SAND2009-4667C

A Rogue’s Gallery of V&V Practice

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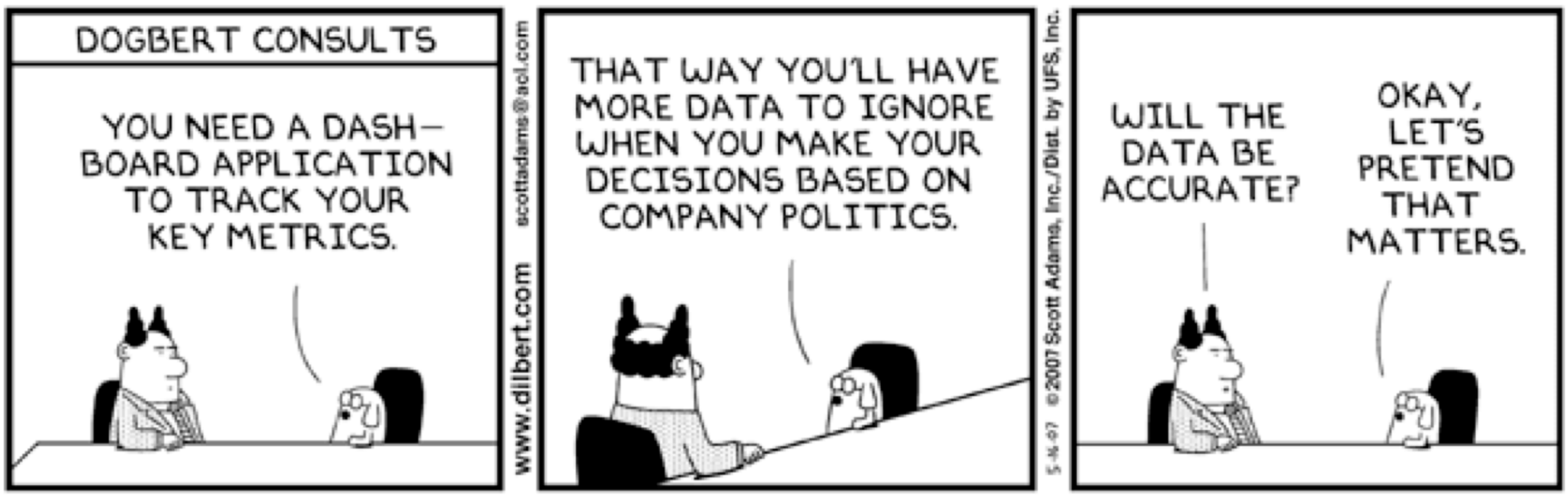
MeV Summer School Lunch Talk

SAND-2009-????P

Quote du jour…

“The purpose of computing is insight, not pictures”–Richard Hamming



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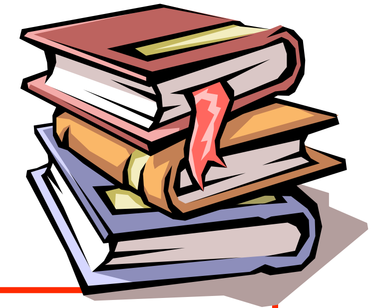
Some definitions used in V&V



Complementary

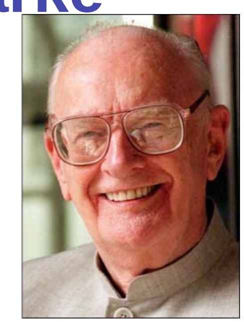
- Verification ≈ **Solving the equations correctly**
  - **Mathematics/Computer Science issue**
  - **Applies to both codes and calculations**
- Validation ≈ **Solving the correct equations**
  - **Physics/Engineering (i.e., modeling) issue**
  - **Applies to both codes and calculations**
- Calibration ≈ **Adjusting (“tuning”) parameters**
  - **Parameters chosen for a specific class of problems**
- Benchmarking ≈ **Comparing with other codes**
  - **“There is no democracy in physics.”***

*L.Alvarez, in D. Greenberg, *The Politics of Pure Science*, U. Chicago Press, 1967.

