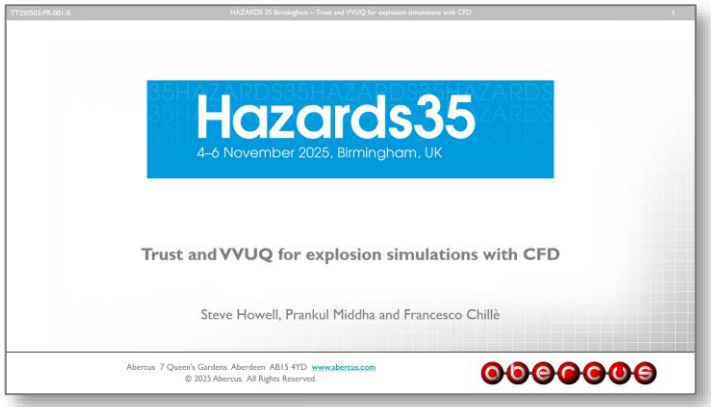




User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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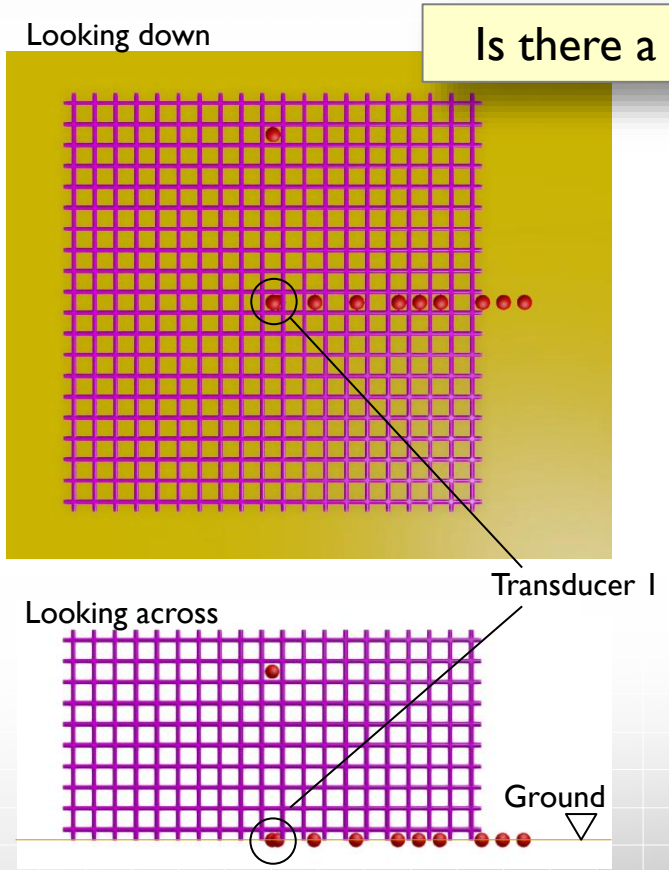
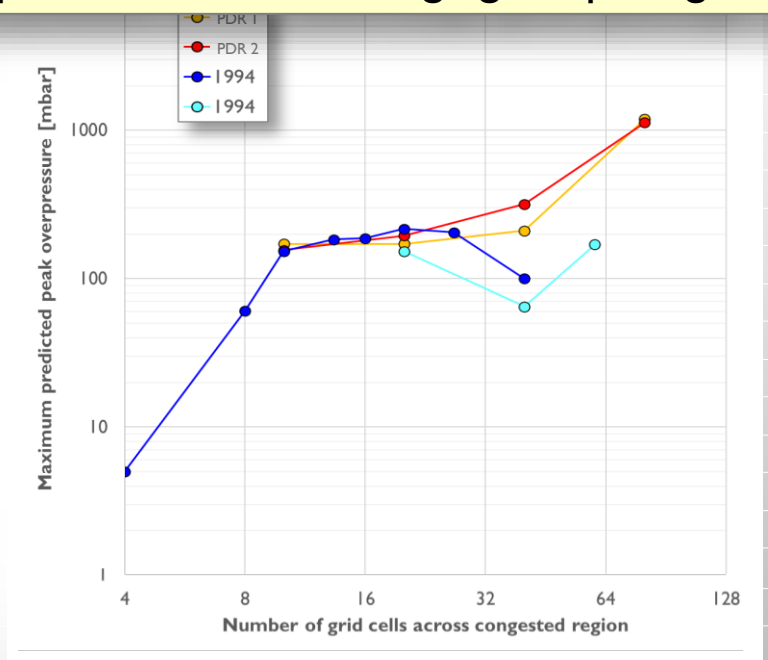
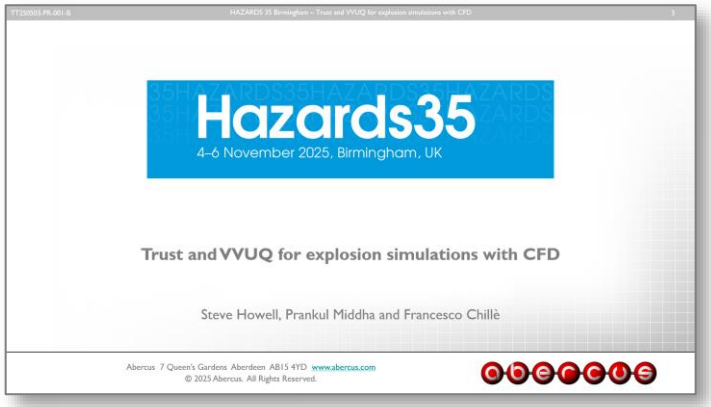


Is there a plateau in the mid-range grid spacing?



User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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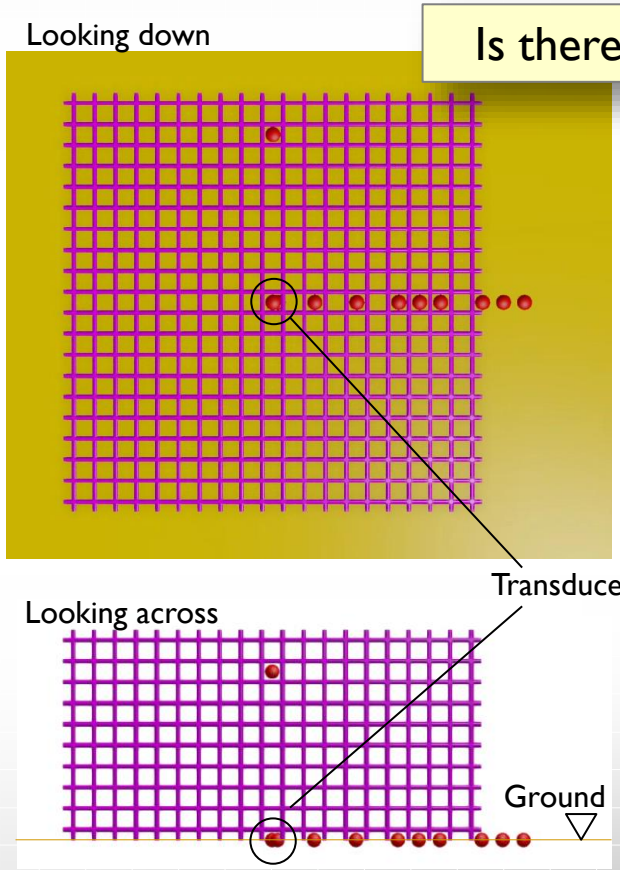

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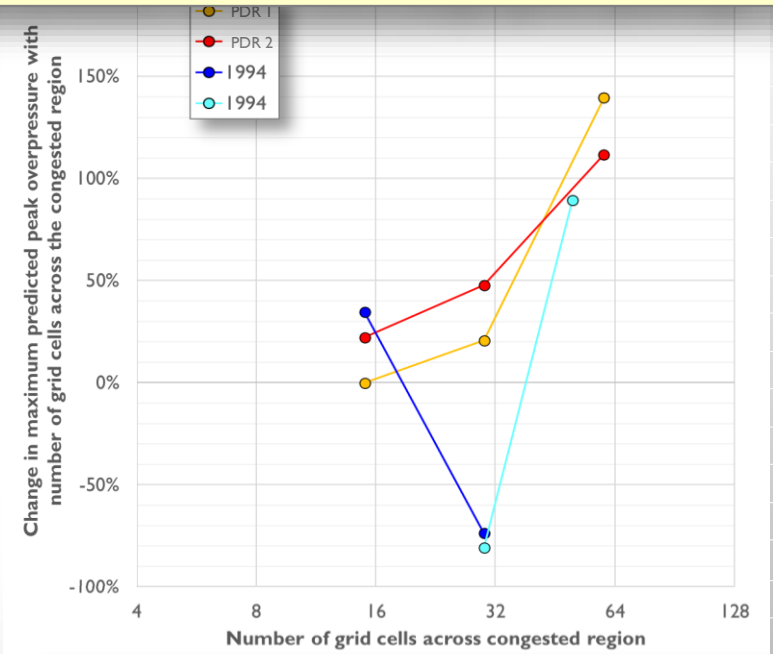
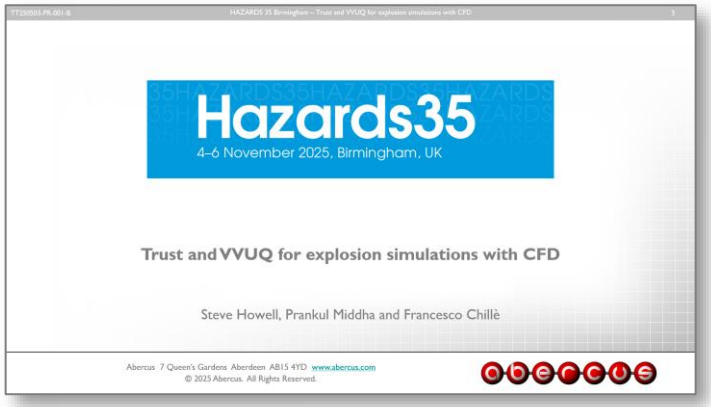


Differentiate and plot the change in overpressure with grid spacing…

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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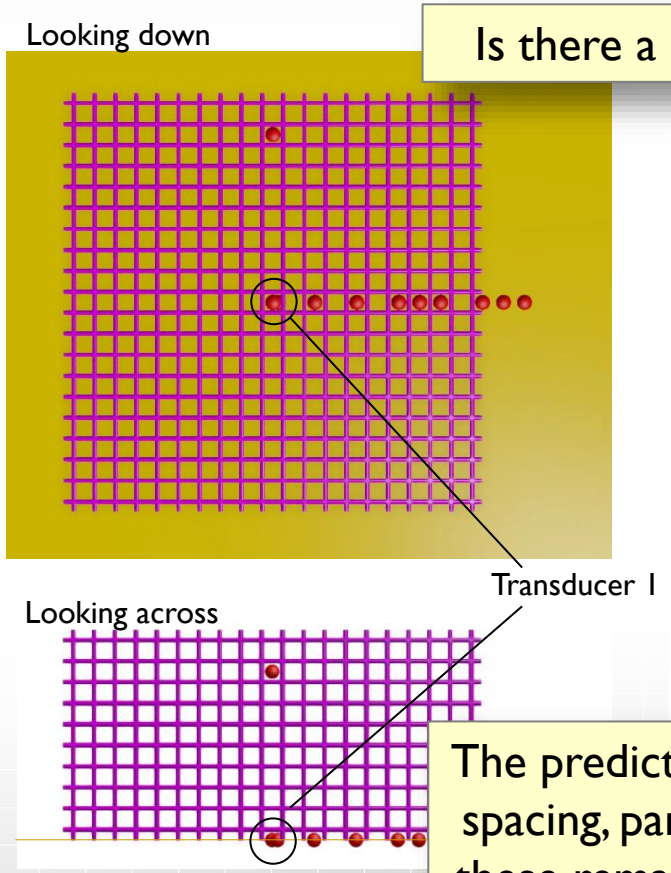

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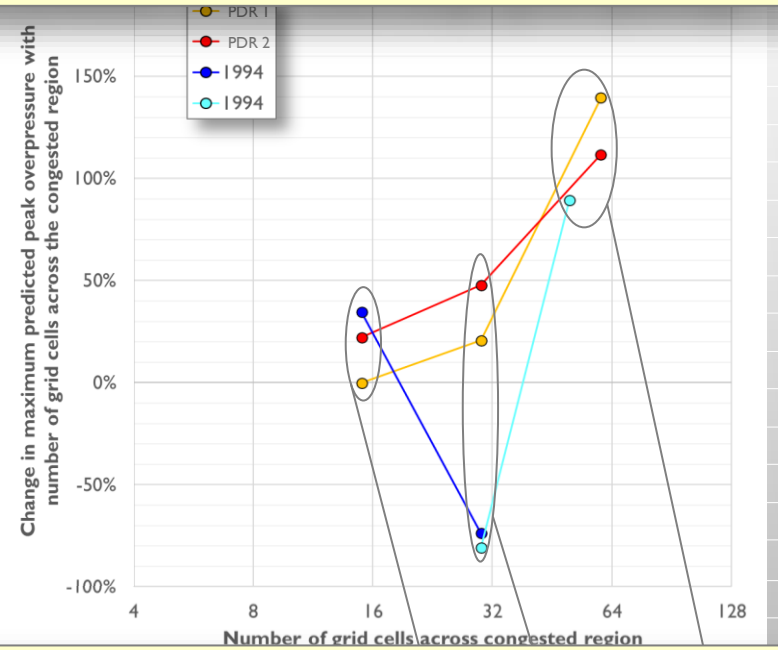
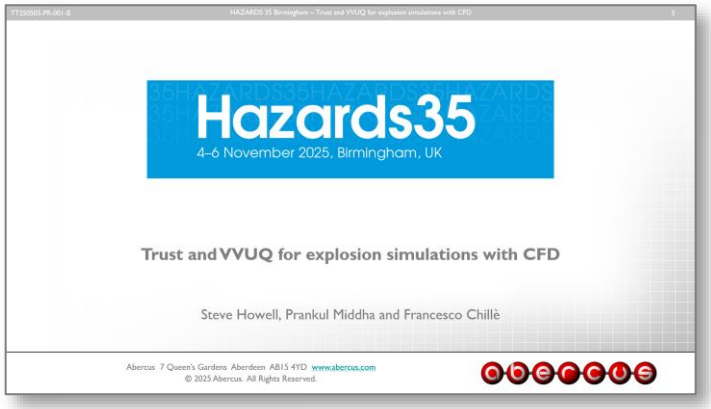


The predicted overpressure is sensitive to the grid spacing, particularly on further refined grids – but these remain within the code's gridding guidelines.

User VVUQ – solution verification

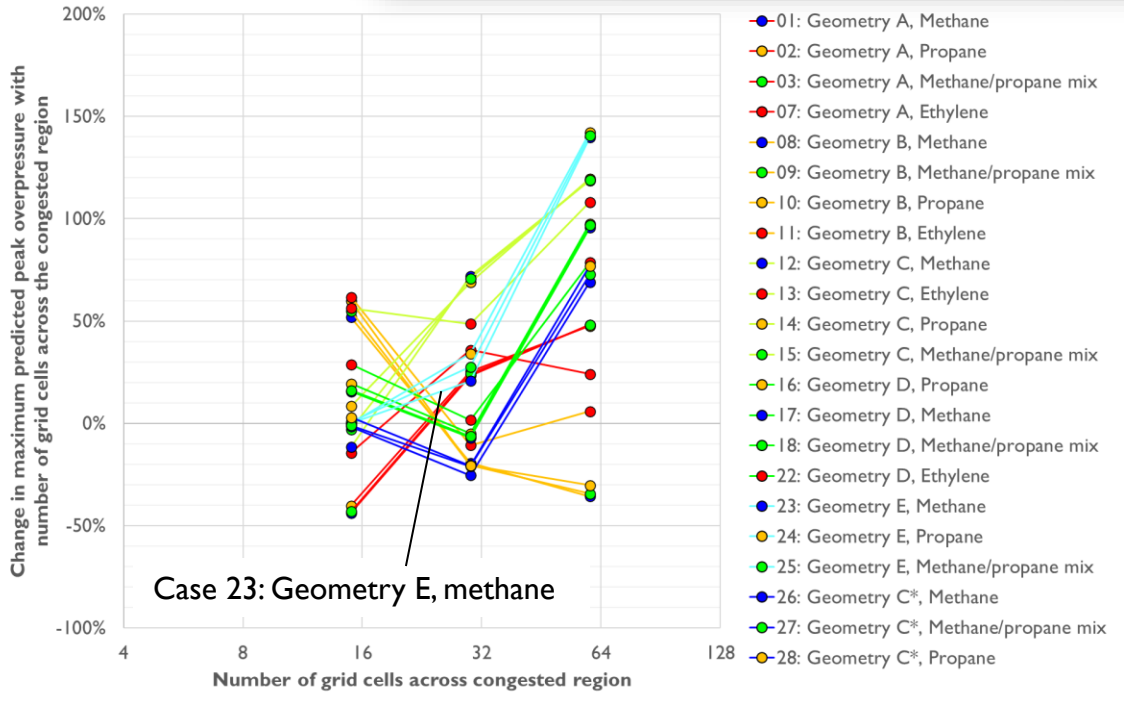
Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



What about the other MERGE geometries?

Is there a plateau in the mid-range grid spacing?

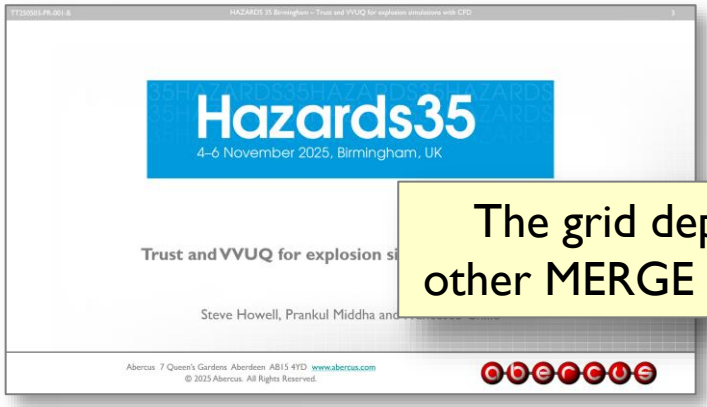
PDR 1



Lines coloured by geometry, markers coloured by fuel.

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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The grid dependence is seemingly greater for other MERGE cases @15 cells than for Case 23…

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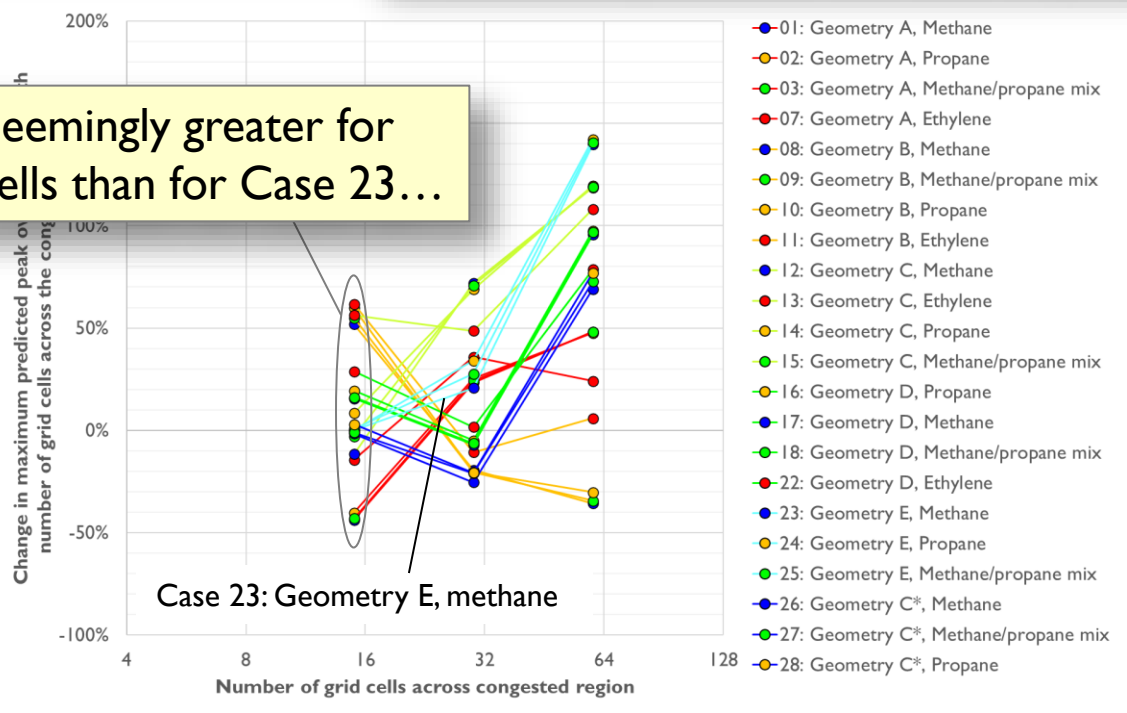

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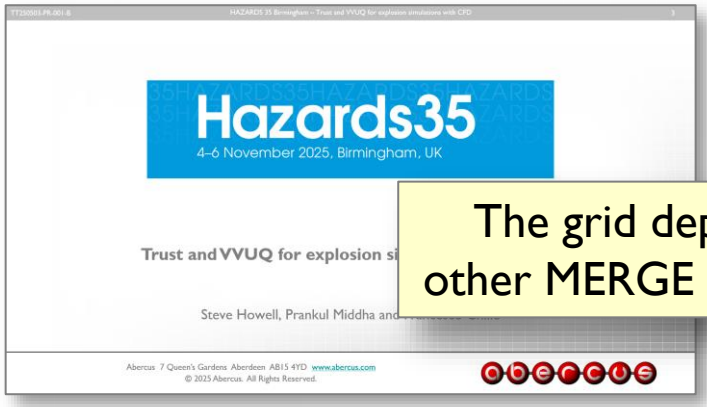

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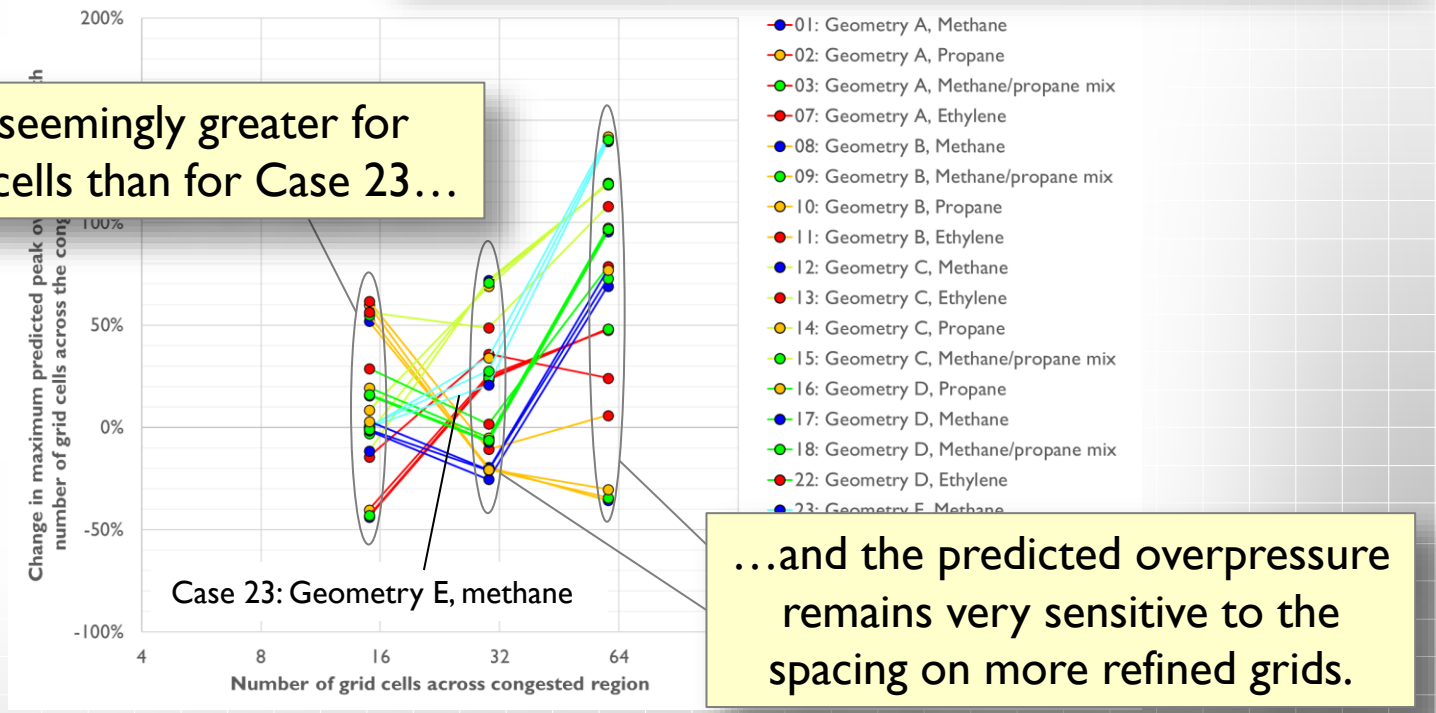

…and the predicted overpressure remains very sensitive to the spacing on more refined grids.