The nature of the code development is a key aspect to consider.

- **How well do the code developers understand what they are working on.**
- **In some cases the key developers have moved on and are not available…**

- **… leading to the "magic" code issue,**
  - **"Any sufficiently advanced technology is indistinguishable from magic." Arthur C. Clarke [Clarke's Third Law]**



  - **Understanding problems can be nearly impossible, or prone to substantial errors,**
  - **Fixing problems become problematic (bad choices are often made!) as a consequence.**

Diffusion of innovation is useful to understand how ideas advance.

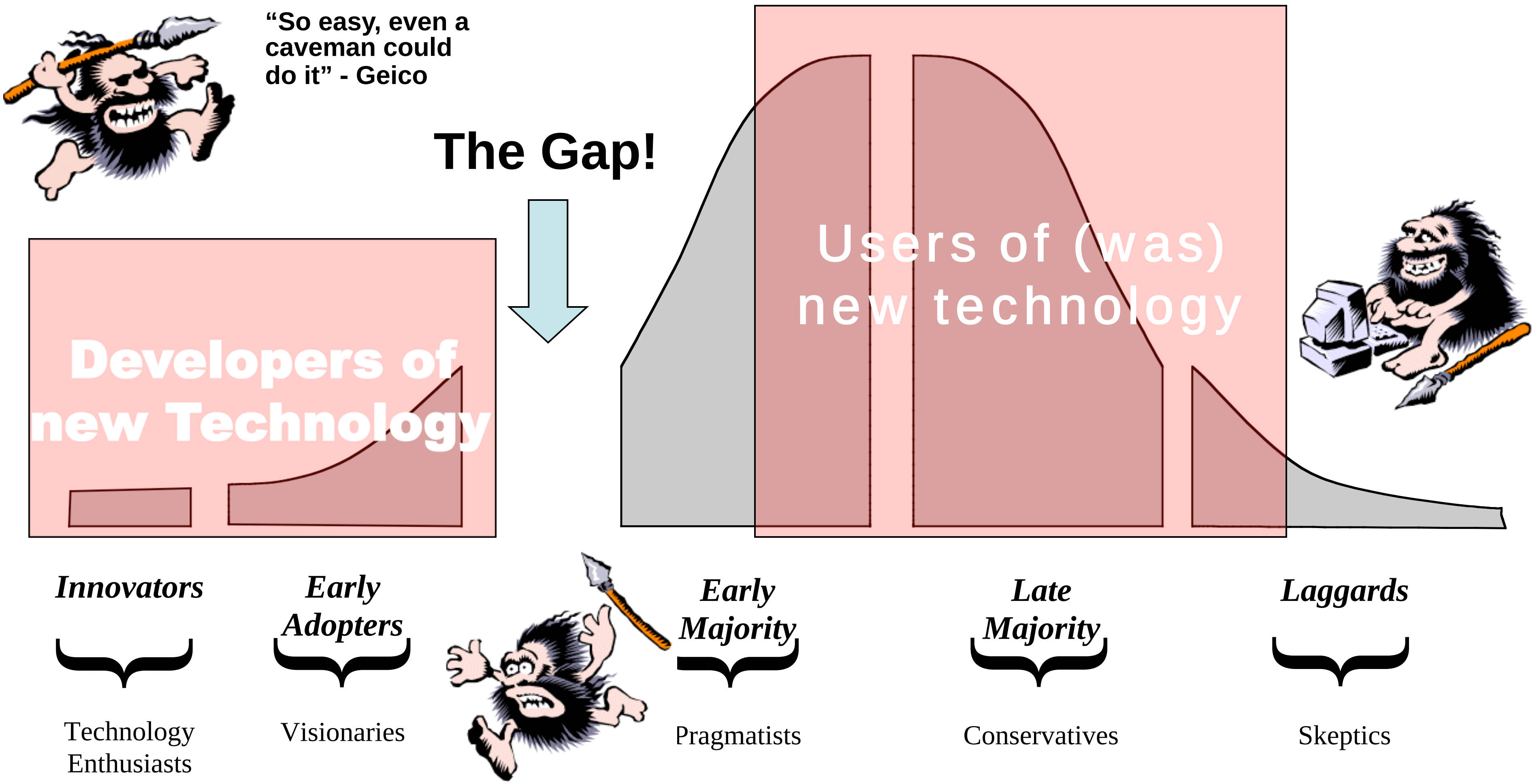
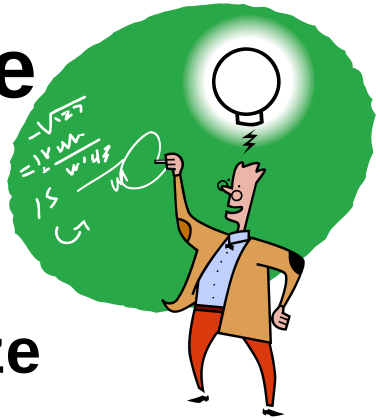