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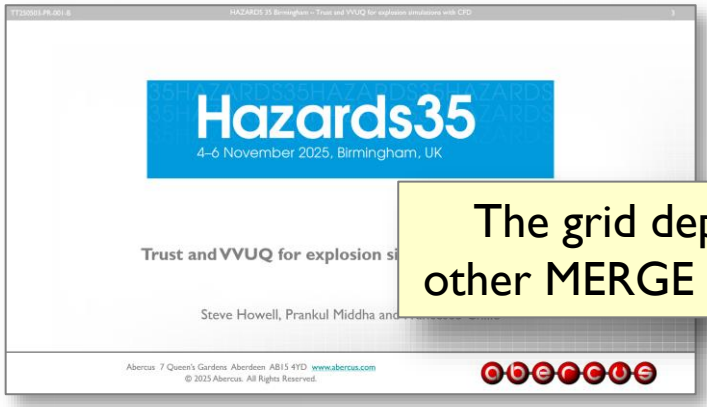
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (MERGE)



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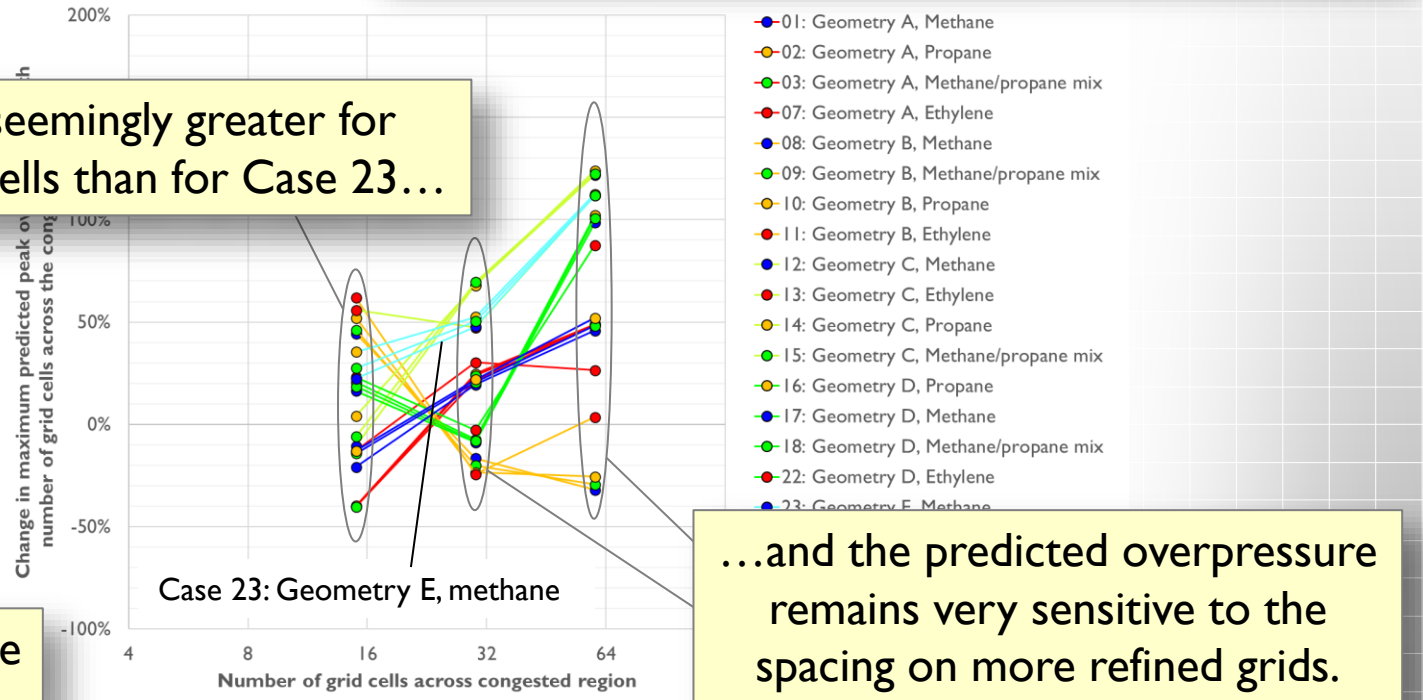

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And the predictions depend upon the version of the PDR-CFD code used.

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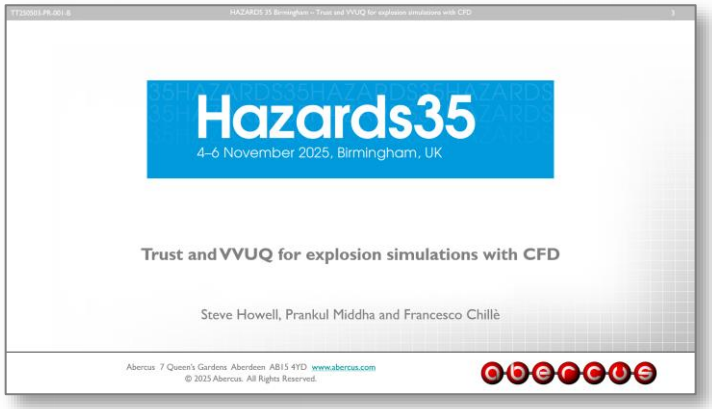
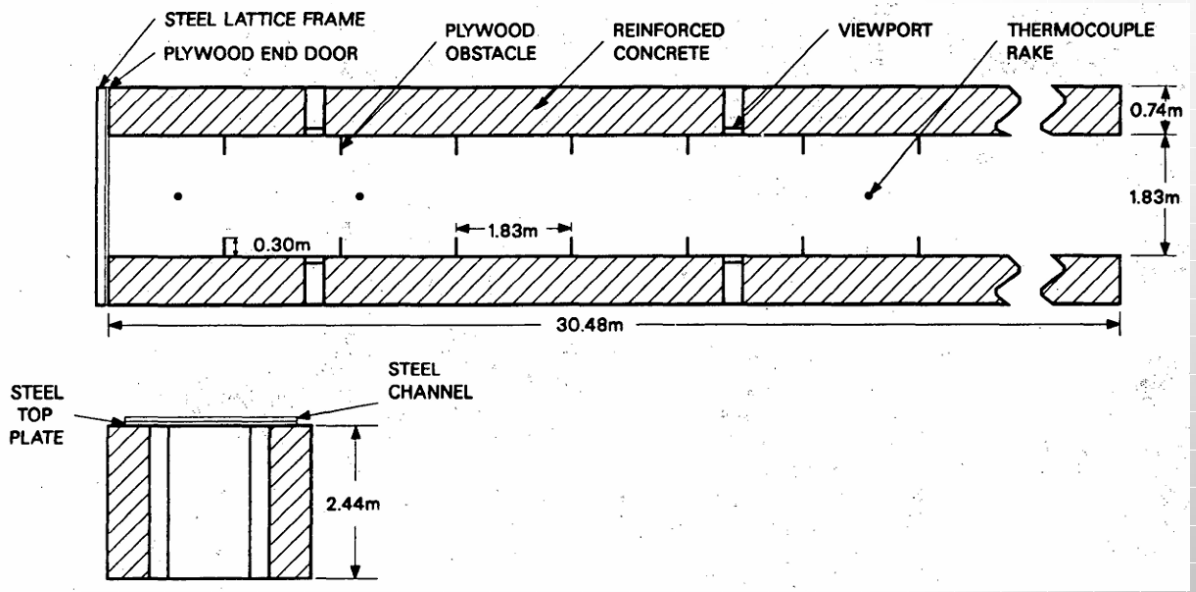
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



What about the other validation cases?:
Sandia FLAME (large-scale hydrogen test)



[Ref. 16]: A. Sherman, Martin Philip and Tieszen, SR and Benedick, William B (1989), FLAME facility: The effect of obstacles and transverse venting on flame acceleration and transition on detonation for hydrogen-air mixtures at large scale. https://www.nrc.gov/docs/ML0717/ML071700076.pdf.

User VVUQ – solution verification

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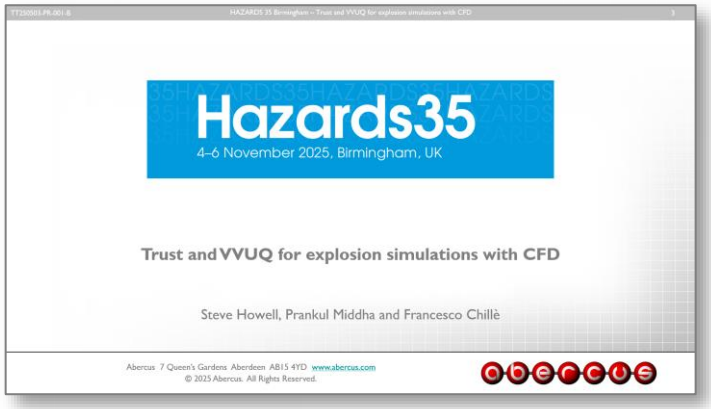

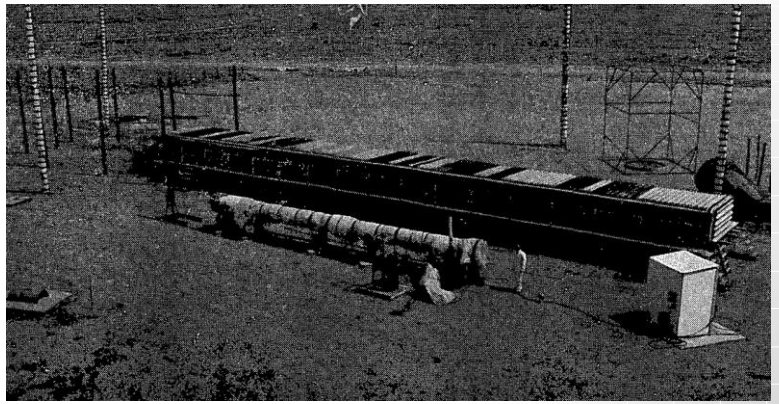

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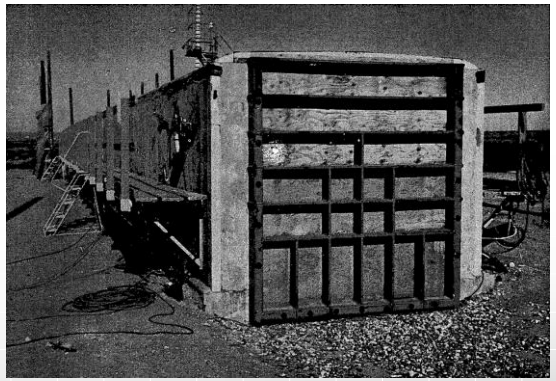

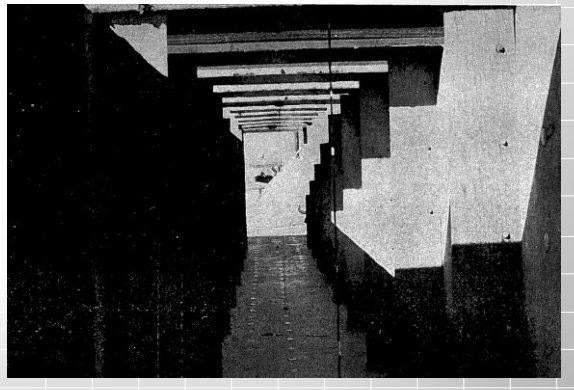

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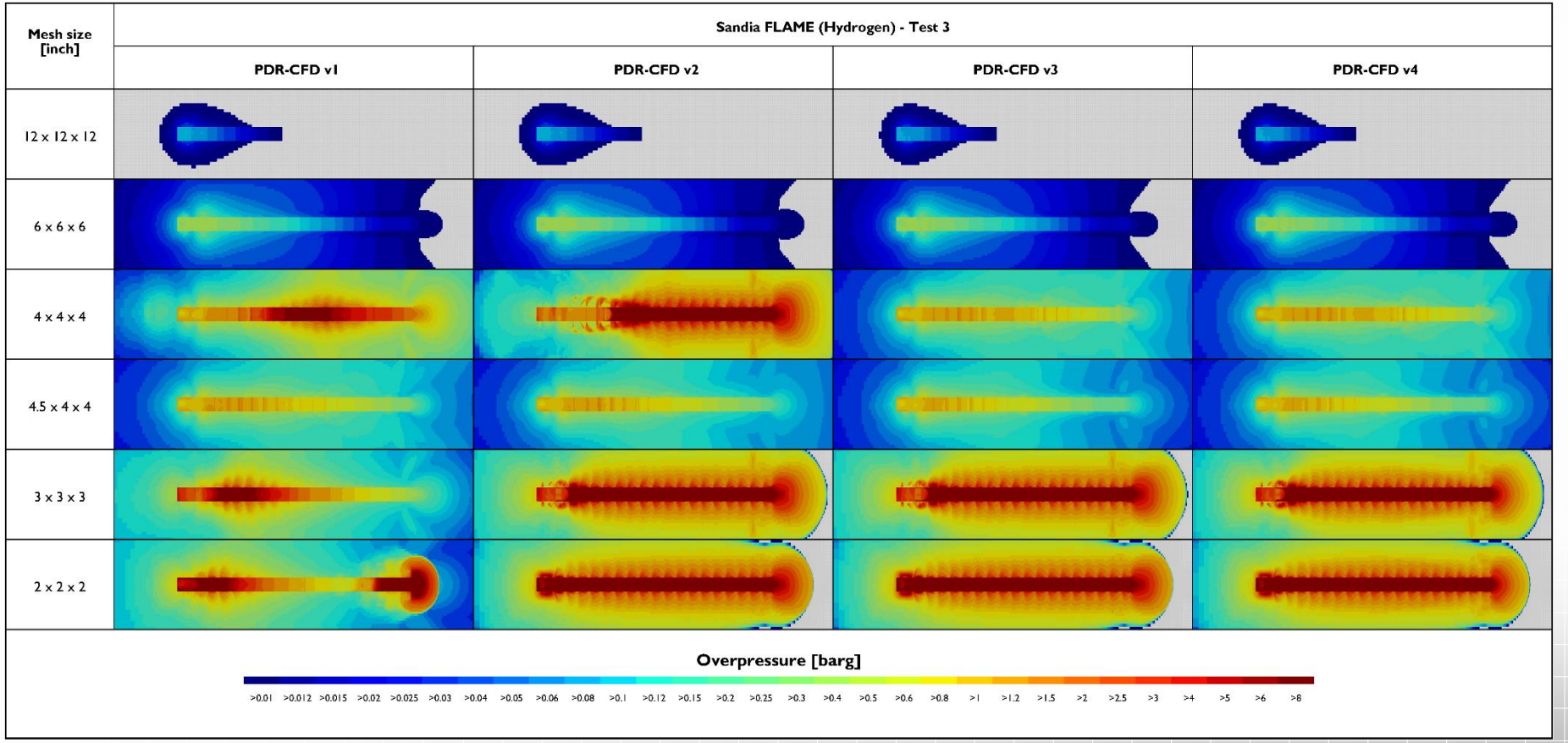
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



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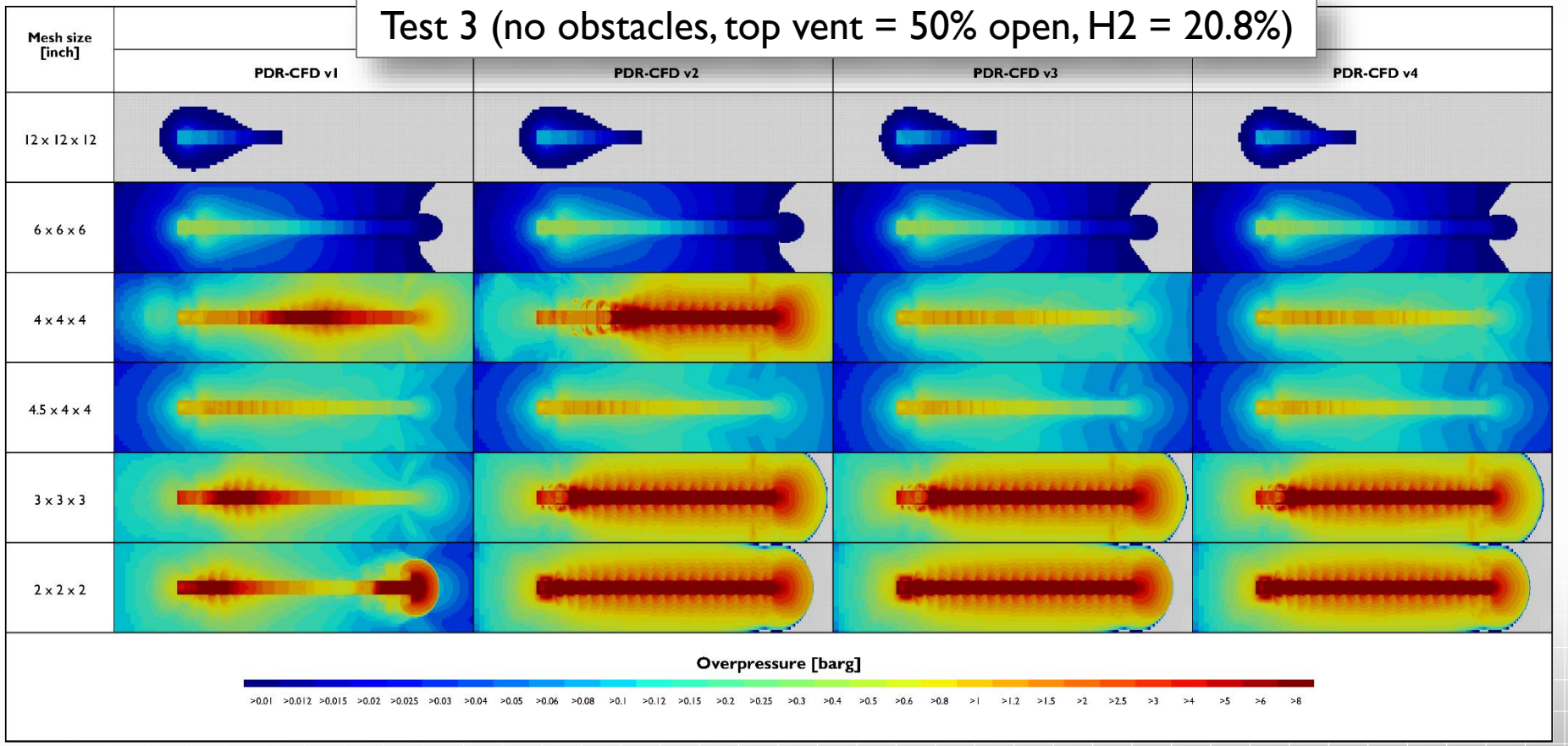

User VVUQ – solution verification

Sensitivity of overpressure to grid spacin

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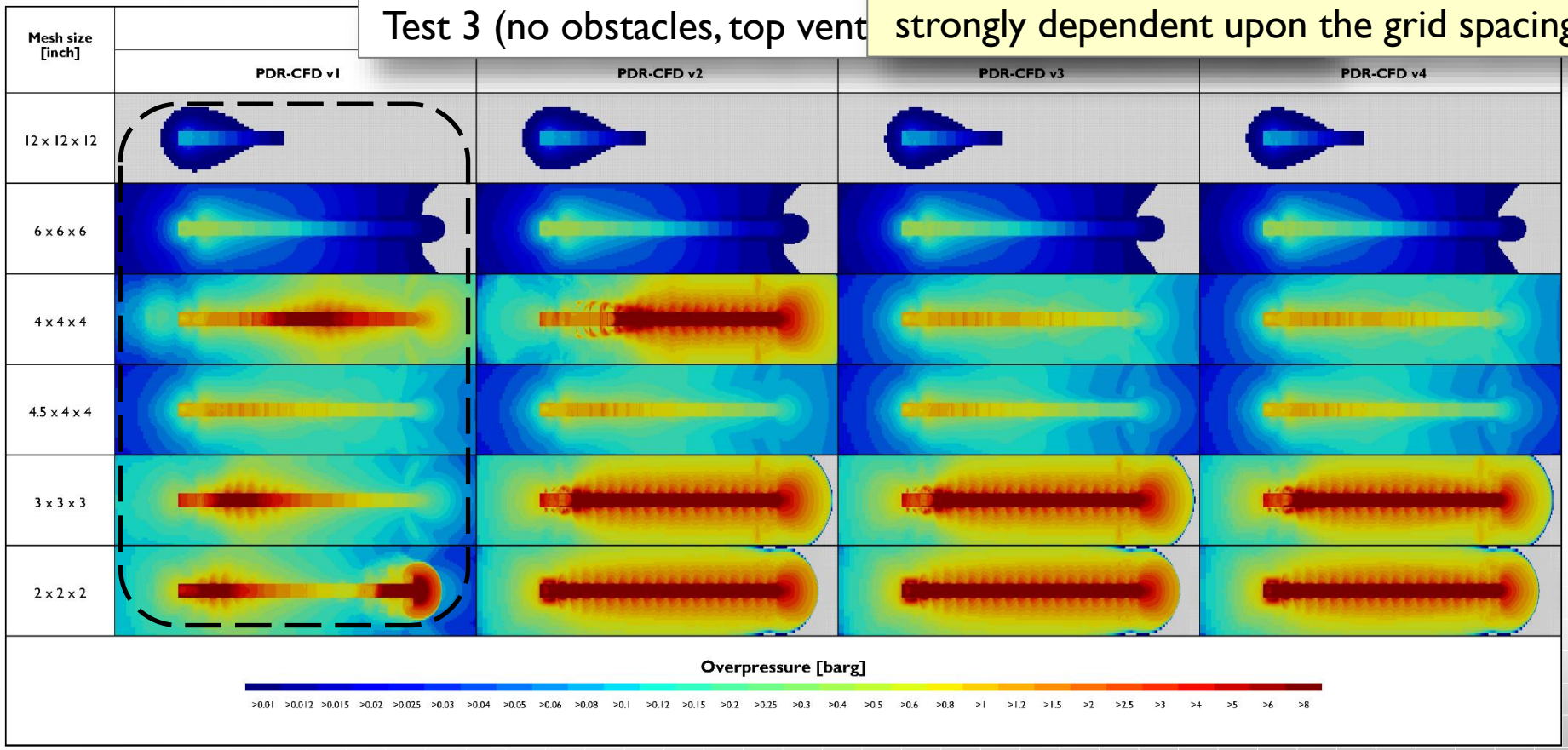

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Sensitivity of overpressure to grid spacin

Test 3 (no obstacles, top vent

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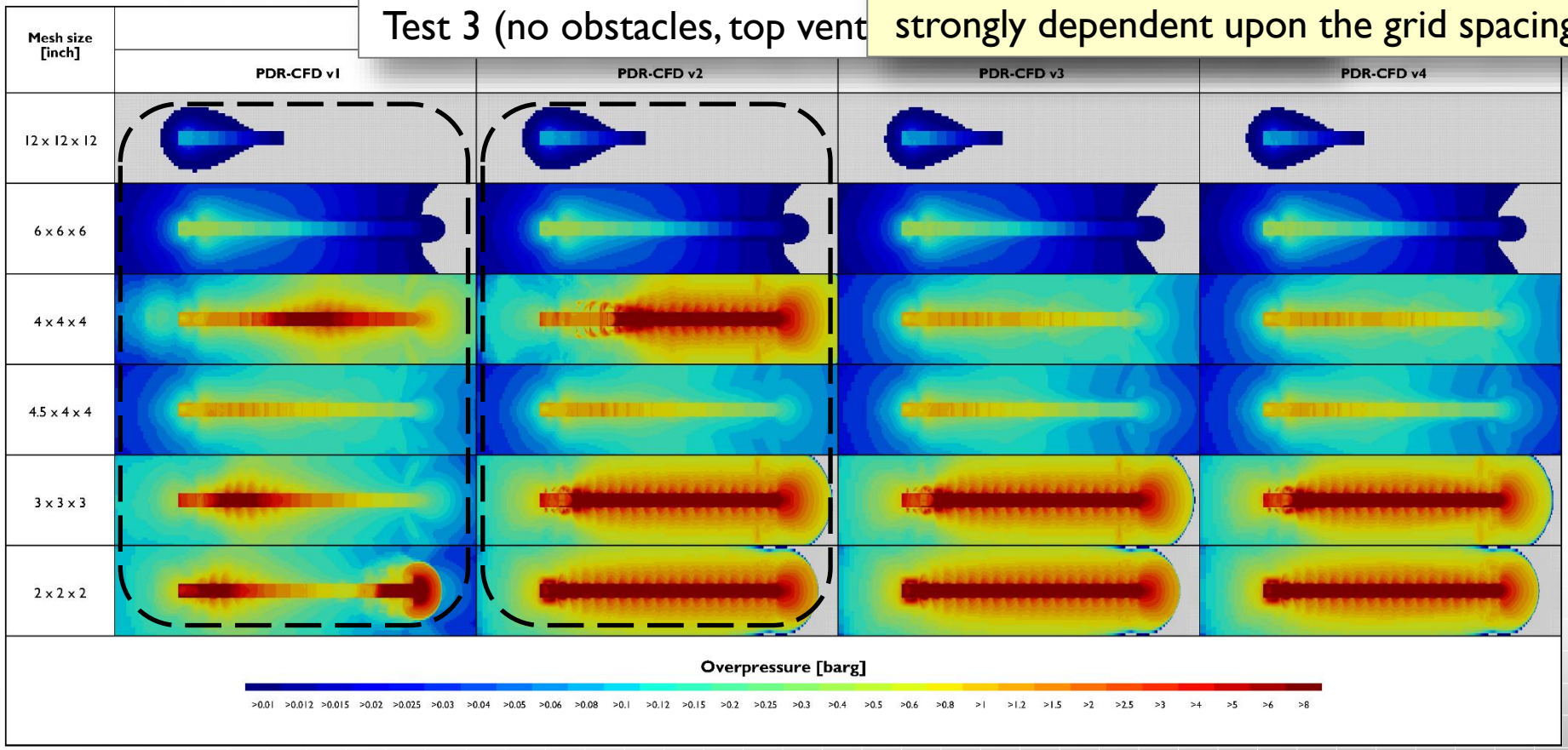

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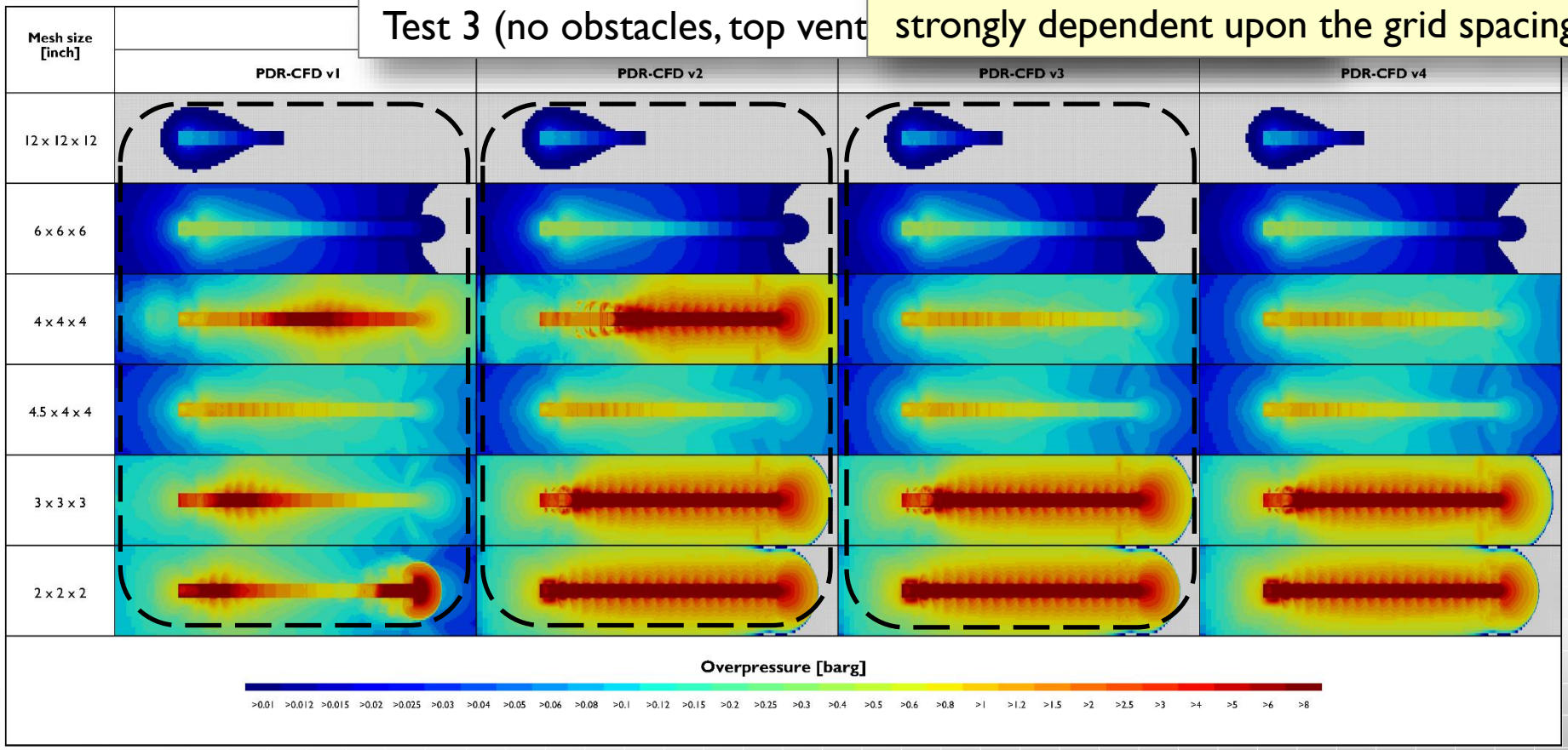