Figure adapted from “After the Goal Rush: Creating a True Profession of Software Engineering” by Steve McConnelll, Microsoft Press 1999

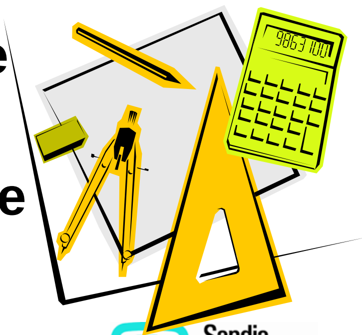
"Most daily activity in science can only be described as tedious and boring, not to mention expensive and frustrating."

Stephen J. Gould, Science, Jan 14, 2000.

We can see how different the user communities can be.



- If one considers that the journals characterize the leading edge of work in an area.
- For fluid mechanics, the engineering community has embraced well-defined standards (using V&V)
- While the physics community tends to embrace a standard based on expert judgment.
- These considerations tend to be reflected in practice:
  - Engineers tend to work to achieve a strong evidence basis for decisions
  - Physicists tend to provide their evidence based more strongly on expertise.



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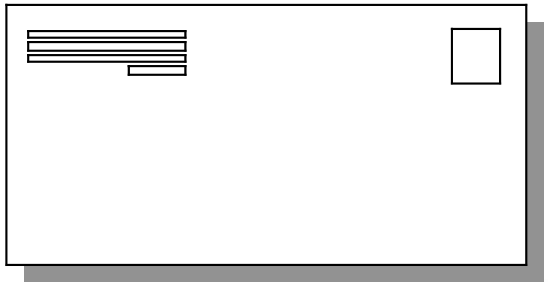
I'm going to go through a set of examples next from the literature.

- The examples are taken from the current (2009) literature for a small subset of journals.
- They *do not* reflect a comprehensive study, the articles were simply chosen from a recent issue of the journal.
- My working thesis is that any issues *are not an indictment of the authors*, but rather a reflection of accepted practice within the communities represented by the journals chosen.

Excerpt from the editorial policy of Physics of Fluids

"Physics of Fluids, published monthly by the American Institute of Physics with the cooperation of the American Physical Society, Division of Fluid Dynamics, is devoted to original theoretical, computational, and experimental contributions to the dynamics of gases, liquids, and complex or multiphase fluids."