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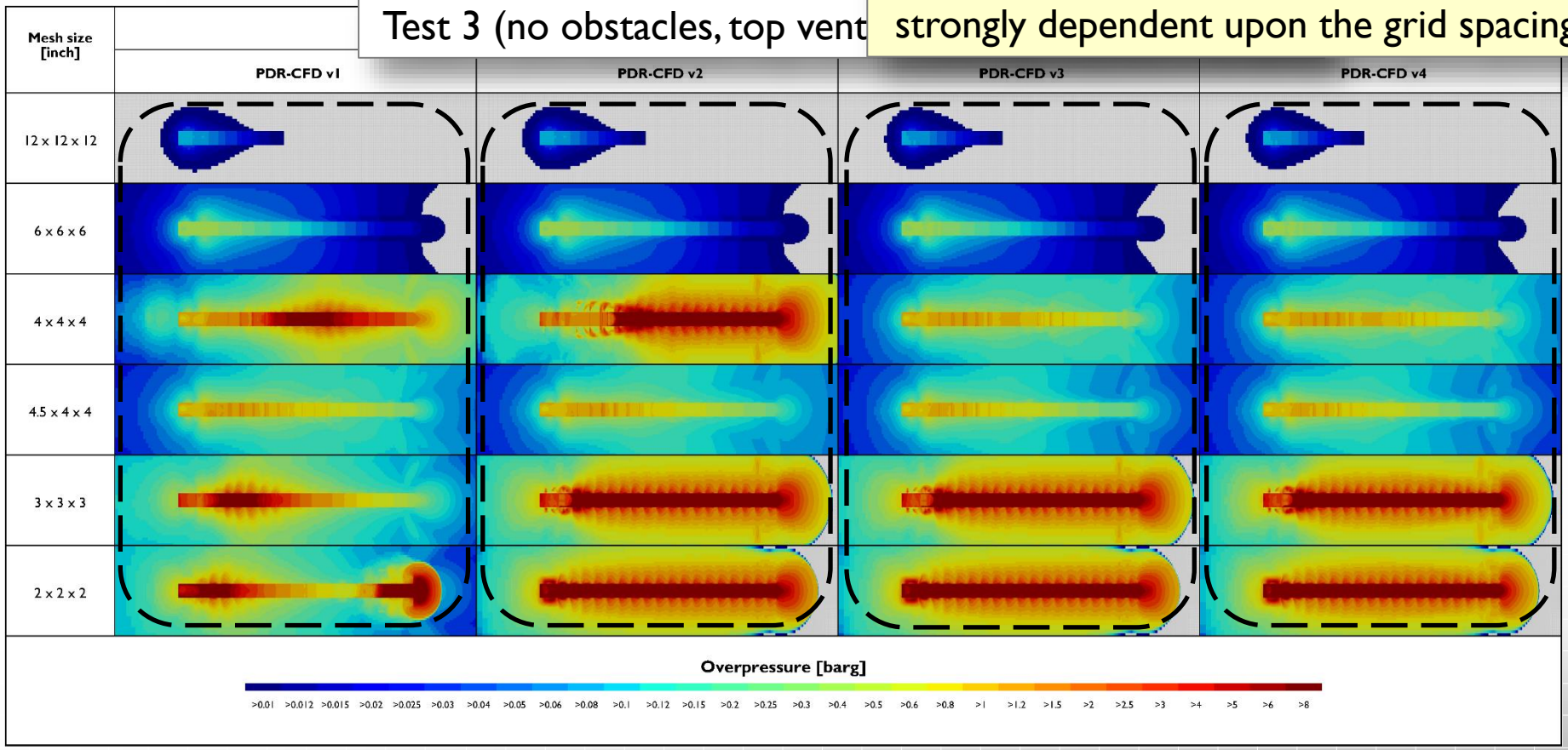

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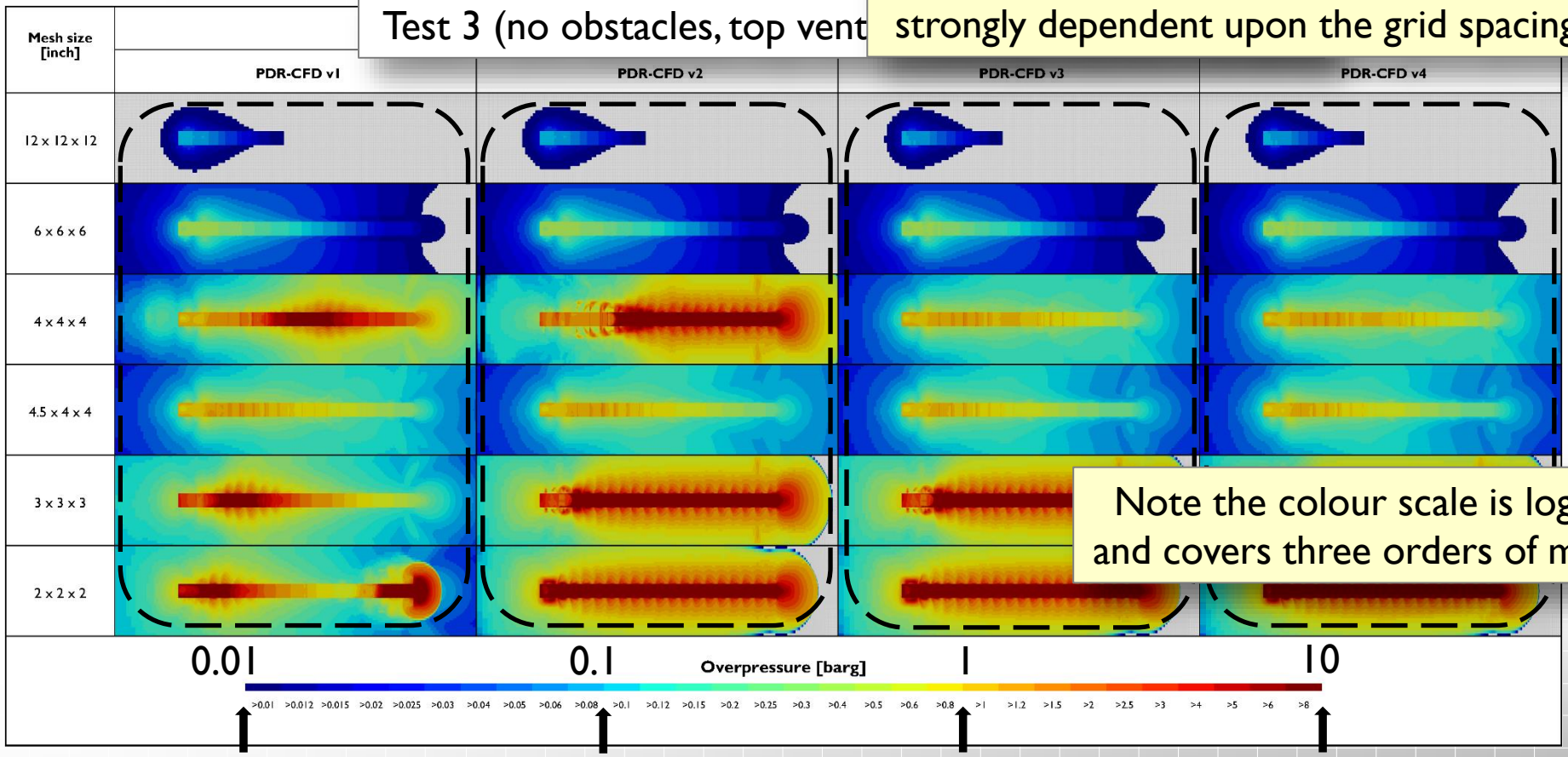

Note the colour scale is logarithmic and covers three orders of magnitude!

User VVUQ – solution verification

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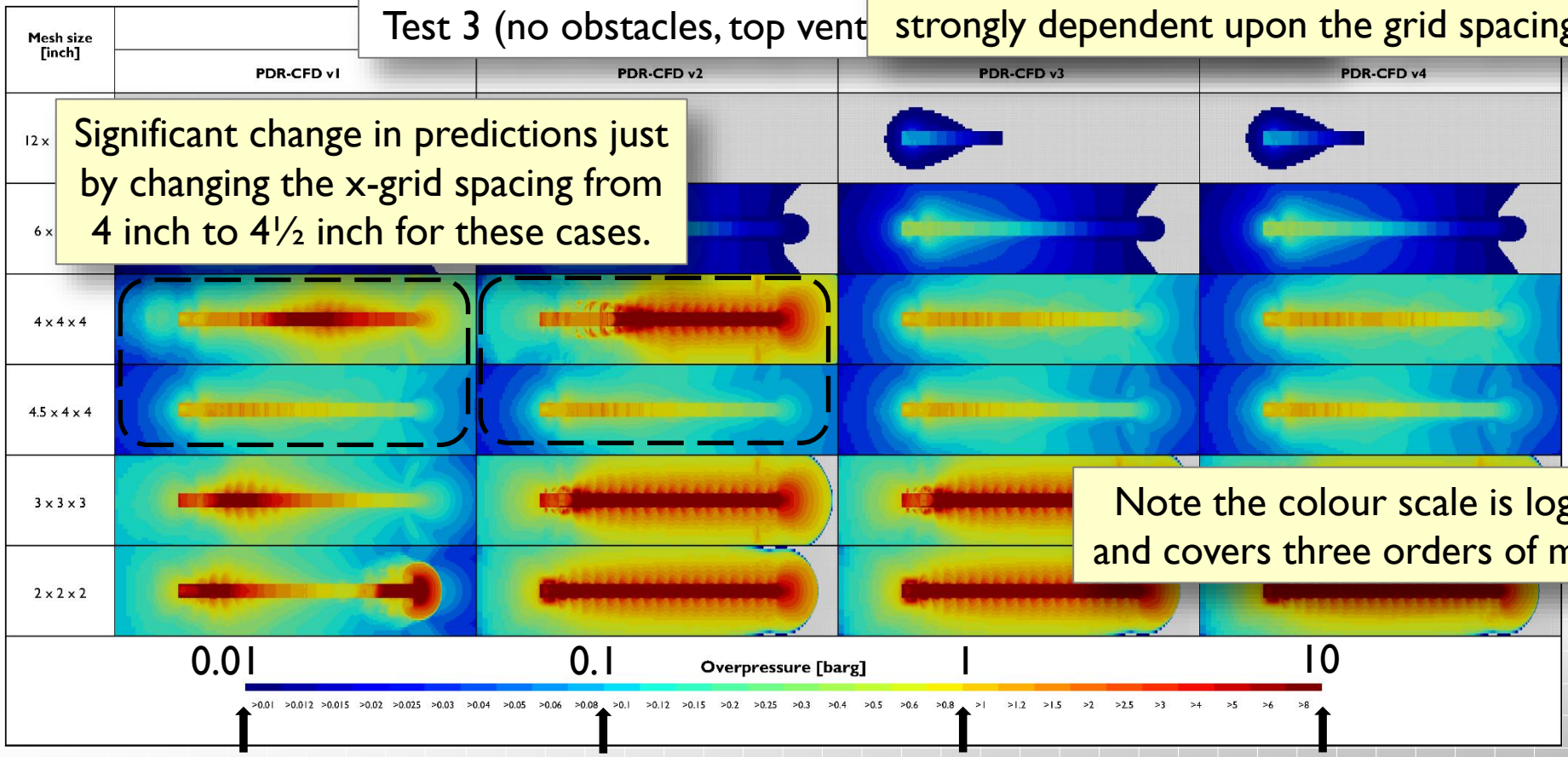
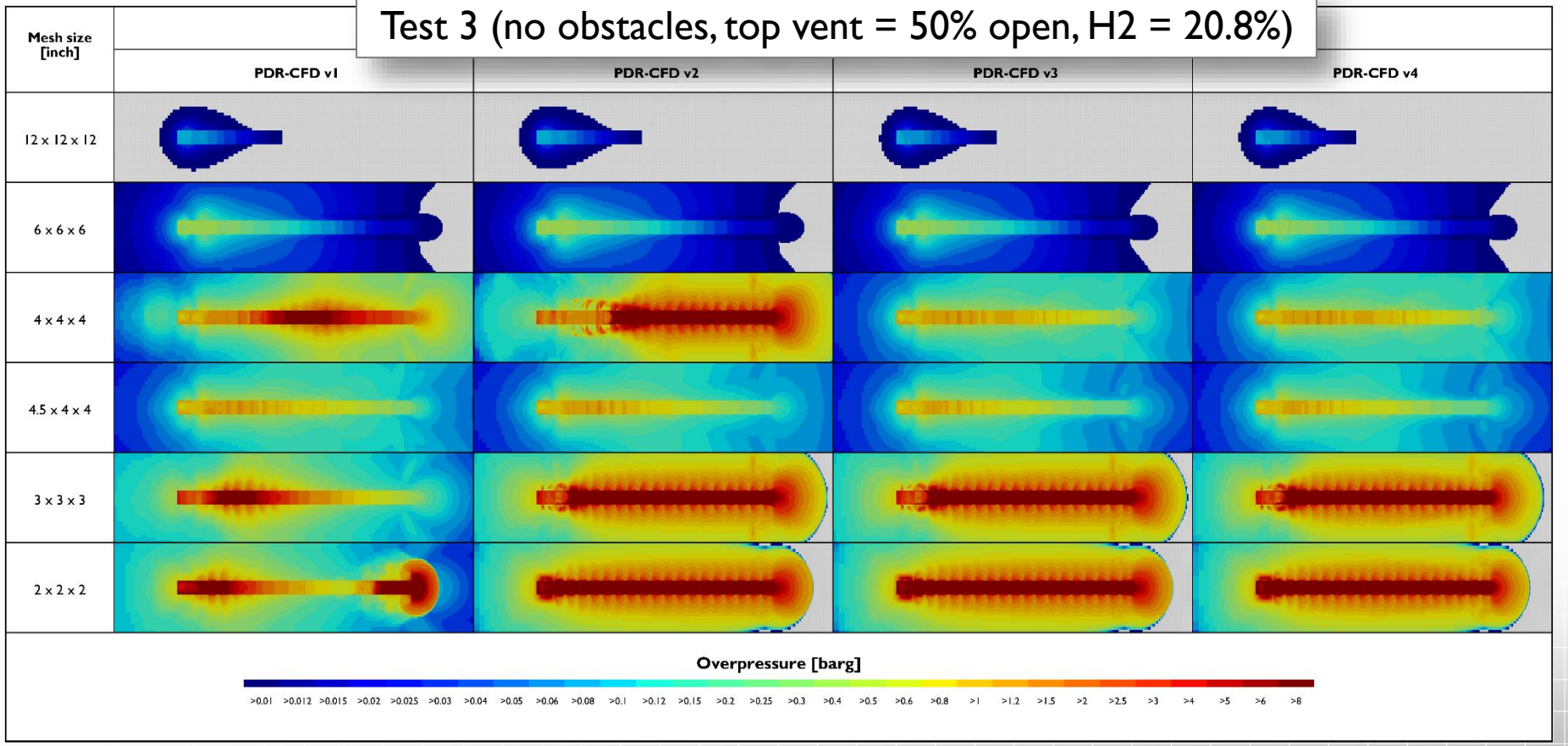


Significant change in predictions just by changing the x-grid spacing from 4 inch to 4½ inch for these cases.

Note the colour scale is logarithmic and covers three orders of magnitude!

User VVUQ – solution verification

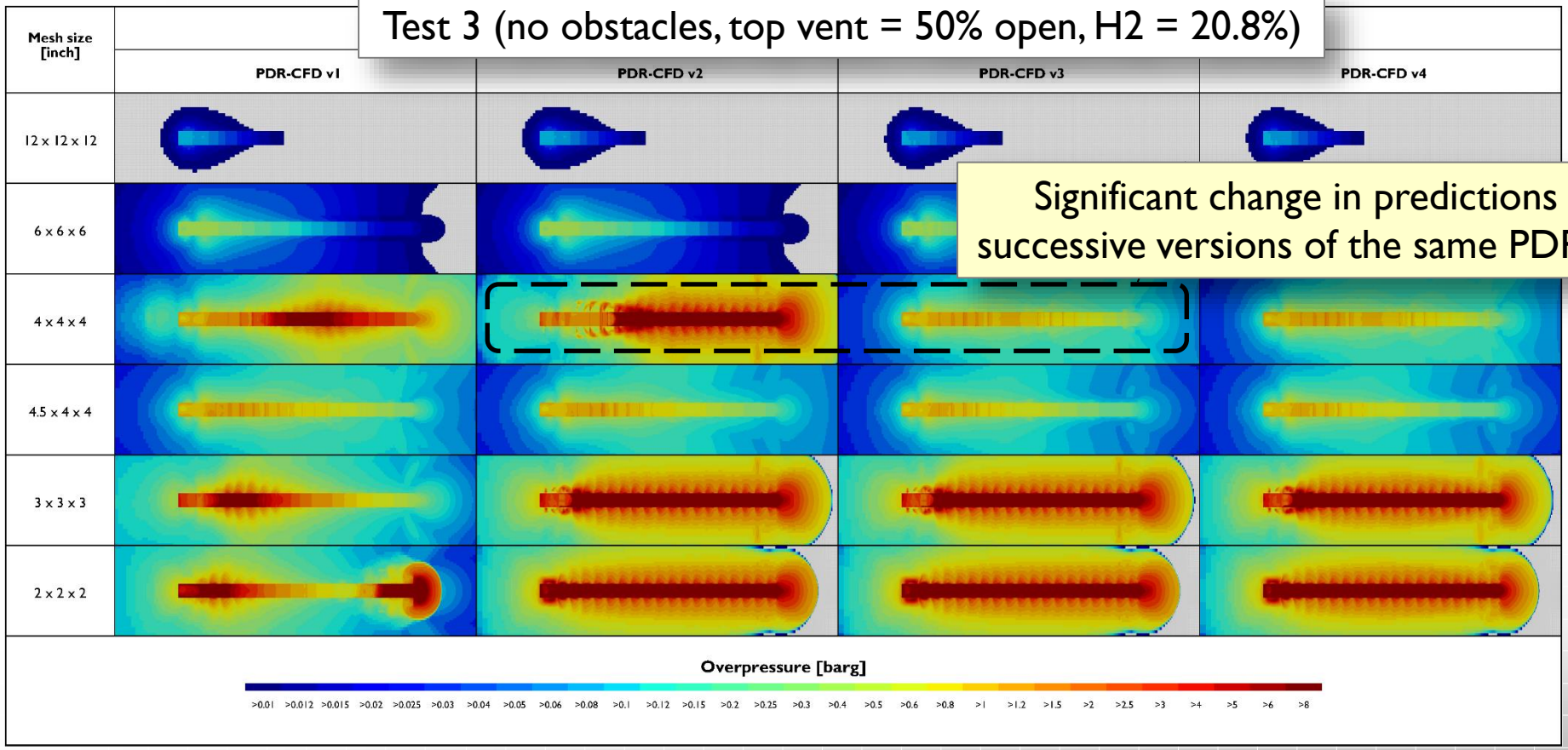
Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

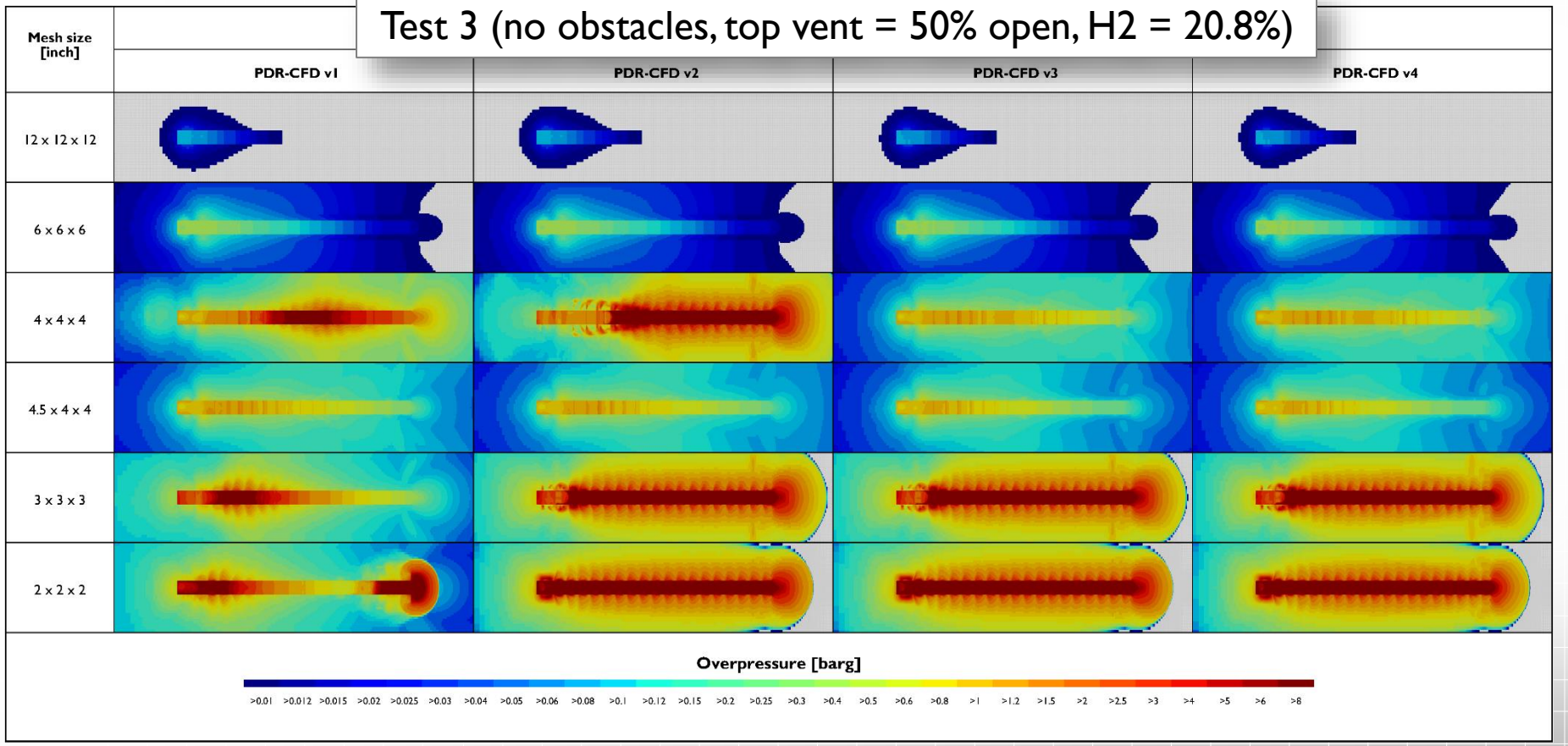
Test 3 (no obstacles, top vent = 50% open, H2 = 20.8%)



Significant change in predictions between successive versions of the same PDR-CFD code

User VVUQ – solution verification

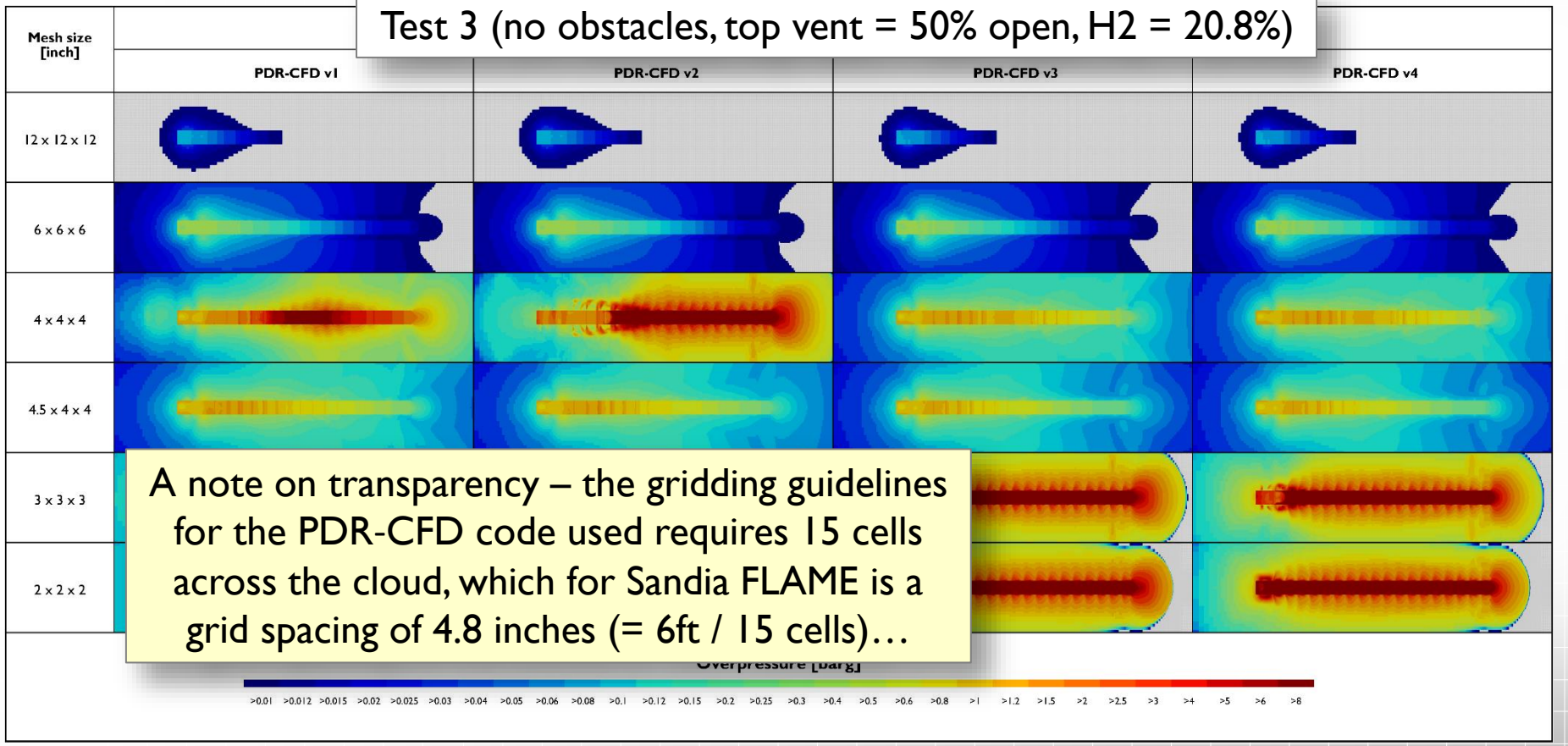
Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Test 3 (no obstacles, top vent = 50% open, H2 = 20.8%)