- **There is nothing about accuracy, validation, verification, convergence, etc…**
- **Everything is in the hands of the editors and reviewers, i.e. the experts.**



I'm not picking on Physics of Fluids, there are many other examples

Example 1: Physics of Fluids

PHYSICS OF FLUIDS **21**, 051702 (2009)

Turbulent boundary layers up to $\mathrm{Re}_\theta=2500$ studied through simulation and experiment

P. Schlatter,[a)] R. Örlü, Q. Li, G. Brethouwer, J. H. M. Fransson, A. V. Johansson, P. H. Alfredsson, and D. S. Henningson
Linné Flow Centre, KTH Mechanics, SE-100 44 Stockholm, Sweden

(Received 4 March 2009; accepted 24 April 2009; published online 20 May 2009)

The computational domain is $x_L \times y_L \times z_L = 3000\delta_0^* \times 100\delta_0^* \times 120\delta_0^*$ with $3072 \times 301 \times 256$ spectral collocation points in the streamwise, wall-normal, and spanwise directions, respectively. The height and width of the computational domain are chosen to be at least twice the largest 99%
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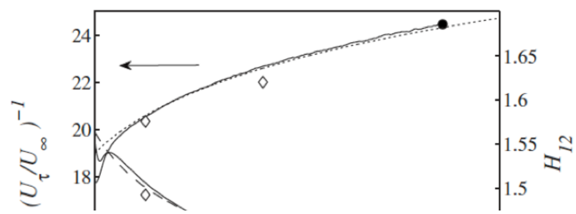
sions, but an increased number of grid points as $4096 \times 385 \times 480$ showing only insignificant differences. Statistics are sampled over $\Delta t^+ \approx 24\,000$ viscous time units, or 30 in units of δ_{99}/U_τ at $\mathrm{Re}_\theta=2500$. Owing to the high computational cost of the simulations, the code is fully parallelized running on $\mathcal{O}(1000)$ processors.



Neither the experiment or the simulation have any error estimate associated with it. The reader cannot have any idea of the quality of either. Is this an acceptable state of affairs?

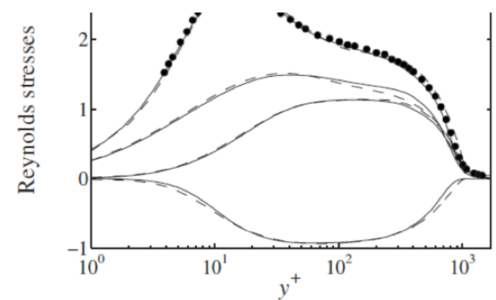


FIG. 3. Turbulent fluctuations u^+_{rms}, w^+_{rms}, v^+_{rms}, and shear stress $\langle u'v'\rangle^+$ (from top). (—) Present DNS at $\mathrm{Re}_\theta=2512$, (●) experiments at $\mathrm{Re}_\theta=2541$. (– – –) Correlations based on the attached-eddy hypothesis (Refs. 14–16).

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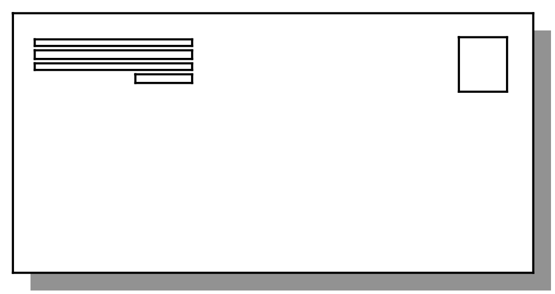
Excerpt from the editorial policy of Journal of Fluid Mechanics

"Journal of Fluid Mechanics is the leading international journal in the field and is essential reading for all those concerned with developments in fluid mechanics. It publishes authoritative articles covering theoretical, computational and experimental investigations of all aspects of the mechanics of fluids. Each issue contains papers on both the fundamental aspects of fluid mechanics, and their applications to other fields such as aeronautics, astrophysics, biology, chemical and mechanical engineering, hydraulics, meteorology, oceanography, geology, acoustics and combustion."

- **There is nothing about accuracy, validation, verification, convergence, etc…**
- **Everything is in the hands of the editors and reviewers, i.e. the experts.**



Example 2: Journal of Fluid Mechanics

J. Fluid Mech. (2009), vol. 628, pp. 43–55. © 2009 Cambridge University Press 43
doi:10.1017/S0022112009006156 Printed in the United Kingdom

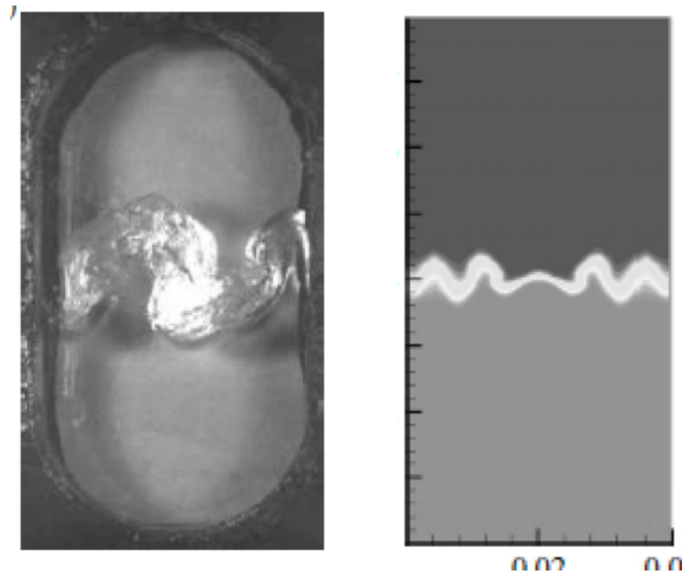
Experimental and numerical study of miscible Faraday instability

F. ZOUESHTIAGH[1]†, S. AMIROUDINE[2] AND R. NARAYANAN[3]

[1]Institut d'Electronique, de Microélectronique et de Nanotechnologie UMR CNRS 8520, Avenue Poincaré, 59652 Villeneuve d'Ascq, France

[2]LPMI-Arts et Métiers ParisTech., 2 Bd du Ronceray, BP 93525, 49035 Angers, France

[3]University of Florida, Department of Chemical Engineering, Gainesville, FL 32611-6005, USA



Equations (3.1) and (3.2) are solved with a finite volume method using the SIMPLER algorithm (Patankar 1980; Amiroudine *et al.* 1997) in a staggered mesh. The space discretization uses the power-law scheme (Patankar 1980) and time discretization is of the first-order Euler type. As the characteristic time t_0 and con
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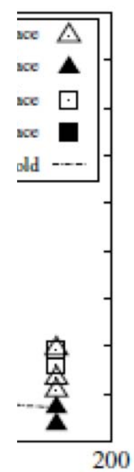
Again both simulation and experiment have no errors estimates. Even the viewgraph norm of the image isn't very convincing. Another telling characteristic is that the simulation is described in very general and vague terms. More importantly the methods used are very old and not very good in modern terms (1st order!!!
How is this good enough?).



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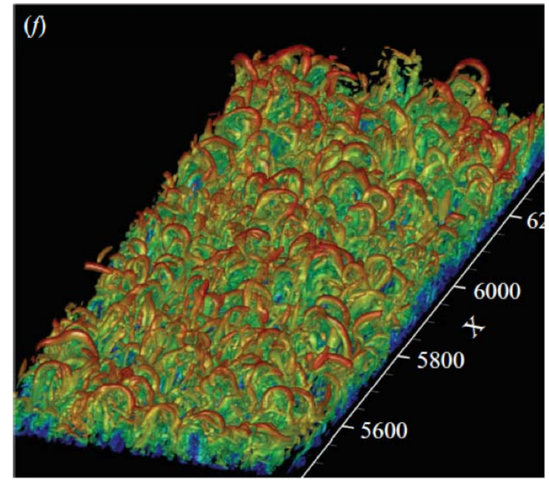
Journal of Fluid Mechanics (continued)

J. Fluid Mech. (2009), *vol.* 630, *pp.* 5–41. © 2009 Cambridge University Press
doi:10.1017/S0022112009006624 Printed in the United Kingdom