Recommended maximum grid size (4.8 inch)

A note on transparency – the gridding guidelines for the PDR-CFD code used requires 15 cells across the cloud, which for Sandia FLAME is a grid spacing of 4.8 inches (= 6ft / 15 cells)…

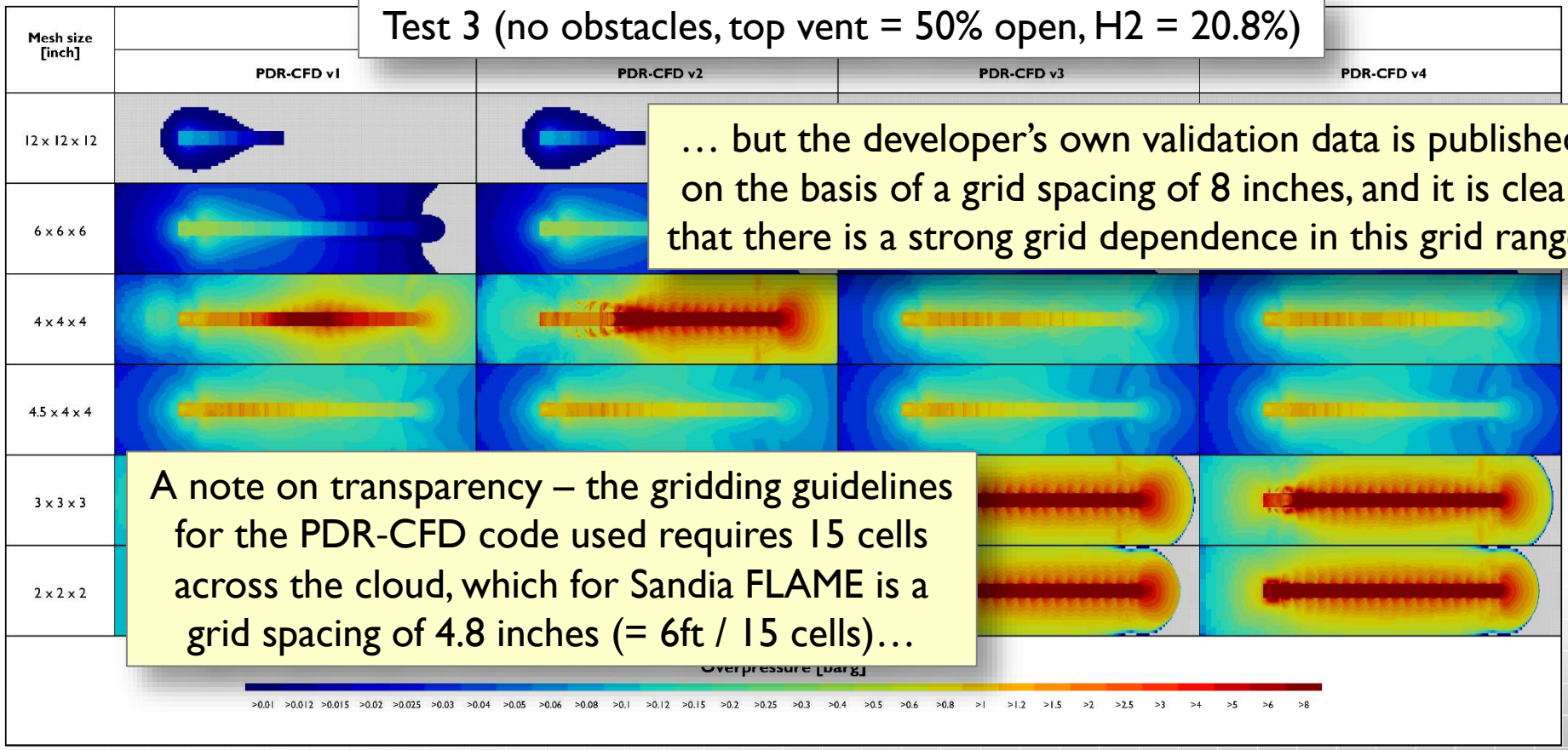
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Test 3 (no obstacles, top vent = 50% open, H2 = 20.8%)

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)



… but the developer's own validation data is published on the basis of a grid spacing of 8 inches, and it is clear that there is a strong grid dependence in this grid range.

A note on transparency – the gridding guidelines for the PDR-CFD code used requires 15 cells across the cloud, which for Sandia FLAME is a grid spacing of 4.8 inches (= 6ft / 15 cells)…

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

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Developer's own validation (8 inch)

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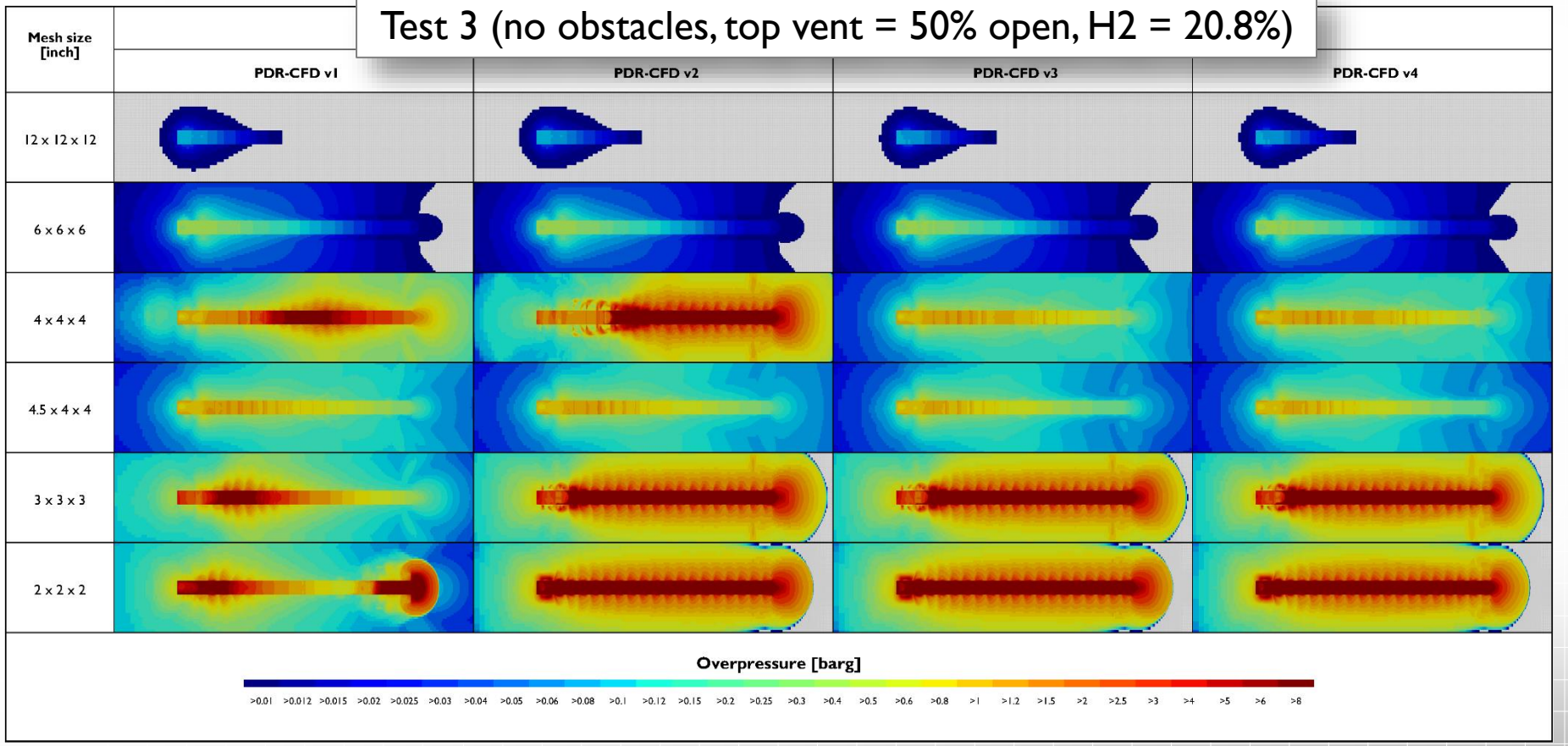


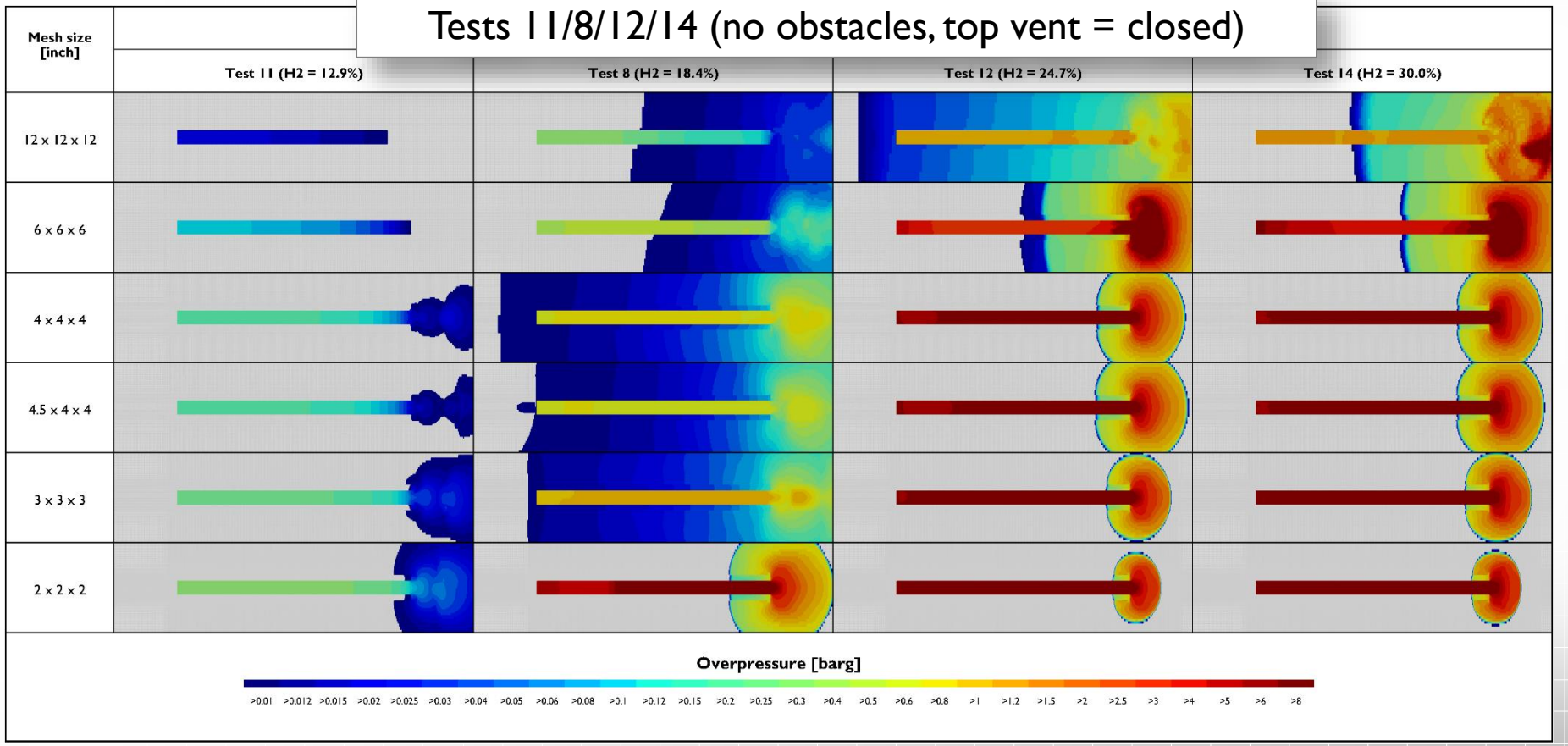
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Tests 11/8/12/14 (no obstacles, top vent = closed)

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)



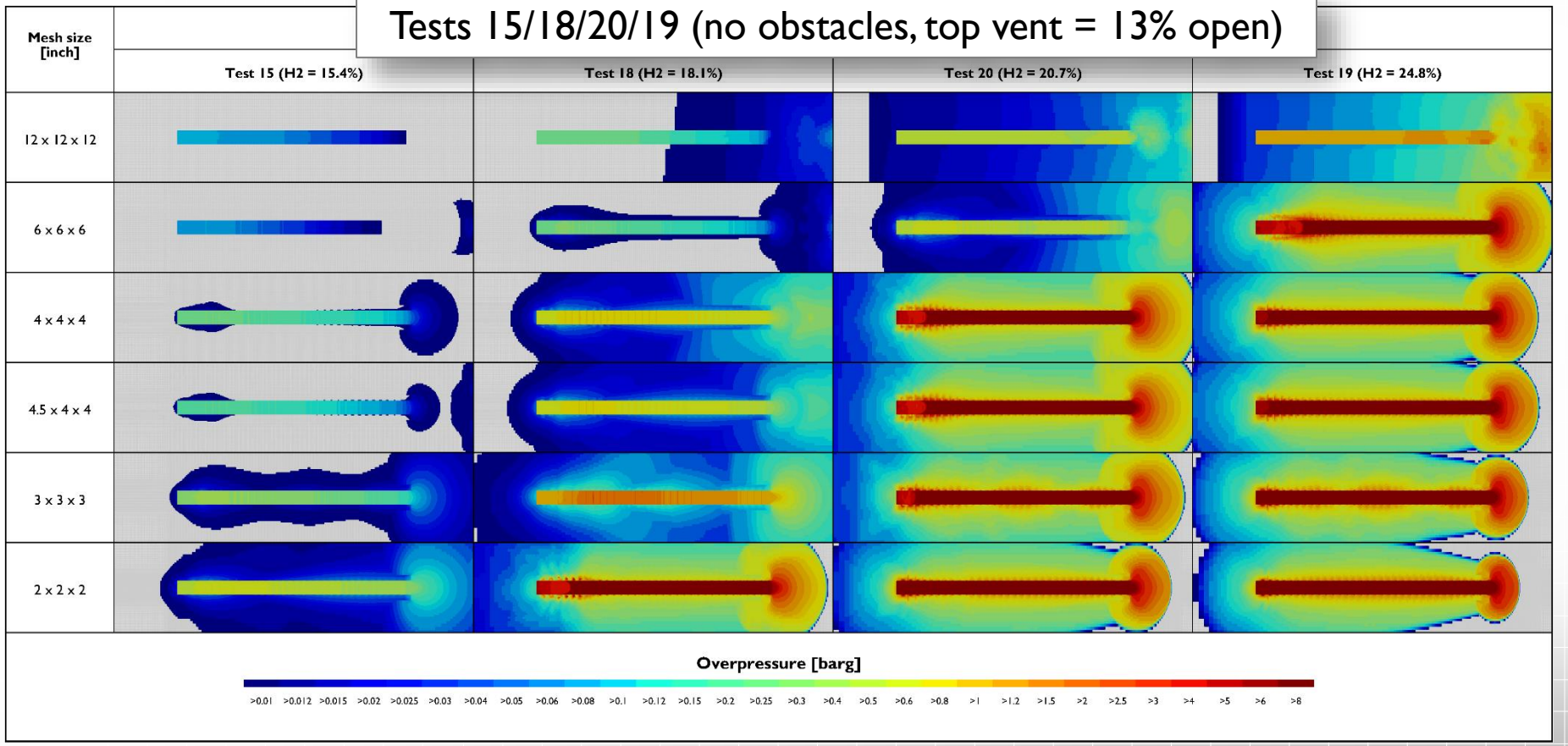
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Tests 15/18/20/19 (no obstacles, top vent = 13% open)

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)



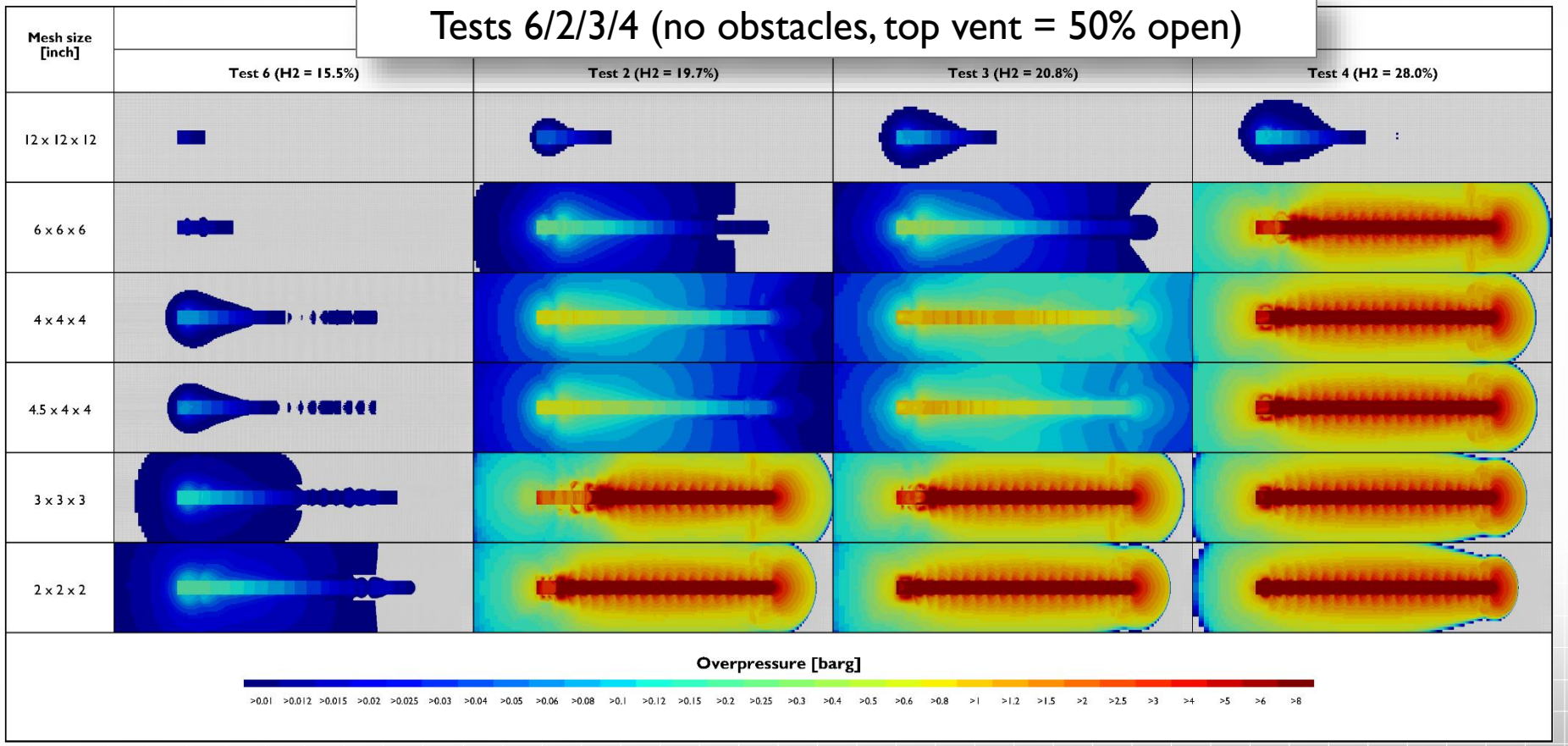
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Tests 6/2/3/4 (no obstacles, top vent = 50% open)

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)

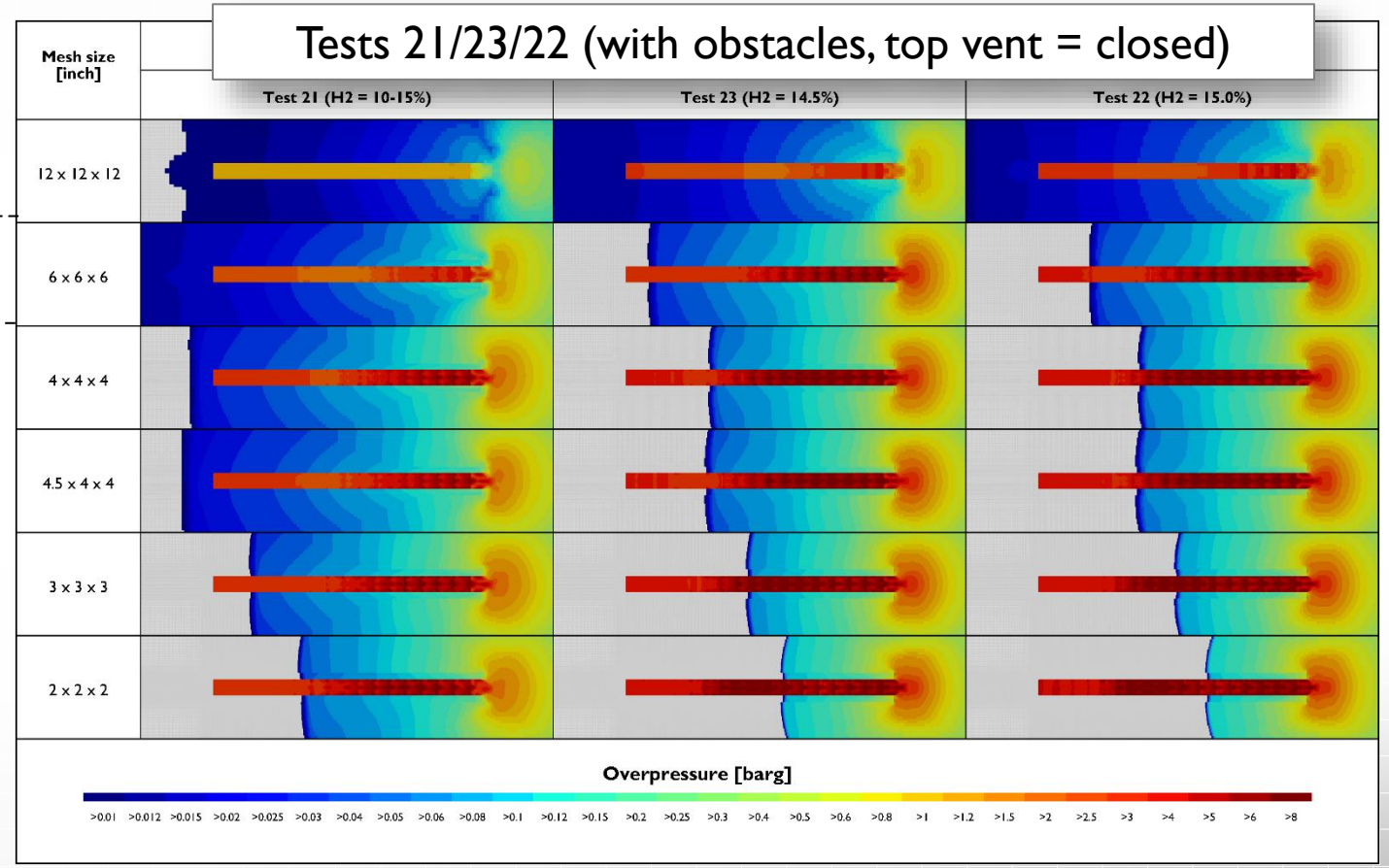


User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)



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Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)

Developer's own validation (8 inch)