Direct numerical simulation of turbulence in a nominally zero-pressure-gradient flat-plate boundary layer

XIAOHUA WU[1] AND PARVIZ MOIN[2]†

The finite-difference grid size is 4096 × 400 × 128 along the x, y and z directions, respectively. Simulation with a coarser grid of 2048 × 400 × 128 was also performed but not presented in this paper. We found that the profile of the skin-friction coefficient C_f obtained from the coarse grid calculation agreed with that from the fine grid to within 0.5 % for the turbulent region $730 < Re_\theta < 930$. Agreement is also excellent in the early transitional region for $80 < Re_\theta < 170$, with a maximum deviation of less than 0.05 %.



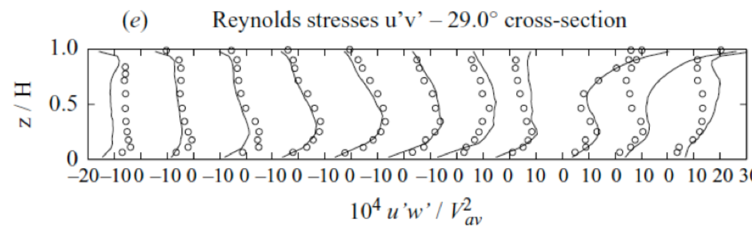
This paper is far better from a V&V perspective than the other JFM papers. The method is described a bit more than other papers. They use two grids! There is a vague error estimate, but no convergence rate. Again, the experimental data is not characterized.

Journal of Fluid Mechanics (continued)

J. Fluid Mech. (2009), *vol.* 630, *pp.* 413–442. © 2009 Cambridge University Press 413
doi:10.1017/S0022112009007277 Printed in the United Kingdom

Large-eddy simulation of a mildly curved open-channel flow

W. VAN BALEN[1]†, W. S. J. UIJTTEWAAL[1]
AND K. BLANCKAERT[1,2]

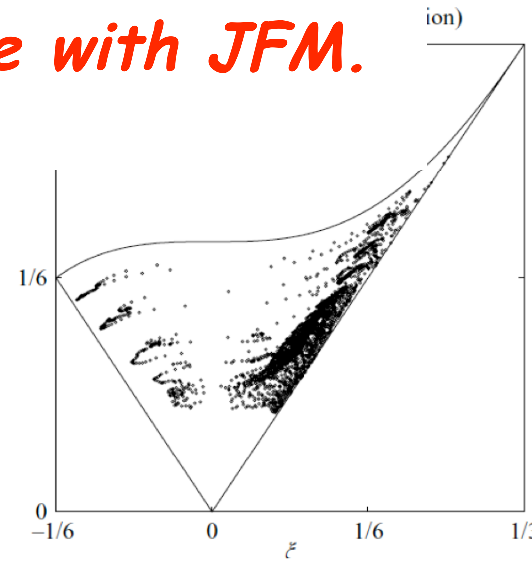


The equations are solved on a staggered mesh using the finite-volume method, with typical grid cells as shown in figure 3, using a pressure-correction algorithm. These equations are numerically integrated in space using the midpoint rule. As a matter of fact, this procedure results in the spatial discretization of the domain following the second-order central scheme. The equations are integrated in time using the explicit second-order Adams–Bashforth scheme. More details on the numerics can be found

This paper is sort of par for the course with JFM. Until…

	Subgrid-scale model	F_i	Boundary conditions	Mesh
Run 1	standard Smagorinsky	0	Non-periodic	3600 × 168 × 24
Run 2	standard Smagorinsky	0	Periodic	300 × 168 × 24
Run 3	dynamic Smagorinsky	$\partial p/\partial x_i$	Periodic	300 × 168 × 24
Run 4	standard Smagorinsky	0	Periodic	300 × 168 × 24
Run 5	dynamic Smagorinsky	$\partial p/\partial x_i$	Periodic	300 × 168 × 24

TABLE 2. Model settings for the different runs. F_i refers to (2.11), the mesh is given as the number of grid cells in streamwise, transverse and vertical direction.