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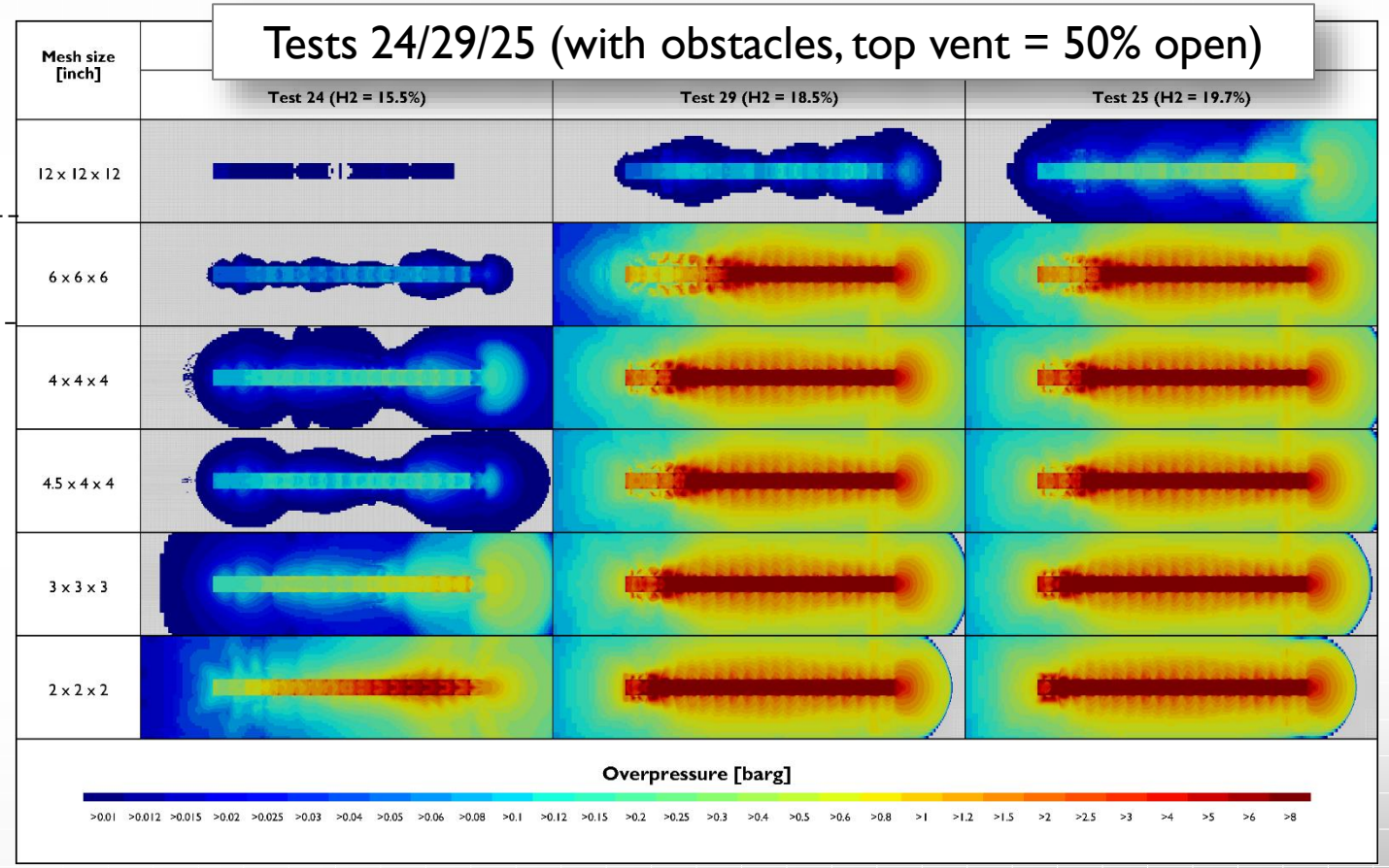
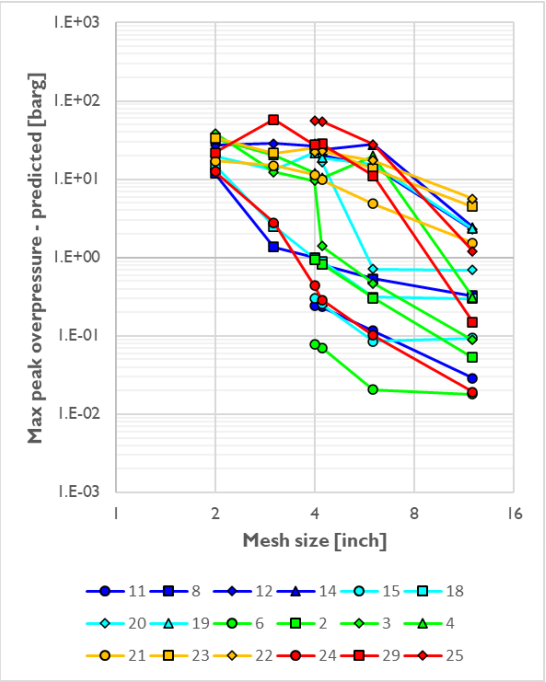
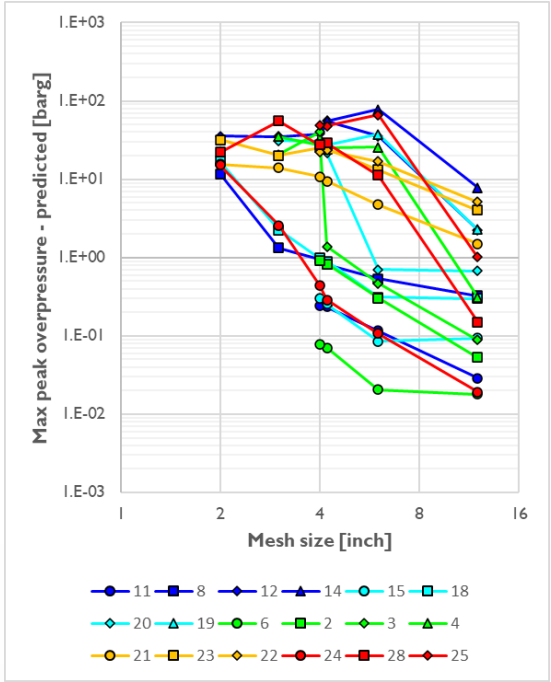


User VVUQ – solution verification

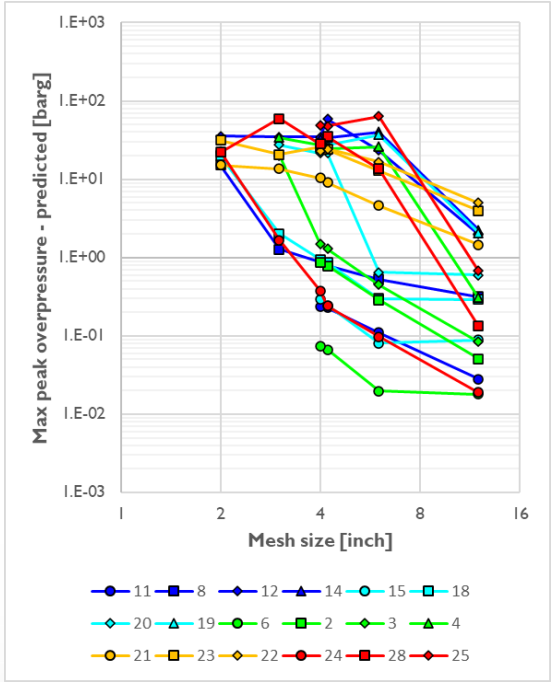
Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



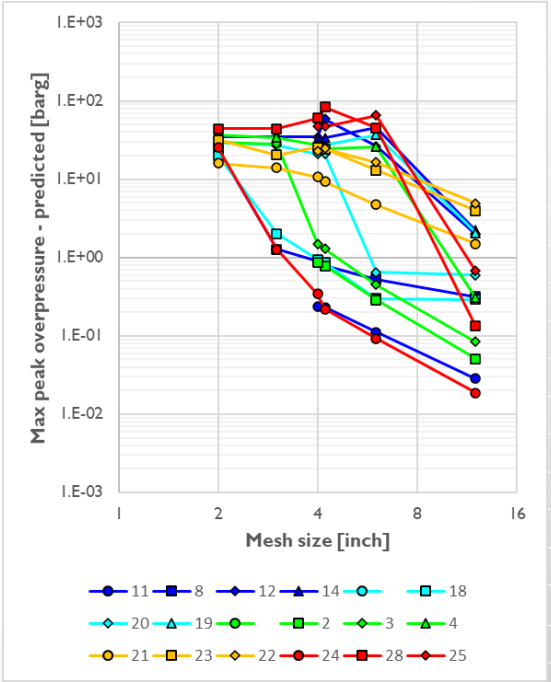
PDR-CFD v1



PDR-CFD v2



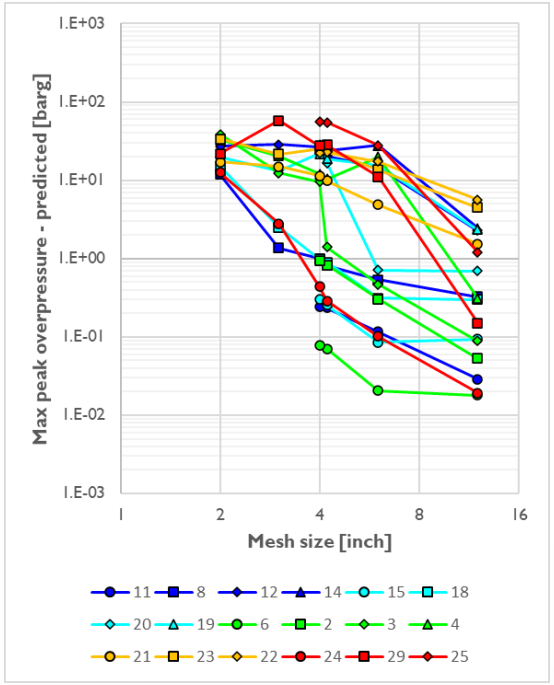
PDR-CFD v3



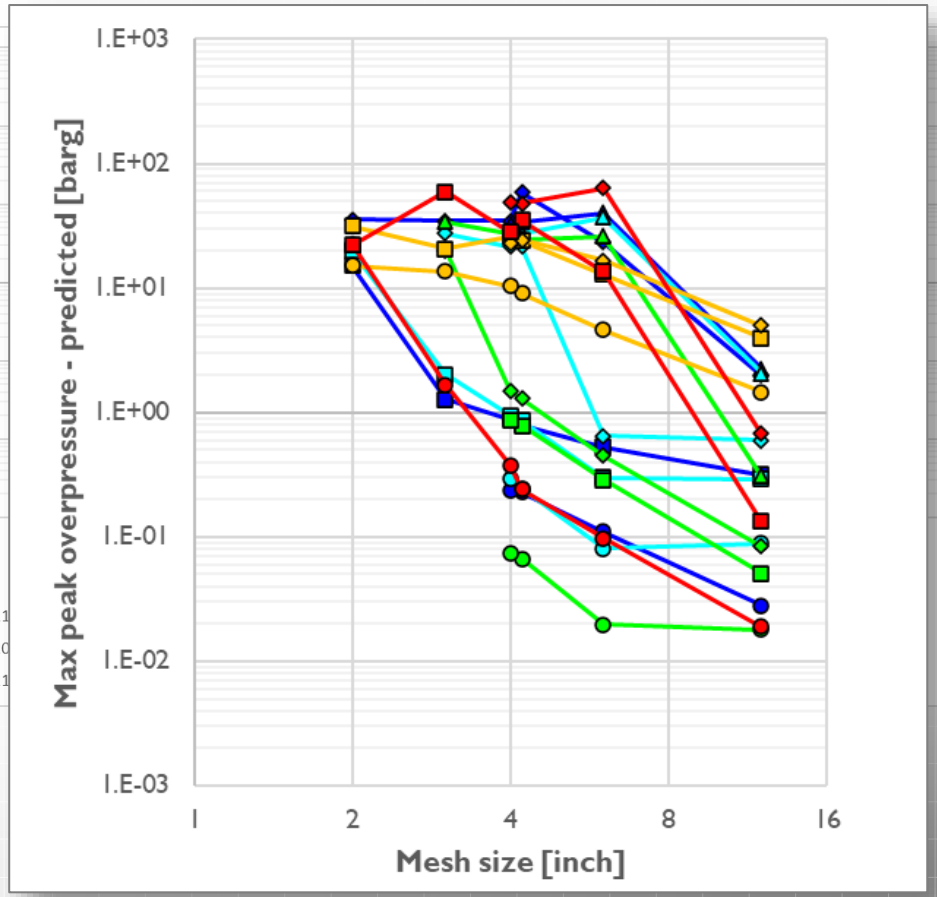
PDR-CFD v4

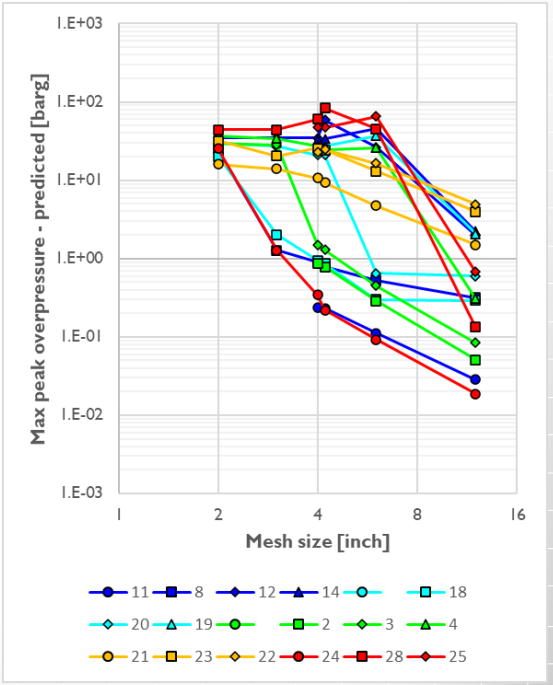
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



PDR-CFD v1

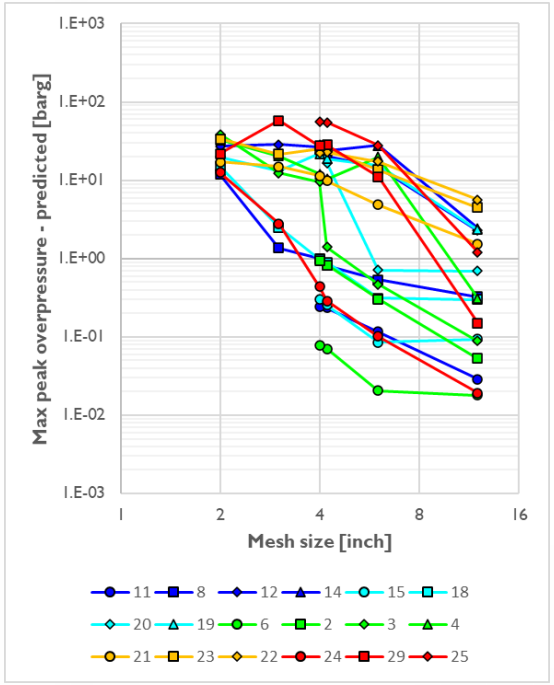




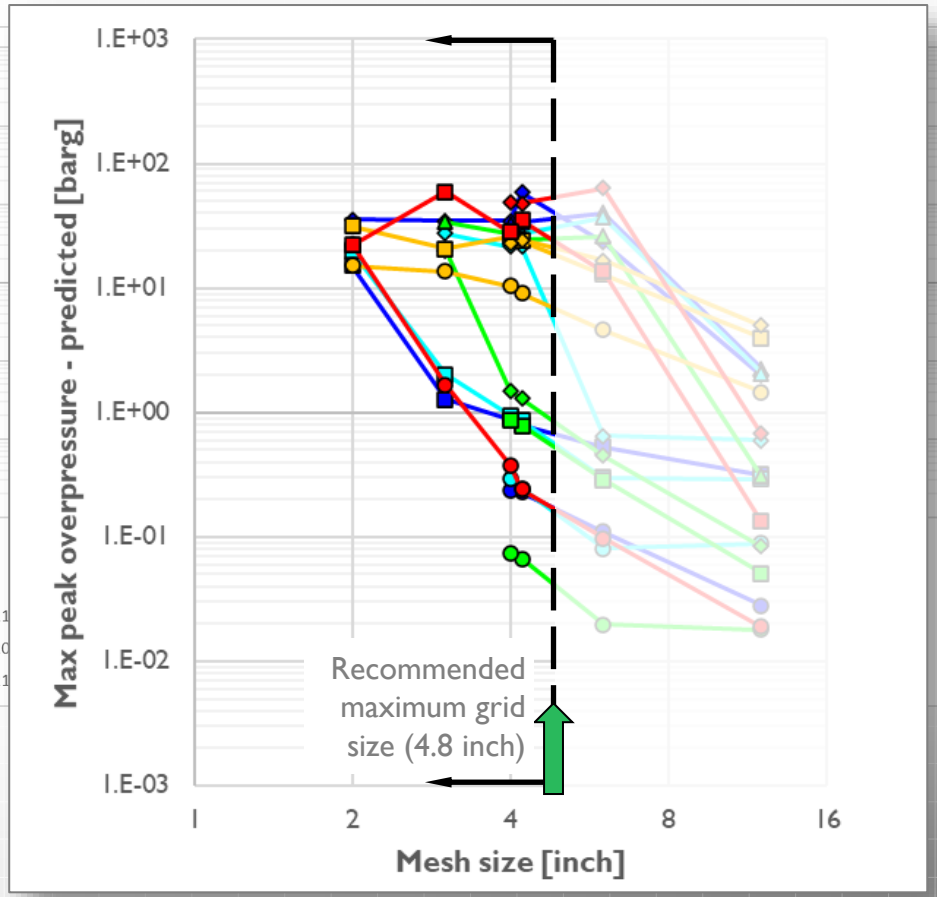
PDR-CFD v4

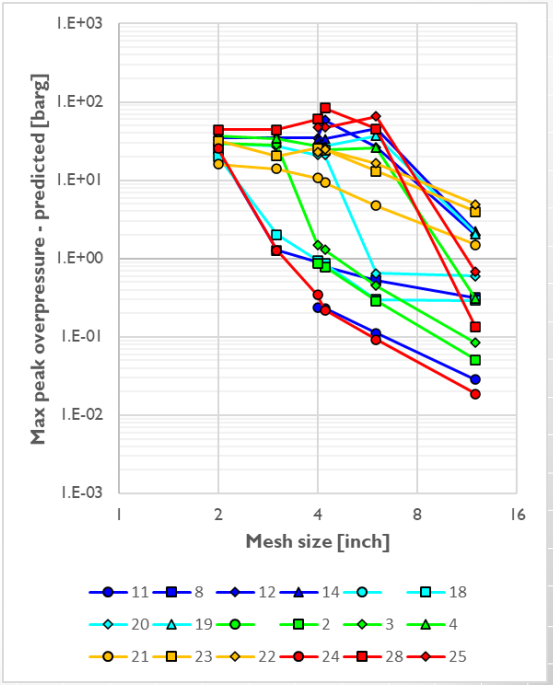
User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



PDR-CFD v1

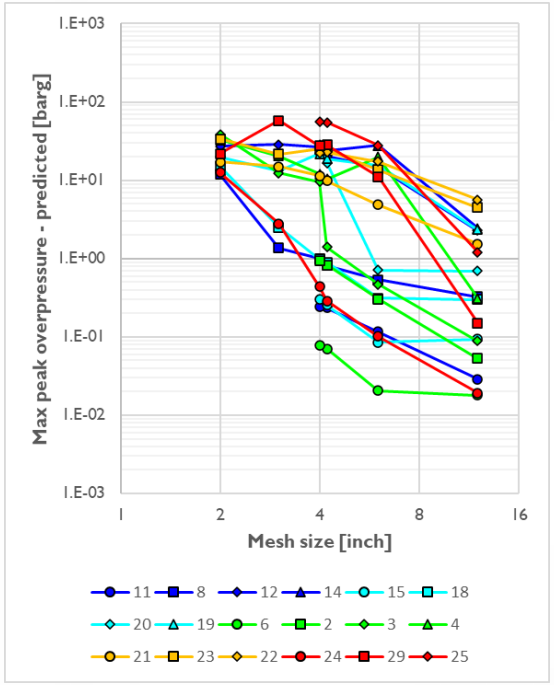




PDR-CFD v4

User VVUQ – solution verification

Sensitivity of overpressure to grid spacing – User VVUQ (Sandia FLAME)



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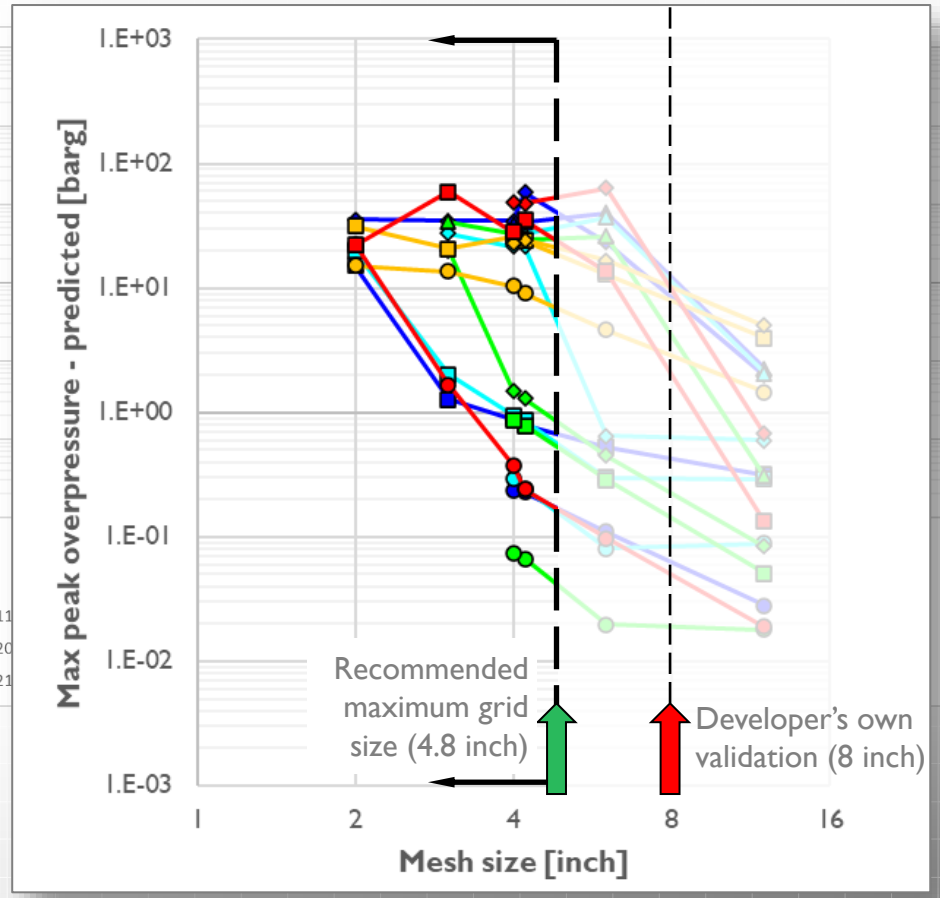

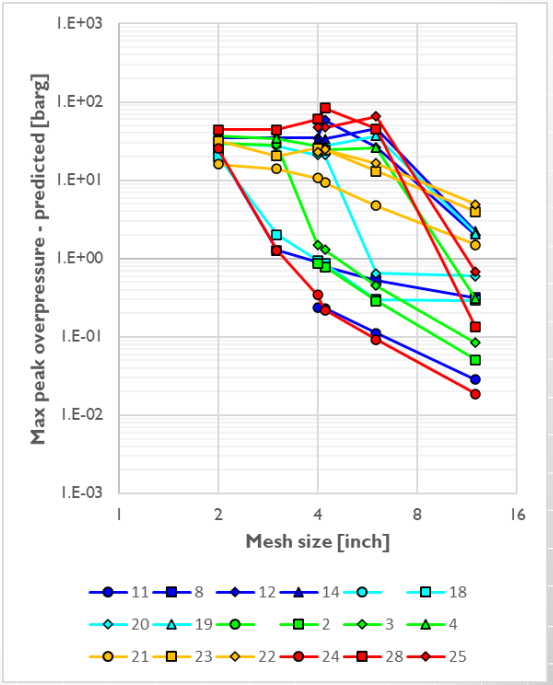

PDR-CFD v4

User VVUQ – solution verification

Summary

- With the PDR approach, predictions for peak overpressure are often strongly dependent upon the grid spacing. Unlike general-purpose (body-fitted) CFD, PDR predictions are typically not convergent as the grid size is reduced to zero.
- Predictions are specific to a particular version of a CFD code:
  - Just because a previous version of a PDR-CFD code has been validated and performs OK, doesn't mean that a later version of the same code will necessarily perform OK.
  - The version of the CFD code used should always be clearly understood and controlled.
- Generally, the validation data by the PDR-CFD code developers is published as graphs in the form of static images:
  - The underlying data and simulation files are not provided so there is no transparency on how the code really performs.

User VVUQ – solution verification

Summary

This has long been known – but does it matter?

- With the PDR approach, predictions for peak overpressure are often strongly dependent upon the grid spacing. Unlike general-purpose (body-fitted) CFD, PDR predictions are typically not convergent as the grid size is reduced to zero.
- Predictions are specific to a particular version of a CFD code:
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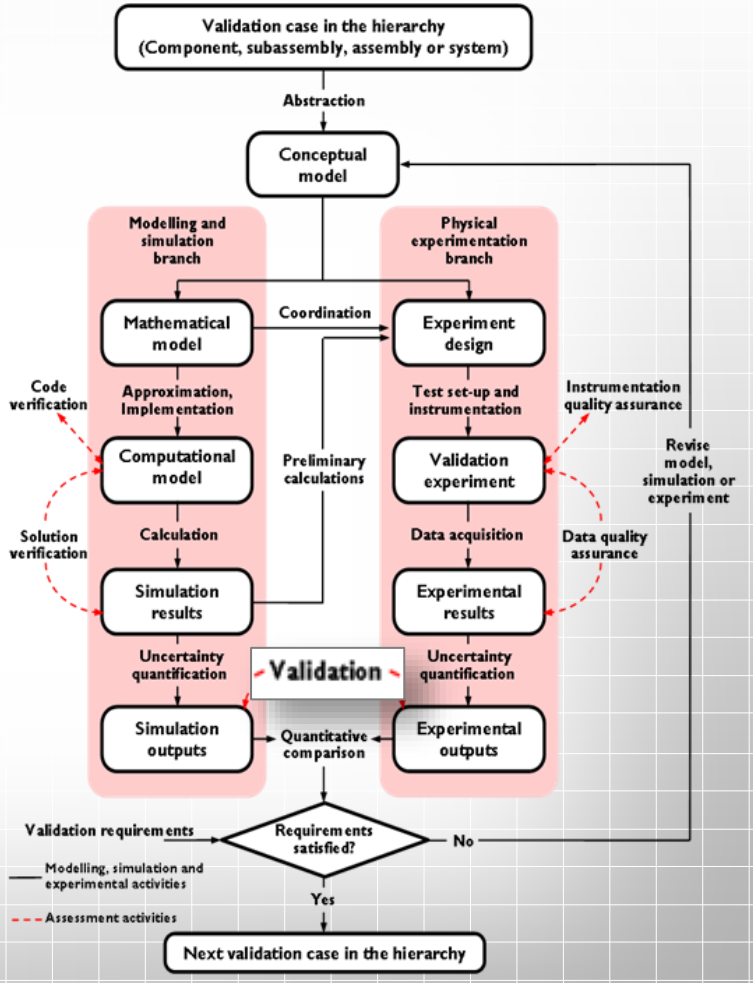
User VVUQ – validation

User VVUQ (Sandia FLAME)

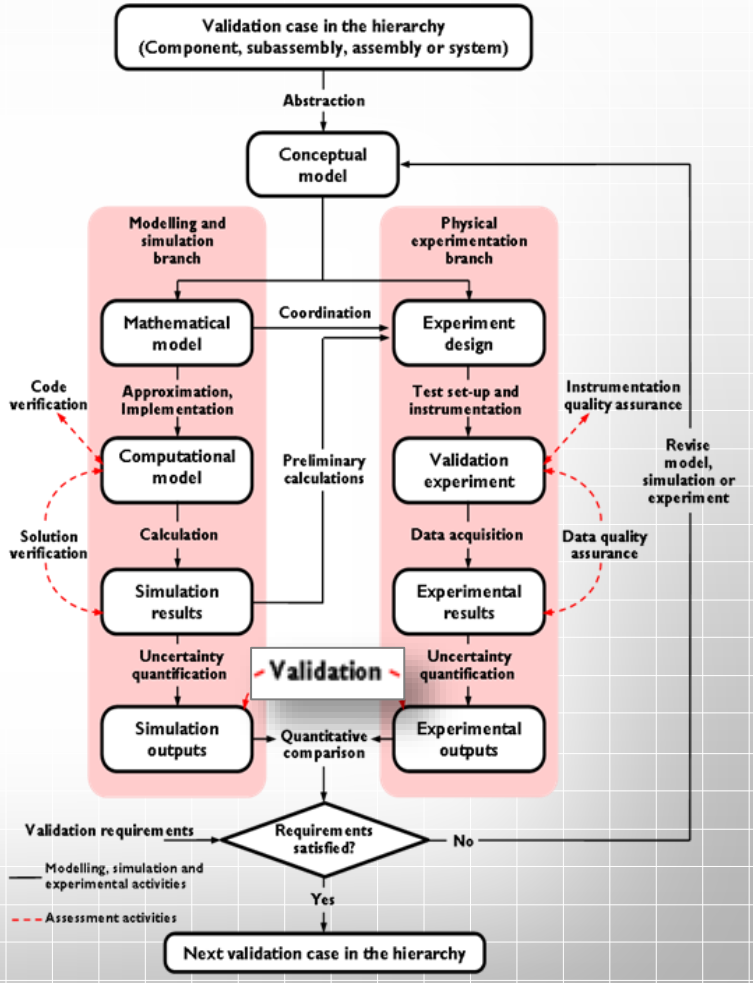
- What is there to present here?