A bonus: same article!

Appendix B. Mesh independency

In order to prove that the solutions of the presented simulations are independent of the mesh, Run 2 from the paper is chosen to be simulated on two other meshes: a coarser mesh and a finer mesh. Recall that Run 2 is the simulation of the axisymmetric flow in the far field of the flow set-up (see figure 5). The big advantage of axisymmetric flow is that periodic boundary conditions can be applied in streamwise direction, thus saving much computational time. An instantaneous result of Run 2, shown in figure 17, also shows the dimensions of the computational domain.

The simulations are run on different meshes: a coarse mesh ($112 \times 200 \times 16$), a medium mesh ($168 \times 300 \times 24$) and a fine mesh ($252 \times 460 \times 36$). The results for the streamfunction ψ and the Reynolds stresses $\overline{u'w'}$ of the three simulations are shown in figure 21 for the outer bank region.

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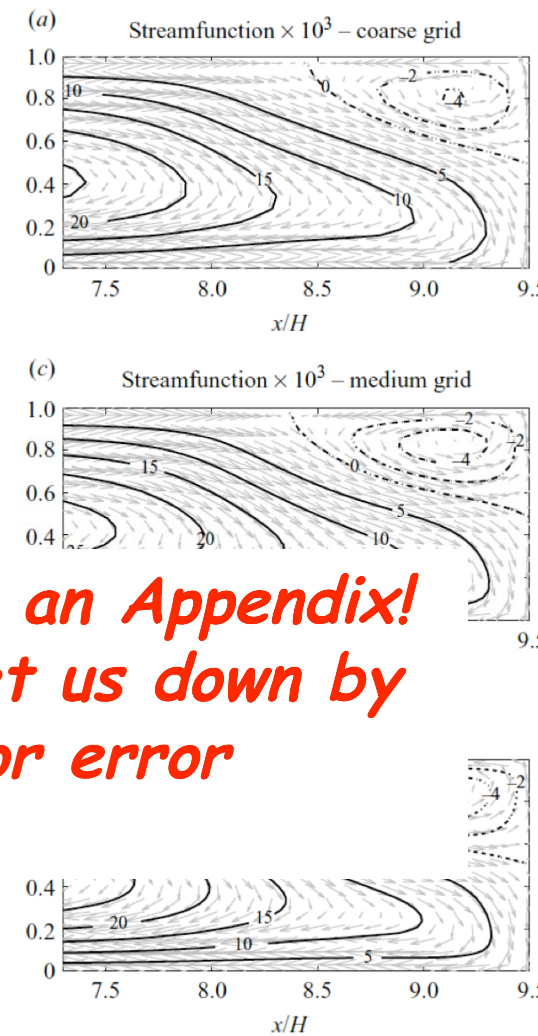
In the background of the pictures in figure 21 the velocity vectors are shown. For this purpose, the velocity fields of the medium and the fine mesh are interpolated to the grid of the coarse mesh to make the comparison comprehensible. It is clearly seen



A mesh refinement study is included in an Appendix! They even use three grids, but then let us down by not even giving us a convergence rate or error estimate. So close, yet so far!