User VVUQ – validation

User VVUQ (Sandia FLAME)

- What is there to present here?
  - Validation is a quantitative comparison of simulation outputs to experimental outputs.
  - If the simulation results from a PDR-CFD code do not converge as the grid size is reduced to zero (and indeed can vary by multiple orders of magnitude), then what are we supposed to compare with the experimental referent?



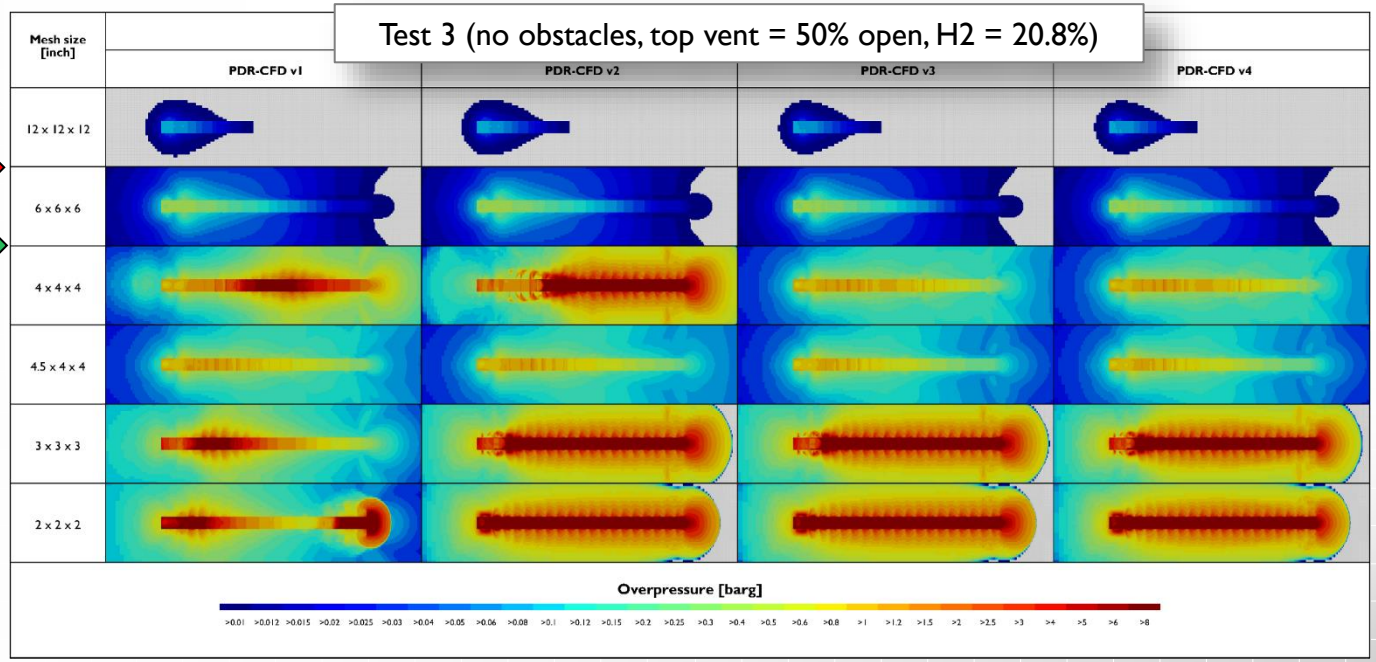
User VVUQ – validation

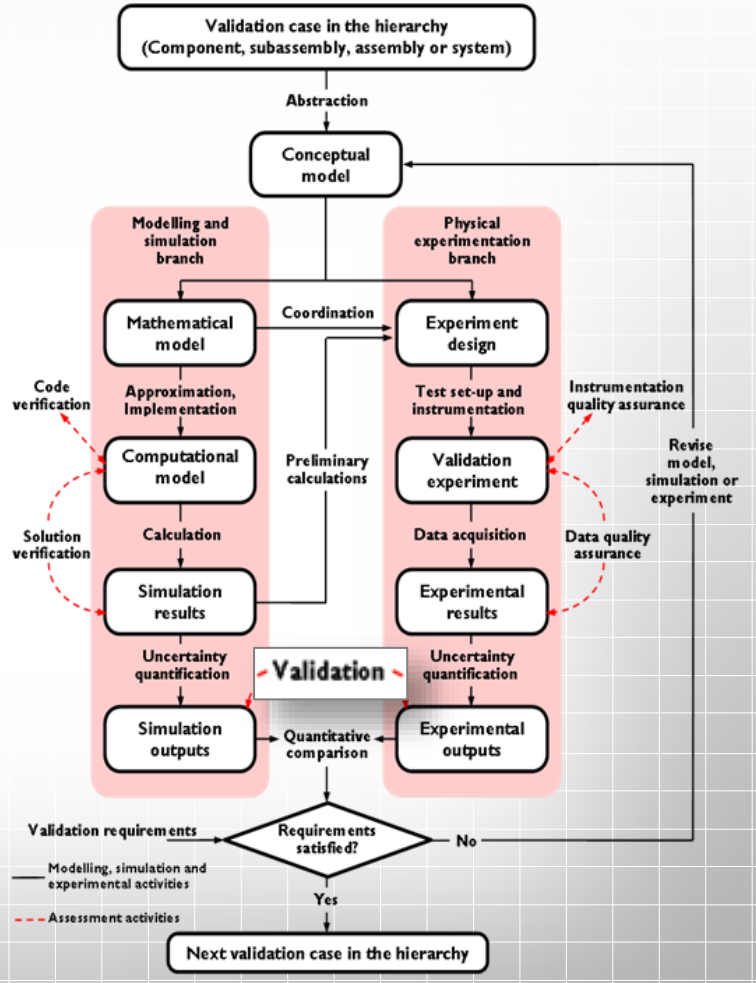
User VVUQ (Sandia FLAME)

- What is there to present here?
  - Validation is a quantitative comparison of simulation outputs to experimental outputs.

Developer's own validation (8 inch)

Recommended maximum grid size (4.8 inch)





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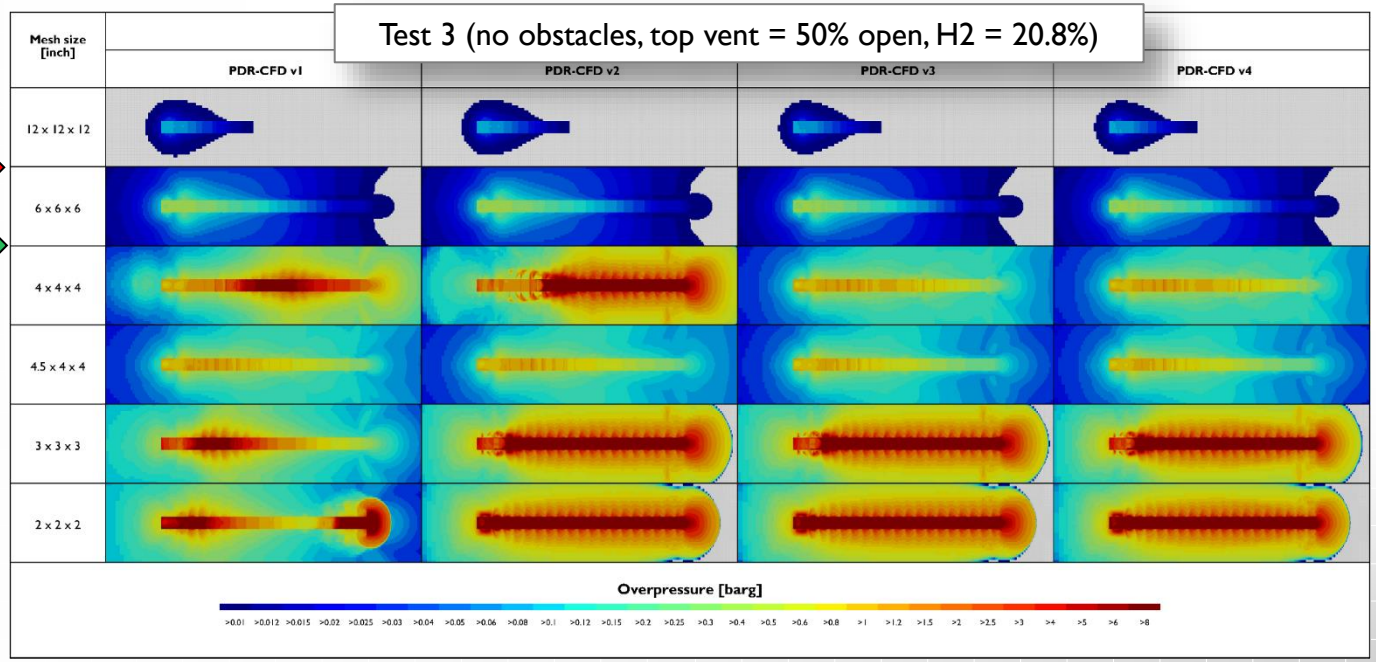

TABLE 6.1
Summary of the Test Parameters and Some Test Results

Test No. F-	Top Vent. %	H_2 Mole Fraction, %	Peak Overpress., kPa	Peak Equivalent Planar Flame Speed, m/s	Comments
TESTS WITH NO OBSTACLES					
1	50	12.4	a	7	
2	50	19.7	2.8	54	
3	50	20.8	a	65	
4	50	28.0	20	126	
5	50	12.6	0.9	4(12)[b]	Top sheet restraint.
6	50	15.5	3.4	19	
7	0	12.0	1.2	16	
8	0	18.4	26	170	
9	0	6.9	a	1.2[c]	Limited burn.
10	0	12.3	2.6	17	
11	0	12.9	4.5	30	
12	0	24.7	95/1100[d,e]	374	DDT near exit.
13	0	12.0			All data lost.
14	0	30.0	250/2100[d,e]	932[f]	DDT near exit.
15	13	15.4	3.1	50	
16	13	17.6	10	75	
17	13	14.9			Some data lost.
18	13	18.1	36	136	
19	13	24.8	65/850[d]	160[g]	DDT at 1/3 length.
20	13	20.7	78	483	
TESTS WITH OBSTACLES					
21	0	10-15%	650	580	No mixing fans
22	0	15.0	3100	700	DDT near exit
23	0	14.5	1200	540	
24	50	15.5	a	46	
25	50	19.7	1500	890	DDT near exit
26	50	28.5	2000	1860	Box obstacles, DDT
27	50	13.1	9	15	
28	50	14.9	9	33.4	
29	50	18.5	23	130	

DDT = Deflagration-to-Detonation Transition
a) Indicates pressure signal within the noise level.
b) Plastic top sheet restraint gave faster value early in test.
c) Indicates horizontal propagation velocity of thin layer below roof.
d) First pressure value refers to deflagration, the second to detonation.
e) Based on dynamic pressure transducers, somewhat uncertain.
f) Peak planar equivalent flame speed is highly uncertain because it was increasing rapidly near the channel exit.
g) Peak planar eq. flame speed highly uncertain due to early DDT.

[Ref. 16]: A. Sherman, Martin Philip and Tieszen, SR and Benedick, William B (1989), FLAME facility: The effect of obstacles and transverse venting on flame acceleration and transition on detonation for hydrogen-air mixtures at large scale. https://www.nrc.gov/docs/ML0717/ML071700076.pdf

User VVUQ – validation

User VVUQ (Sandia FLAME)

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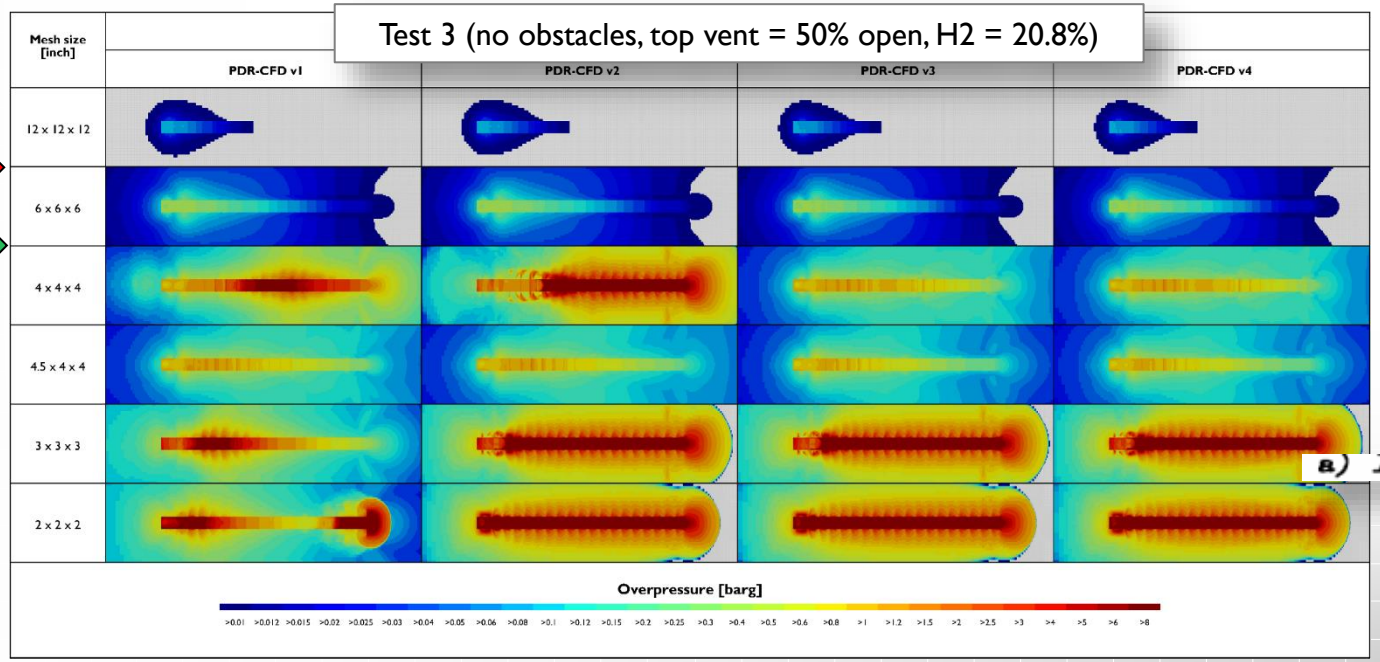

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13	0	12.0			Al data lost.
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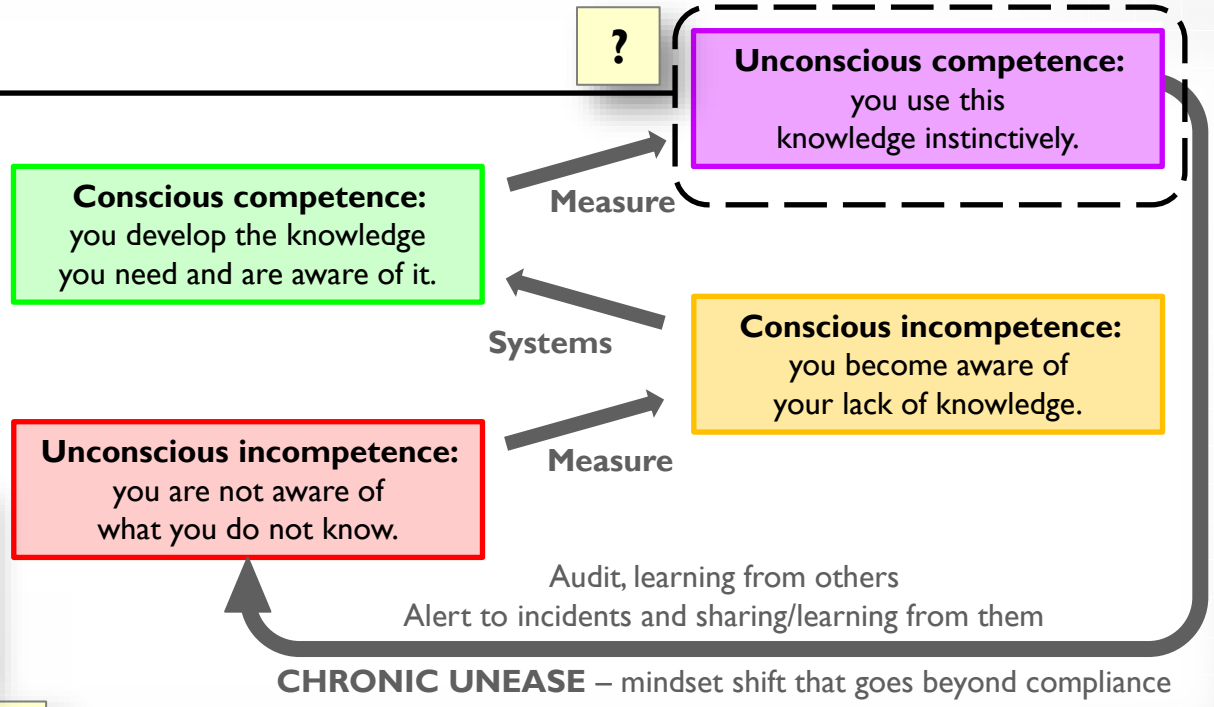
Today

Trevor Kletz Keynote Lecture – Ken Rivers (UK HSE, former IChemE President)

- *"With over 40 years of validation from real-world experiments,* [our PDR-CFD software] *delivers reliable modelling results".*
- *"Our automated framework checks simulations against real-world data from lots of experiments and incidents, ensuring accurate and reliable results".*
- *"With* [our PDR-CFD software], *you get results you can trust to control risks and improve safety".*

In his presentation, Ken pointed out that very often, a state of *unconscious competence* can look very much like a state of *unconscious incompetence*…

Where are we in terms of CFD for simulating explosions?



[Ref. 10]: Rivers (2025), "*Process Safety Leadership: meeting emerging challenges in the UK industry*", Hazards 35, Birmingham, November 2025.
[Ref. 11]: www.macmillancentreforlearning.co.uk/the-journey-from-unconscious-incompetence-to-unconscious-competence-adapted-from-noel-birch-1970s-by-malcolm-macmillan/

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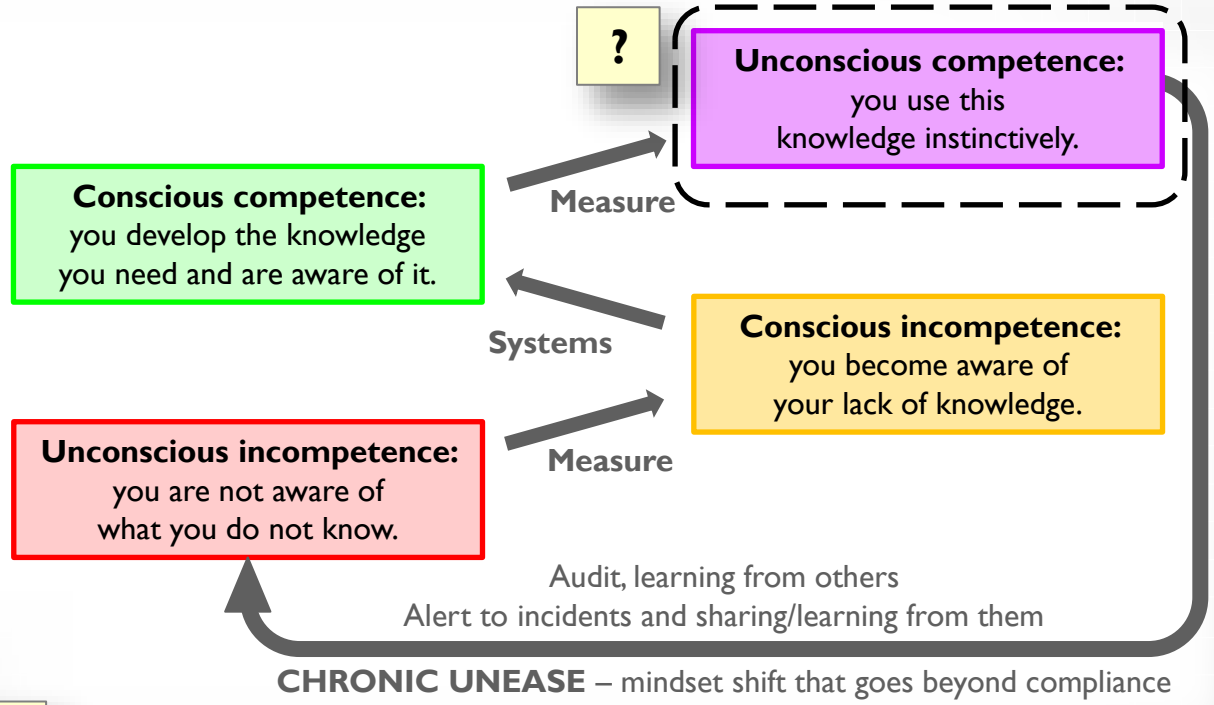
"With [our PDR-CFD software], *you get results you can trust".*



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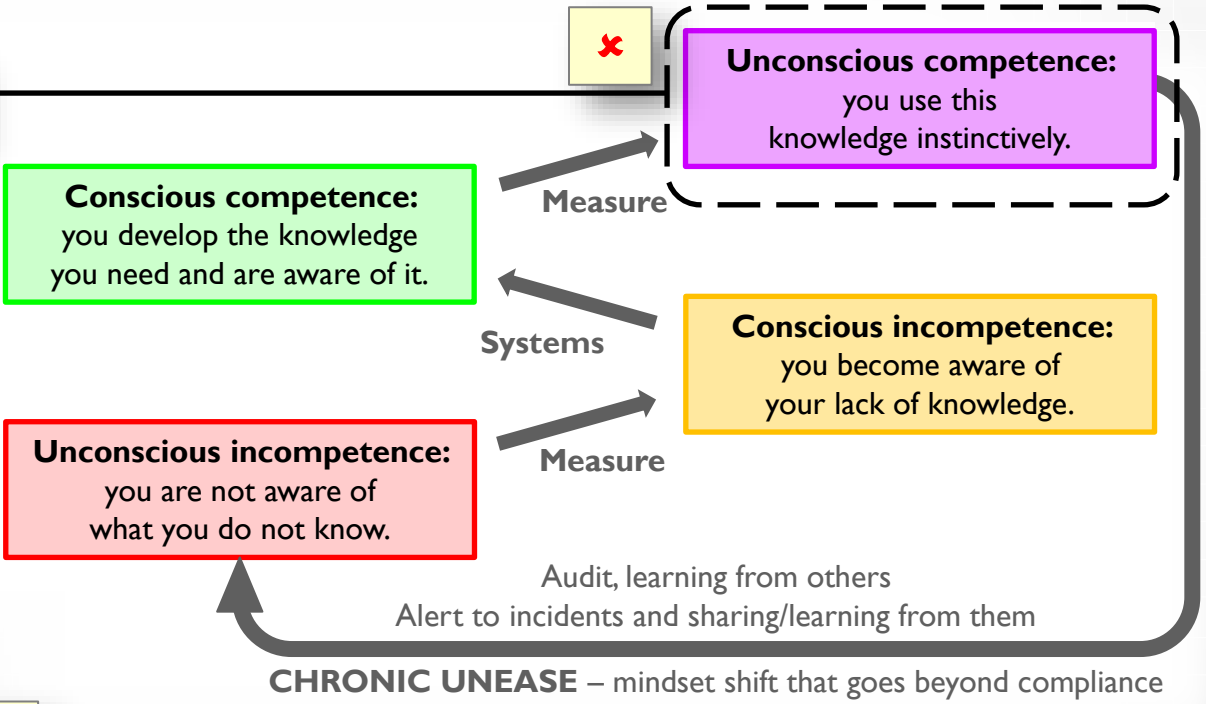

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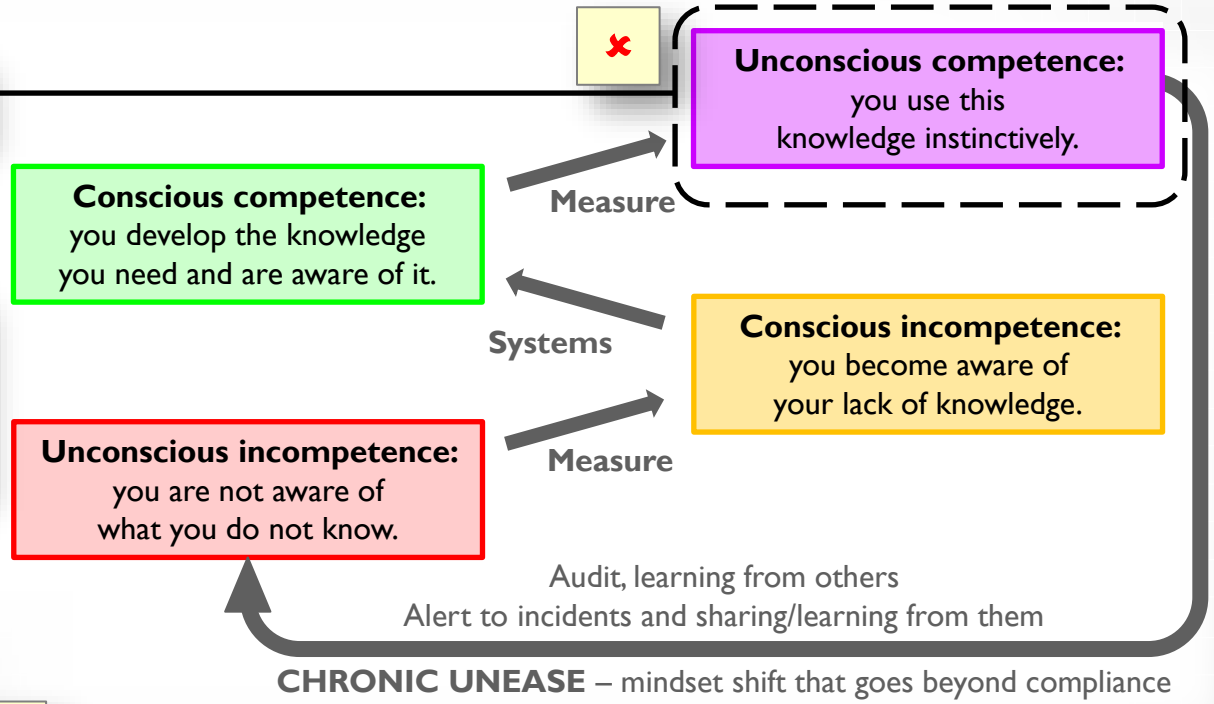

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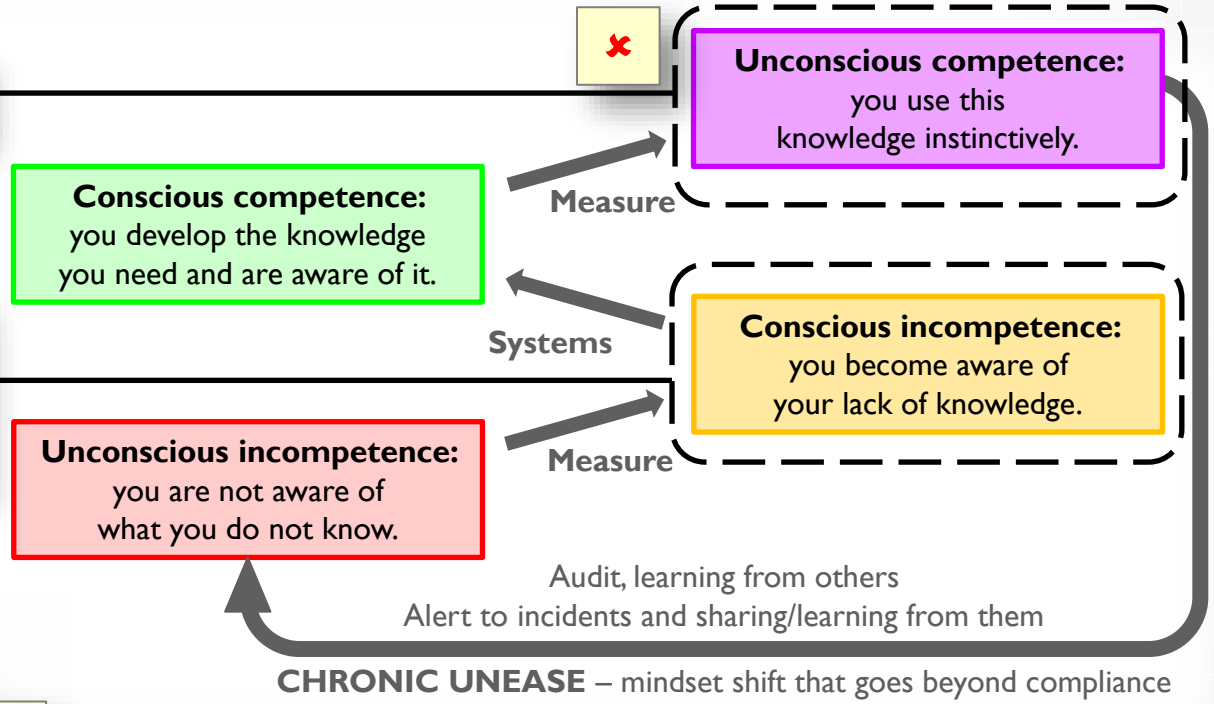

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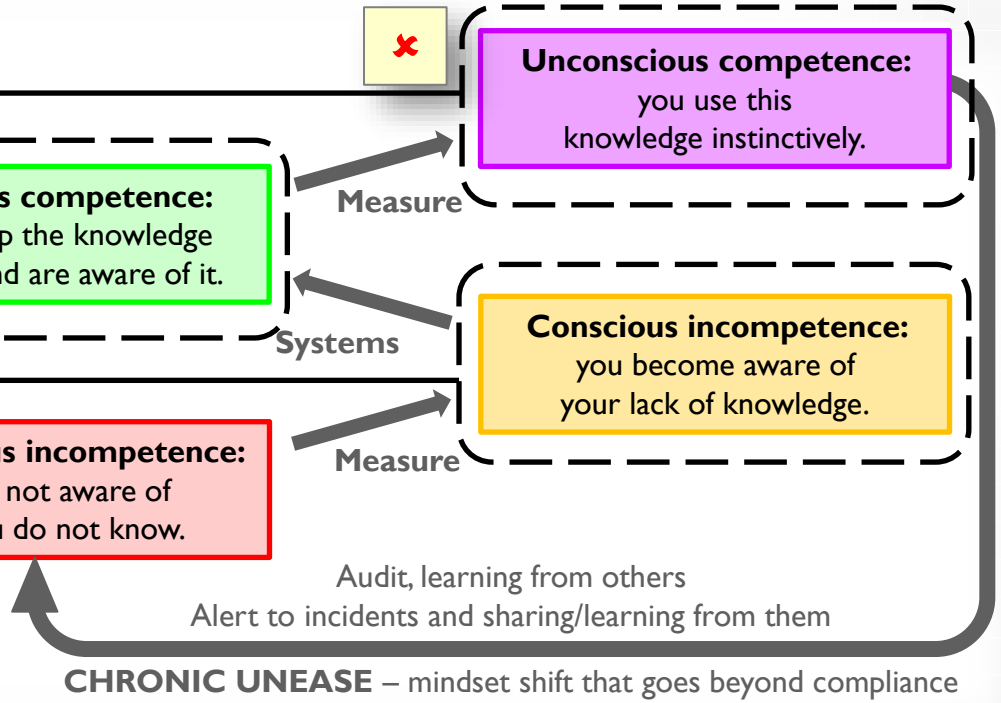

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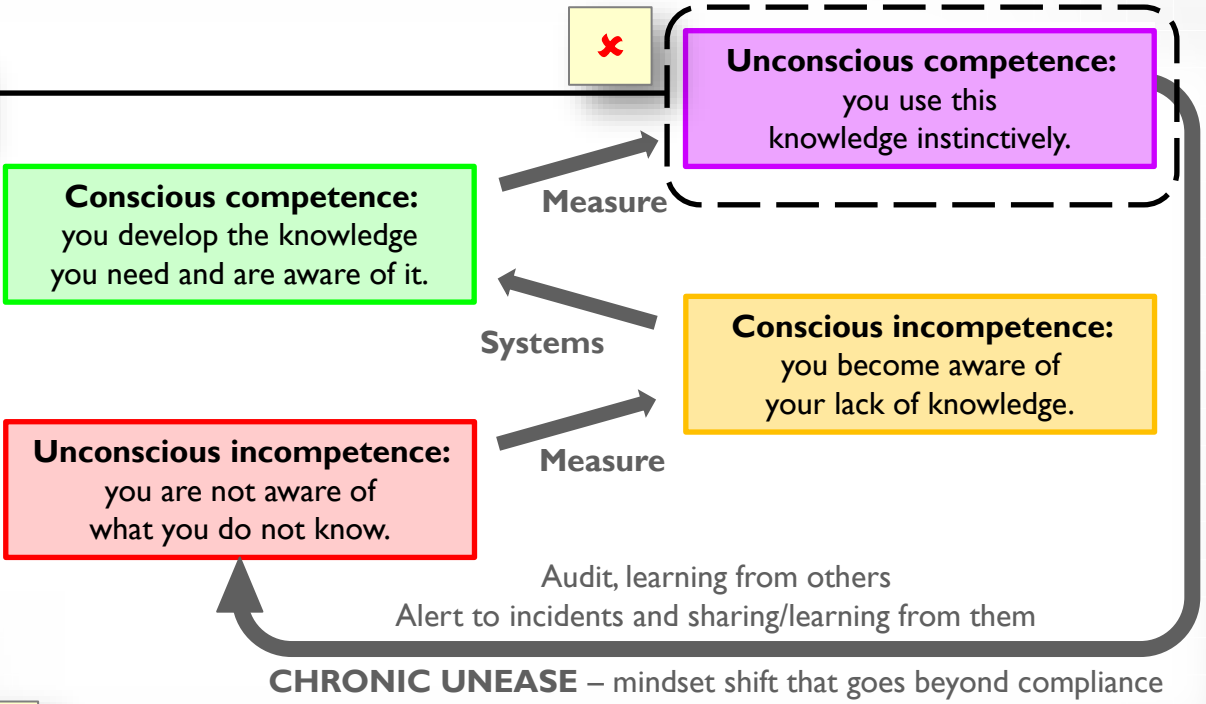

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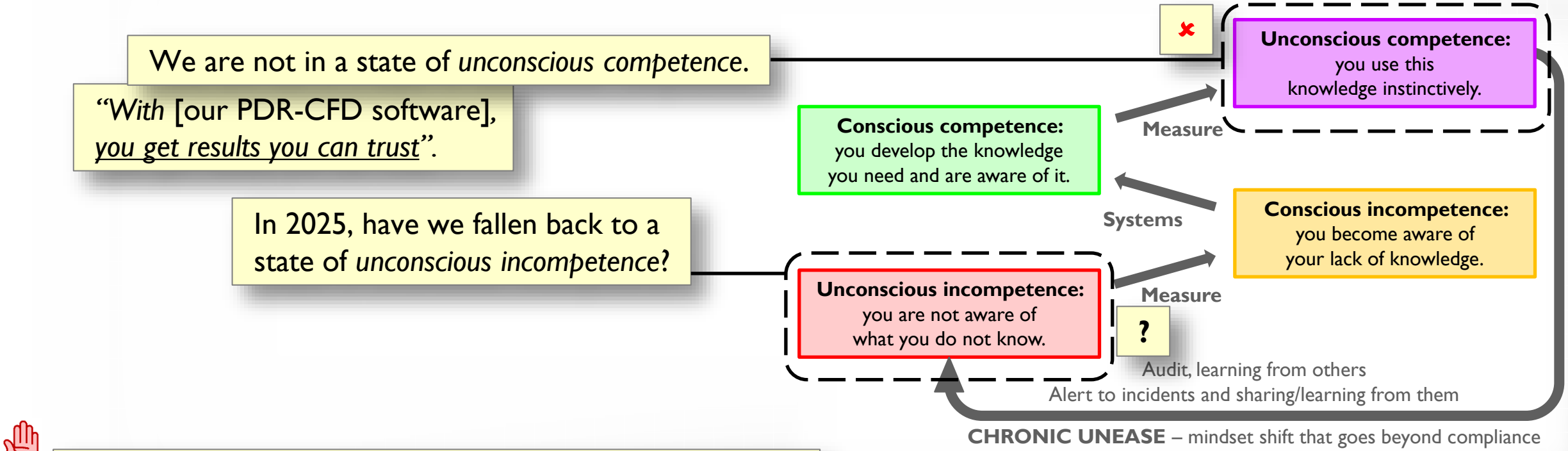

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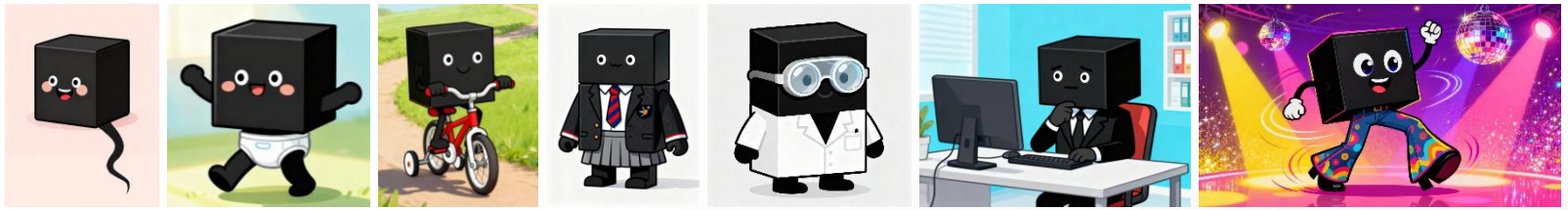

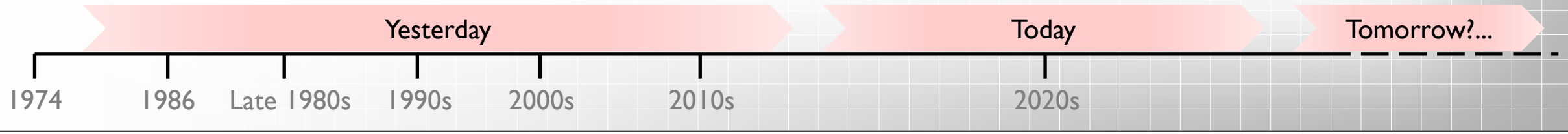

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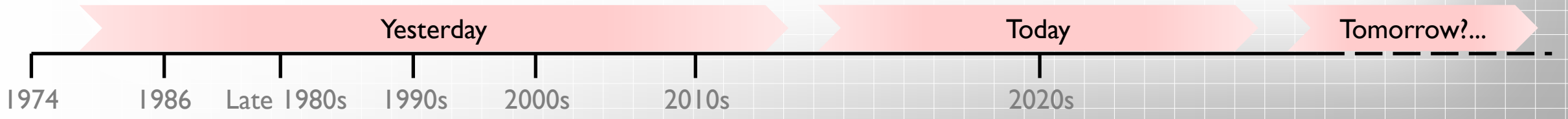

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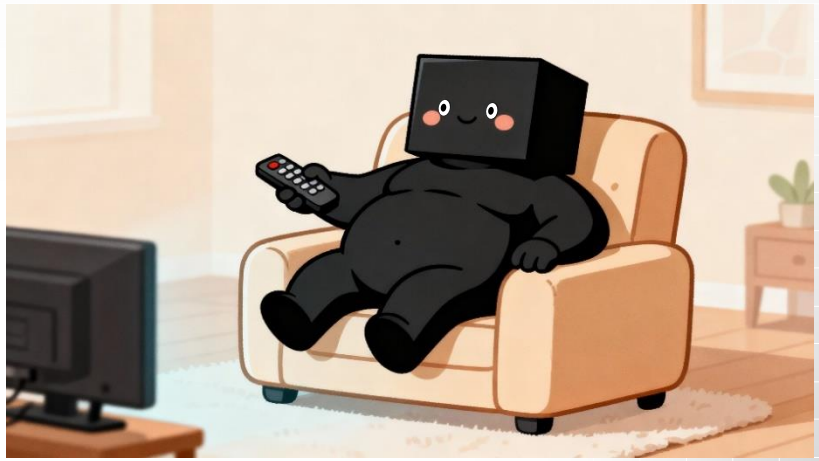

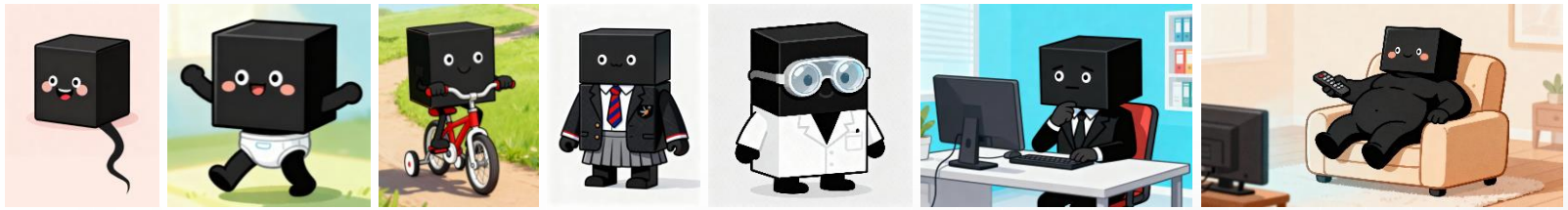

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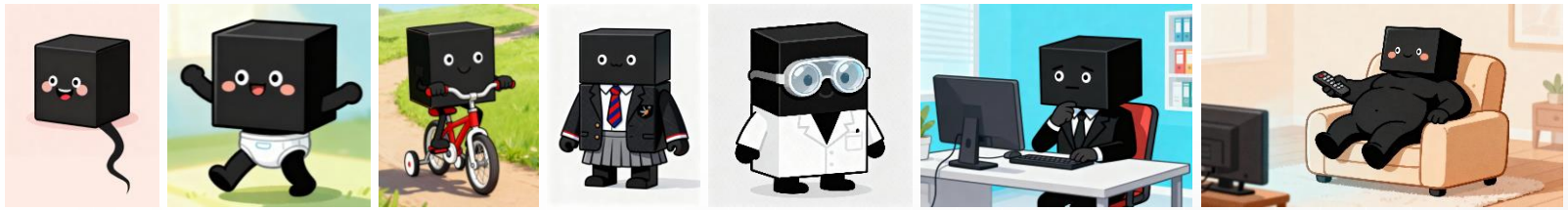
https://www.ibm.com/think/topics/ai-hallucinations



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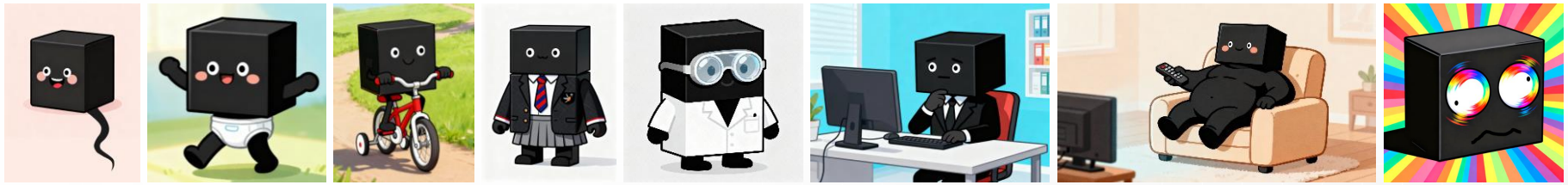

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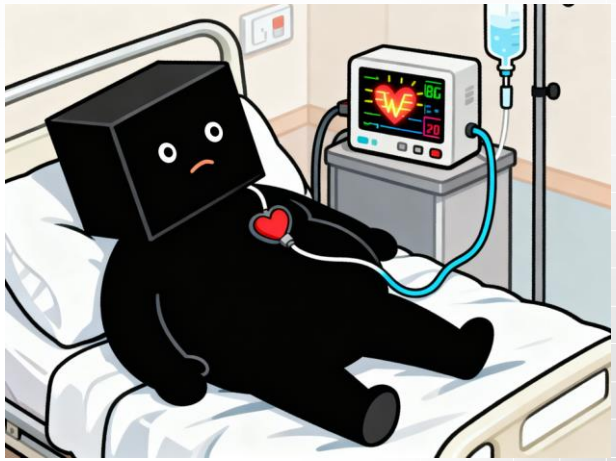

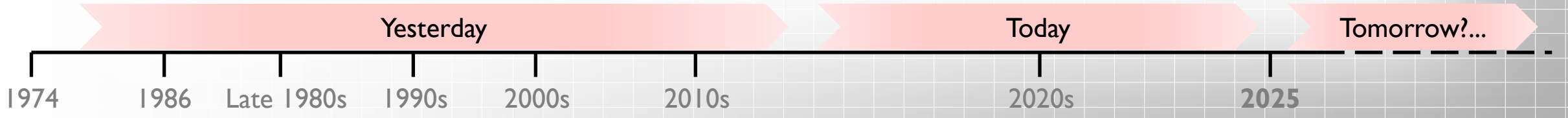

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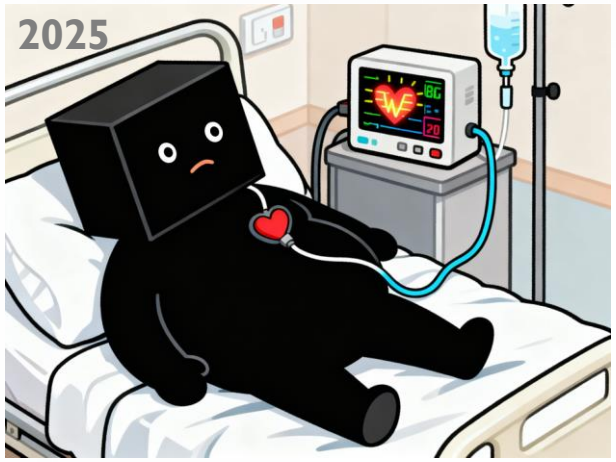

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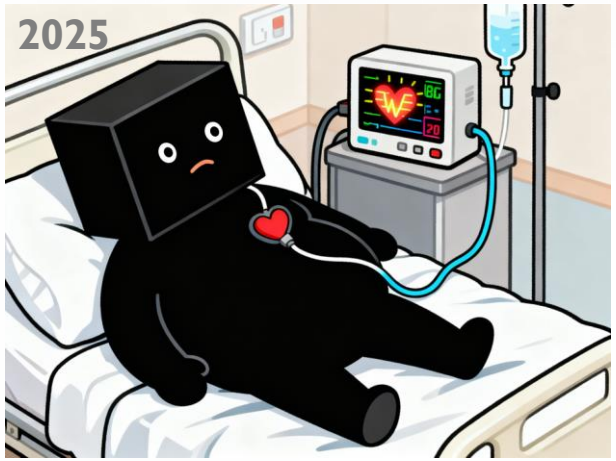

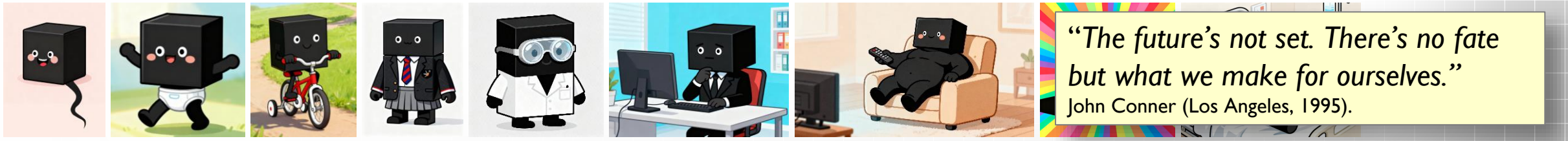

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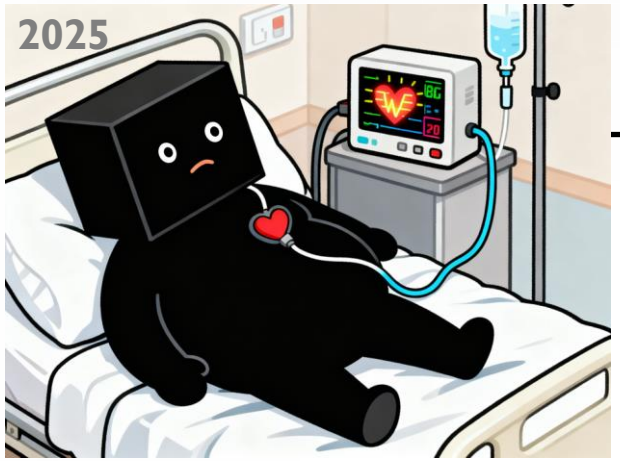

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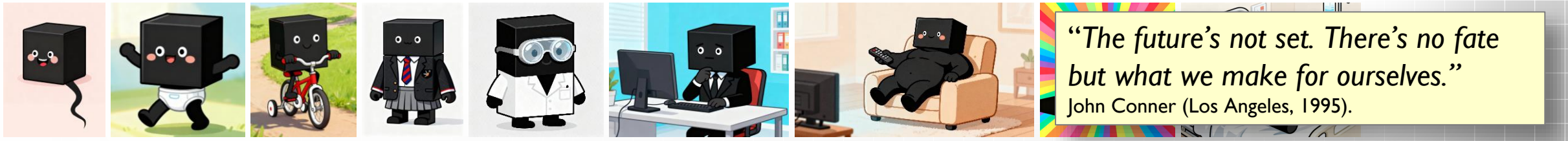

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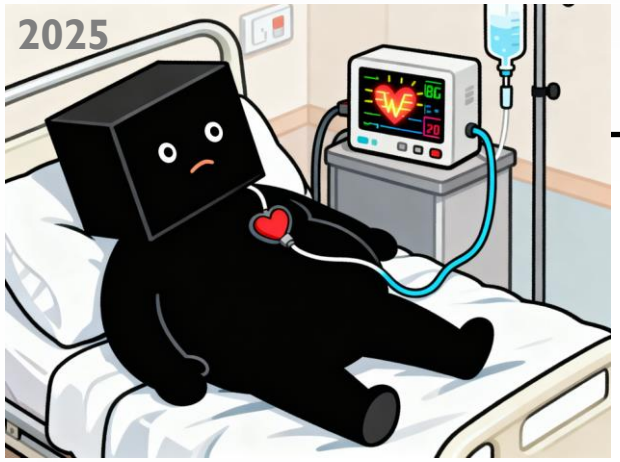

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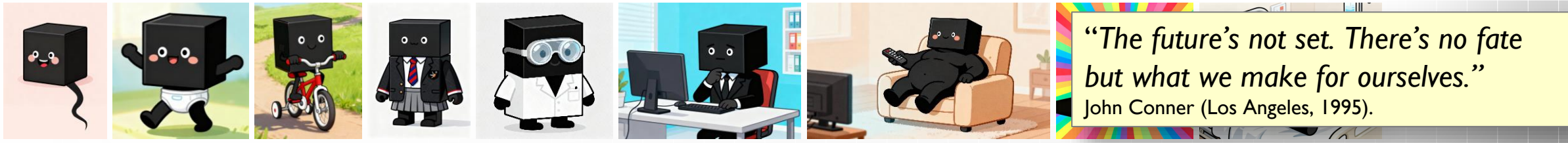

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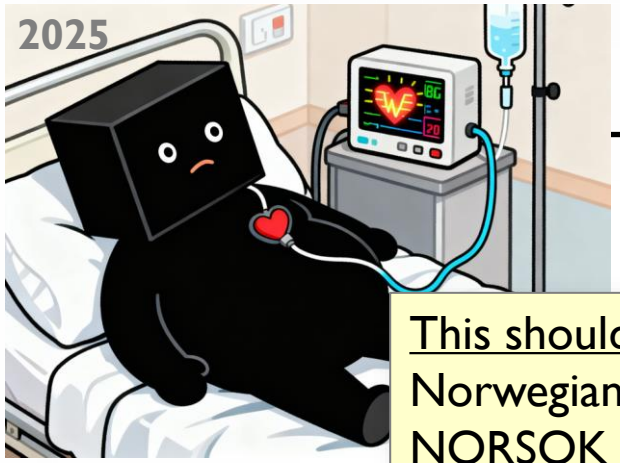

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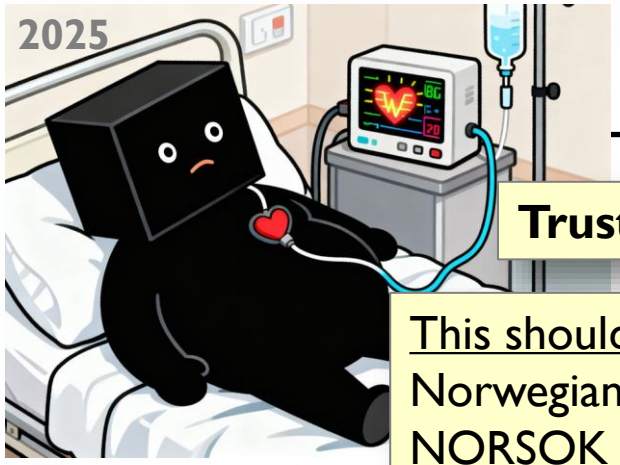

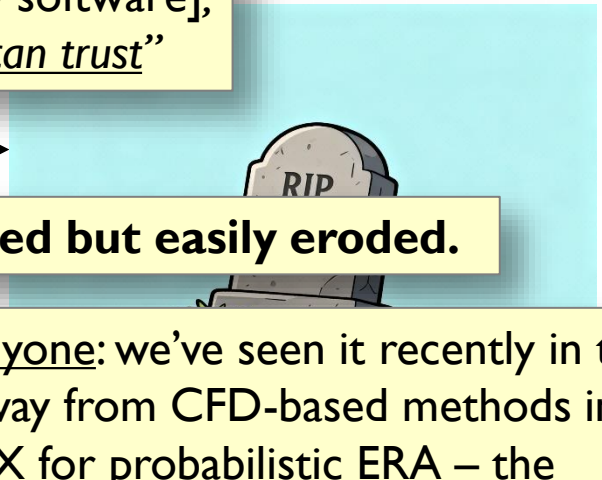

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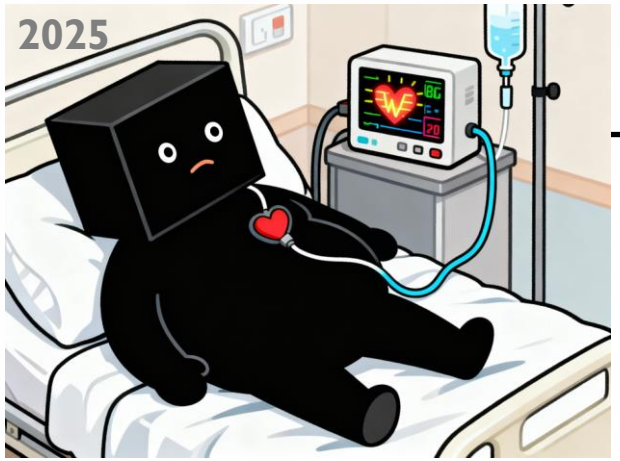

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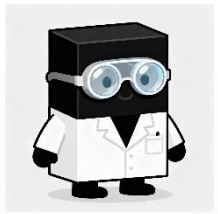

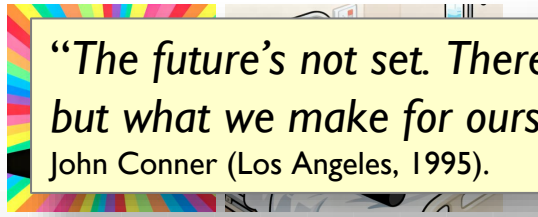

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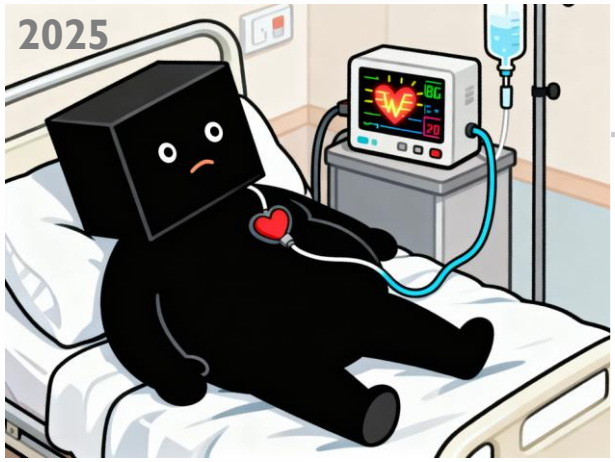

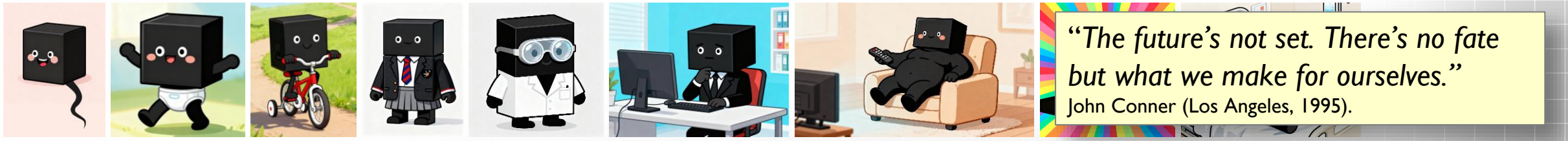

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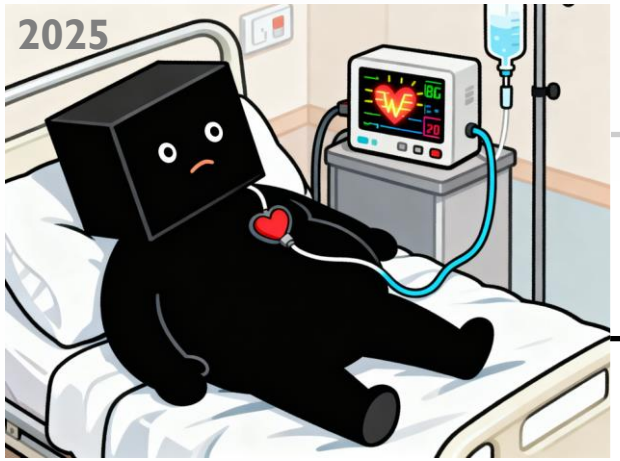

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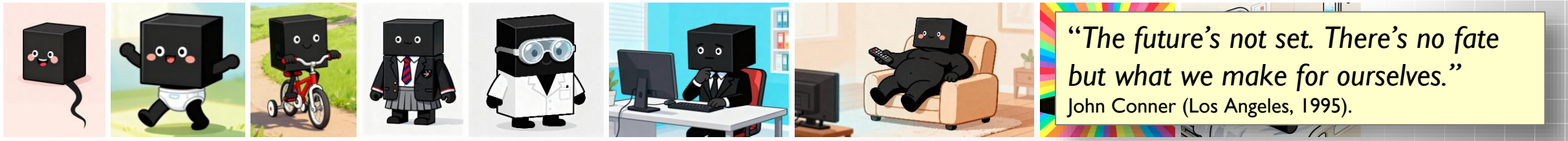

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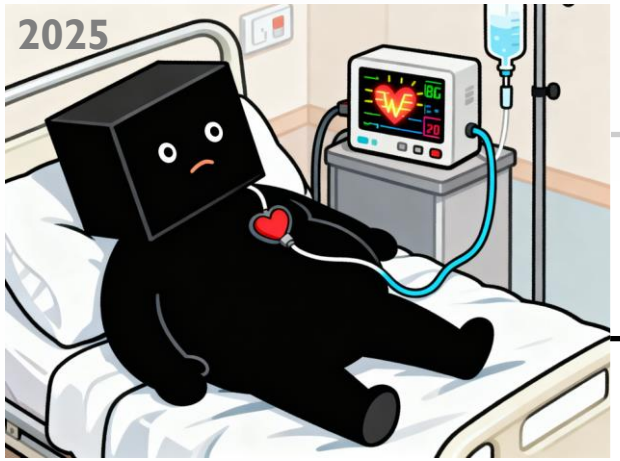

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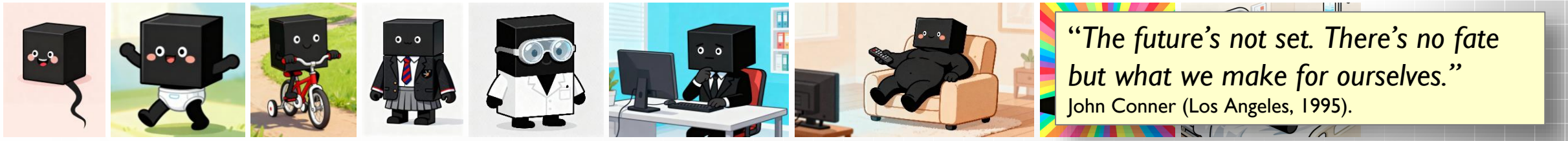

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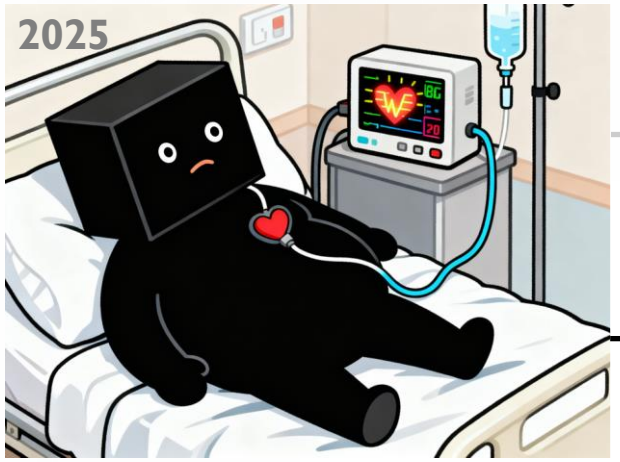

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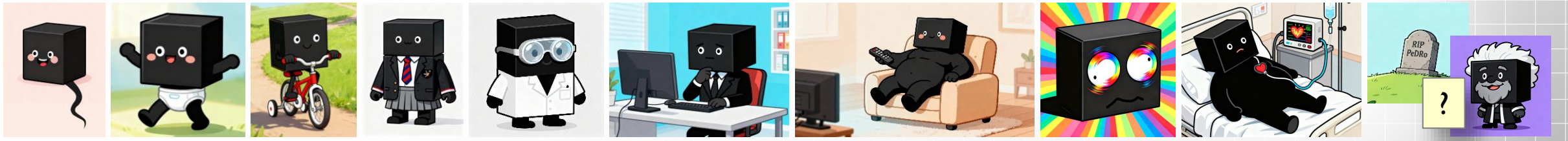
… there might still be life in the PDR-CFD approach yet!



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Closing remarks

- **George Box: *all models are wrong but some are useful*.**
  - In order to understand whether the PDR approach is useful for simulating vapour cloud explosions, we really need to understand how it behaves with respect to:
    - Geometry handling – code verification.
    - Grid size and time step – solution verification.
    - Version to version – code verification, validation.
    - Industry sector to industry sector – validation domain.
  - We need to develop methodologies around handling **uncertainties** in our modelling approaches – not just for CFD, but for all of the predictive tools we have in our toolbox.
  - We need to **acknowledge the issues, not hide them**! Then we can **address them**.

Closing remarks

- ***"With* [our PDR-CFD software], *you get results you can trust*".**

- This is only a marketing statement, so what is all of the fuss about?...

Closing remarks

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- This is only a marketing statement, so what is all of the fuss about?...

  … but is it just a statement? Or is it indicative of the culture within the PDR-CFD community in 2025?

  It is not aligned with safety culture thinking, and in the long run, **it will erode hard-earned trust in CFD**, and rightly so.

- **We are all marketing folks** – all experienced users of the PDR approach have a responsibility to call out this kind of misleading statement…

Closing remarks

- Democratisation will come to PDR-CFD for vapour cloud explosions, eventually, but we must not force it prematurely – we are not ready for it yet…

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… **slow and steady is the safe way forward**, otherwise we risk **eroding our hard-earned trust in PDR-CFD** for simulating vapour cloud explosions.

Closing remarks

- This may not be an easy message for us to receive…

  … but equally, this is not an easy message to deliver either.
- Along the **improvement journey** we may encounter **CHRONIC UNEASE**, but we need to **face it and embrace it rather than avoiding the journey**.

- Regarding the VVUQ presented herein, **don't take Abercus' word for it!**:
  - Go and **examine the VVUQ section** in the manual for your chosen PDR-CFD software and please check for yourself. PDR-CFD users – **this is your responsibility, as a minimum**.
  - The VVUQ section presents VVUQ work activities performed by the PDR-CFD developer – it represents what they get from their own CFD code and does not necessarily reflect what any other user will get from the code, so you should **undertake your own VVUQ for yourself**…

The way forward…

- Private message in reaction to some of Abercus' recent conference presentations (from an operator): "*I received your papers, thank you for sharing them. You guys do a lot of good work. If only the industry had the same rigour and energy to work through the technicalities!!*"

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- Thank you for your encouragement…

  … but **Abercus worries that it does not do enough**!

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- Thank you for your encouragement…

  … but **Abercus worries that it does not do enough**!

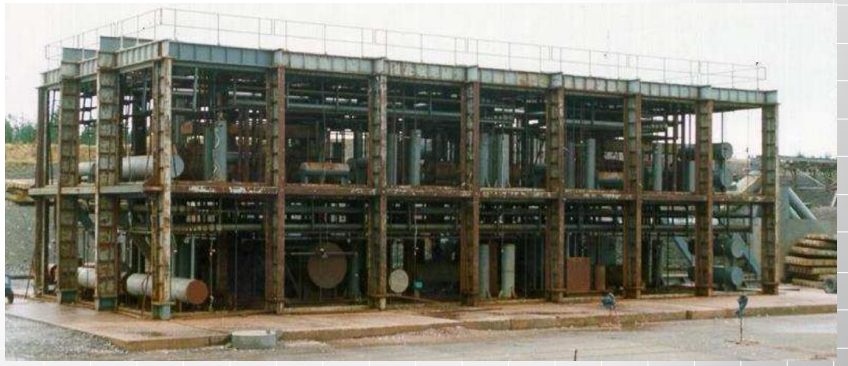
- And it becomes very difficult to have rigorous conversations with some of our clients when this conversation is not an open conversation within our community.

The way forward…

- The community needs your help!:
  1. We need folks at the top of the hierarchy to **ask for evidence of VVUQ by users** of the PDR-CFD codes.

     If no one in a position of authority is asking for it, what are the drivers to voluntarily undertake VVUQ?
  2. We need **access to experimental validation data** in order to enable users to perform their own VVUQ.

     This has been a significant barrier to users' VVUQ in the past – unless you were party to the original JIPs, for example BFETS in the 1990s, much of the information needed for VVUQ has not been available…



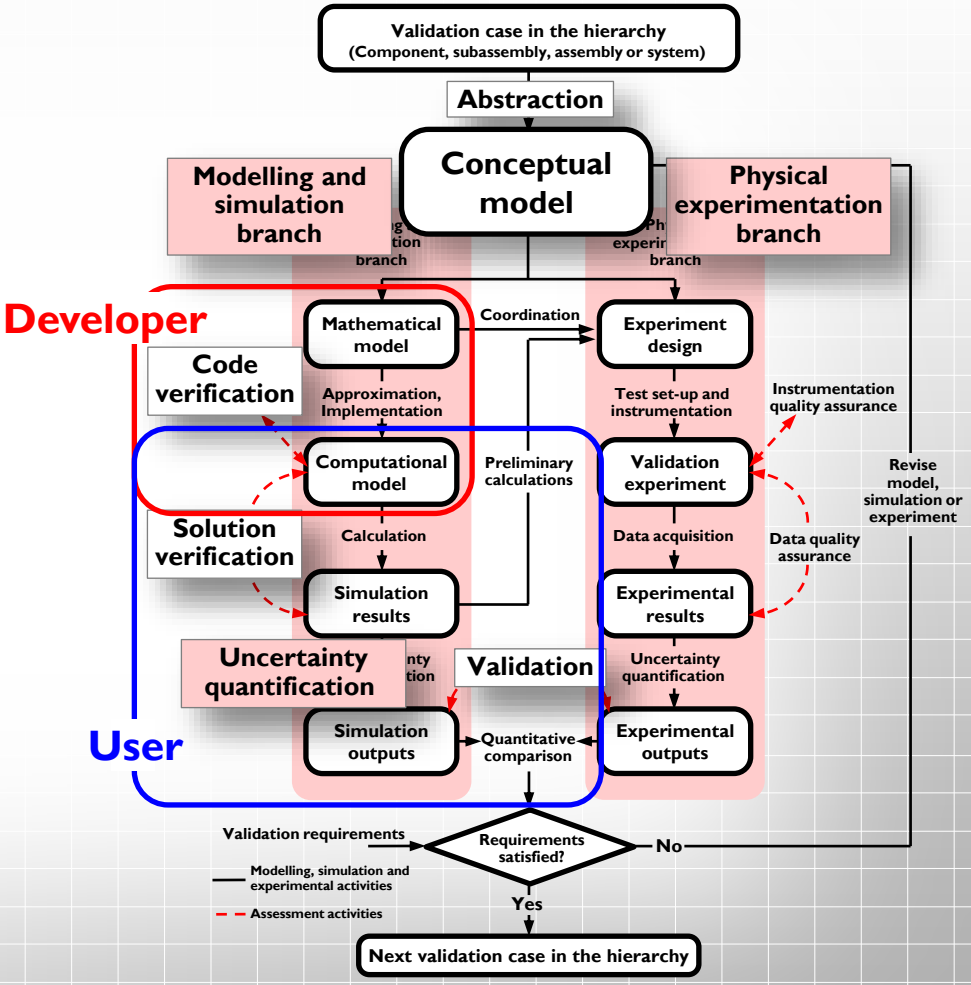
[Ref. 17]: Johnson DM, Allason D and Cronin PM, "*Large scale experimental research of VCEs – A summary from one viewpoint*", J. Loss Prev. Proc. Ind. 89,105287, 2024.

The way forward…

- The community needs your help!:
  3. We **urgently need to have clarity on who is responsible for VVUQ**! Users or PDR-CFD developers?

     Unless a PDR-CFD code owns the entire left-hand branch, such that a user cannot interfere with it, **validation is not of the code, but of the combination of code plus user/workflow**.

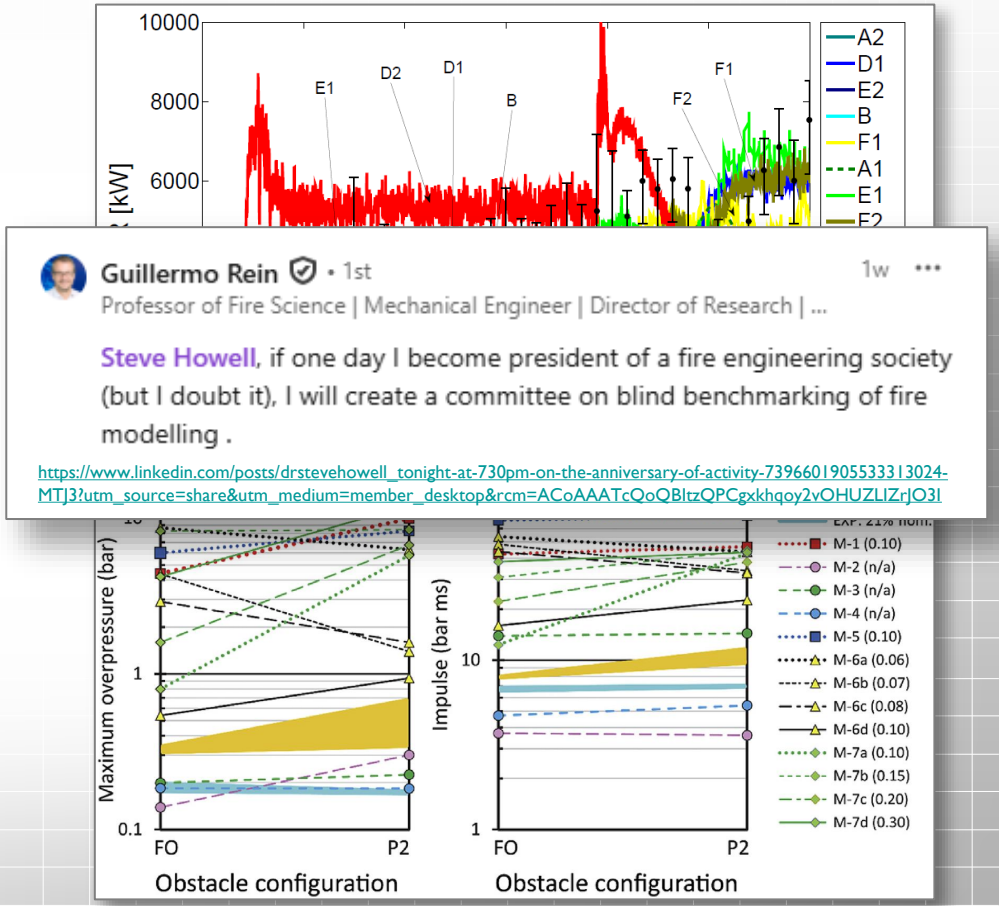
     We don't have complete agreement on this, even within the authorship of this paper, let alone within our industry! Without clarity on this issue, there exists a **responsibility gap** that needs resolution.



The way forward…

- The community needs your help!:
  4. We need PDR-CFD developers to release the **underlying data for their validation studies** – static images in the validation section of a user manual is not good enough, it cannot be rigorously scrutinized.

     Ideally PDR-CFD developers would develop this into **validation tutorials**, taking users through the VVUQ process and comparing with real experimental validation referents…
  5. We need to organize **regular blind benchmarking** exercises, so that we can identify user variation with the PDR approach and address it together, within the PDR-CFD community – this should become normality.

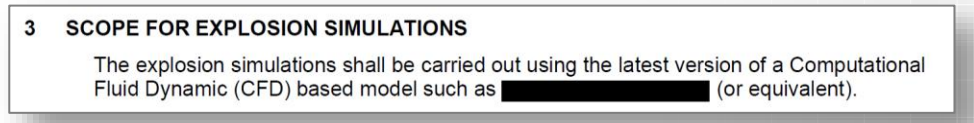


The way forward…

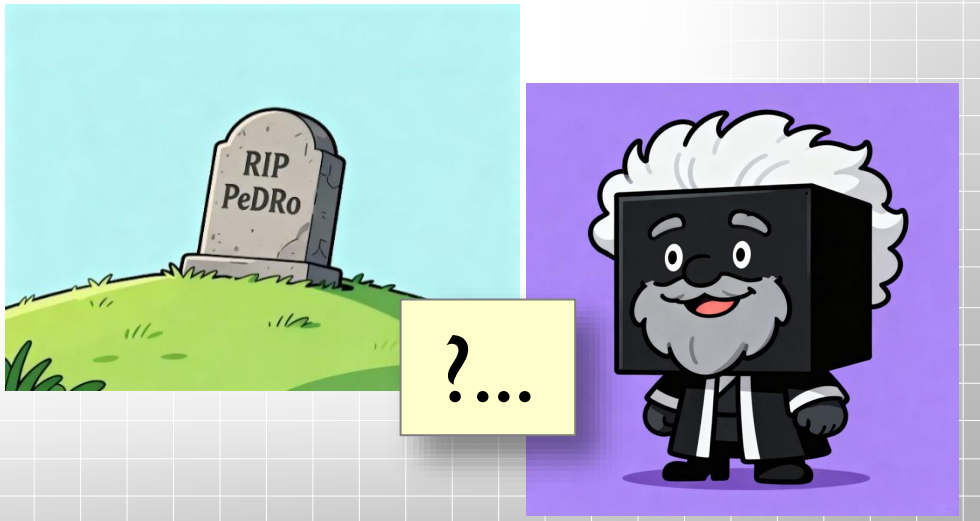
- The community needs your help!:
  6. When procuring CFD explosion studies, we need to stop demanding that studies be completed with the latest version of a particular CFD code. The choice of CFD code should be **dictated by rigorous VVUQ**.

     Who owns the **legal liability** when the latest version of a specific software is demanded by procurement?
  7. In our **marketing**, we need to be **honest** about the **current status** of the PDR approach for simulating VCE explosions. Statements like *"With* [our PDR-CFD software], *you get results you can trust"* do great damage to the credibility of the approach in the long-run.

     Trust in CFD is hard earned but easily eroded.


3 SCOPE FOR EXPLOSION SIMULATIONS

The explosion simulations shall be carried out using the latest version of a Computational Fluid Dynamic (CFD) based model such as [redacted] (or equivalent).

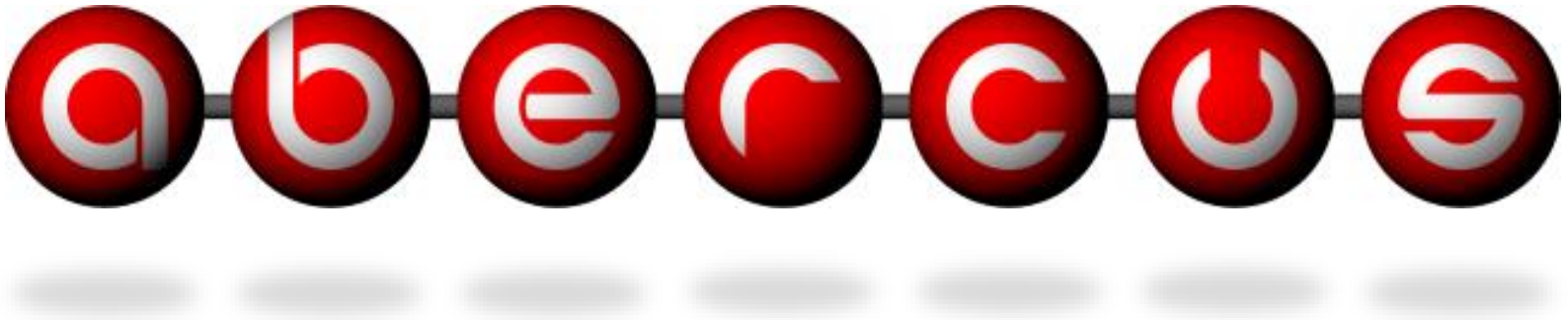


The way forward…

- The PDR Alliance has recently been established to provide an open forum to explore issues relating to the PDR approach (www.pdr-alliance.org):
  - Trygve Skjold and Helene Hisken (University of Bergen).

The way forward…

- The availability of experimental validation data may have previously been a barrier to users undertaking VVUQ, but there are some important recent developments:
  - PHMSA has recently prepared a validation database for vapour cloud explosions and dispersion (2025 – Filippo Gavelli, Blue Engineering and Consulting, USA):
    - https://primis.phmsa.dot.gov/rd/projects/854/
    - https://primis.phmsa.dot.gov/rd/FileGet/20198/03903-PP-008_(Model_Validation_Database_for_Vapor_Cloud_Explosion)_-_Appendices.zip
  - There is also a sister database for fire (OSTI, USA):
    - https://www.osti.gov/biblio/2588296
    - https://www.osti.gov/servlets/purl/2588296
  - FABIG (Fire And Blast Investigation Group) will soon release the BFETS geometries, to complete the data needed for VVUQ – keep an eye on the FABIG website in the coming weeks.
- If you have or know of any experimental data suitable for validation – **get in touch**!



Contact us

Enquiries can be directed to:
steve.howell@abercus.com
www.abercus.com

www.linkedin.com/in/drstevehowell