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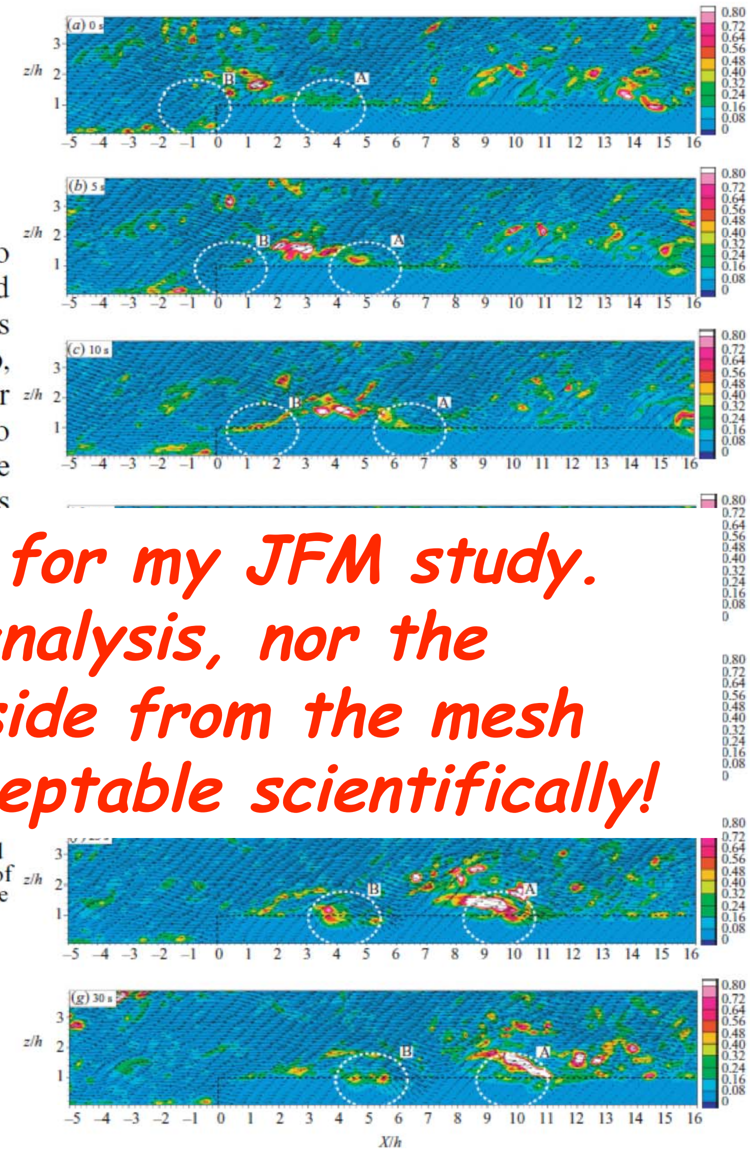
Journal of Fluid Mechanics (continued)

J. Fluid Mech. (2009), vol. 630, pp. 93–128. © 2009 Cambridge University Press
doi:10.1017/S0022112009006739 Printed in the United Kingdom

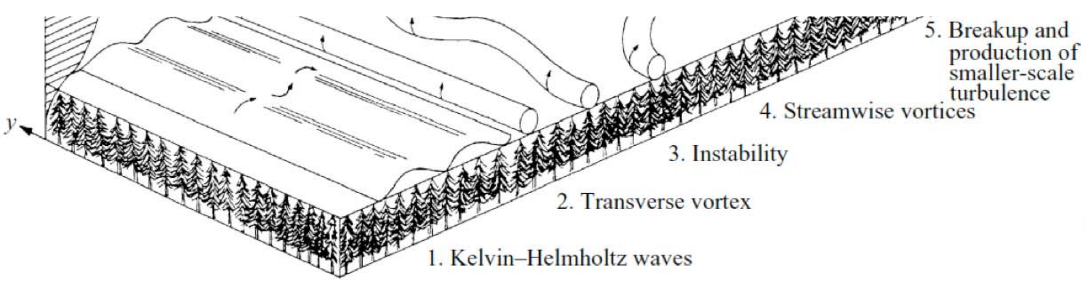
Coherent structures in canopy edge flow: a large-eddy simulation study

S. DUPONT† AND Y. BRUNET

The computational domain extends over 668 × 200 × 200 m^3, corresponding to 345 × 100 × 65 grid points in the x-, y- and z-direction, respectively, with 2 m grid spacing below $z = 84$ m and a vertically stretched grid above. This resolution allows us to simulate turbulent structures induced by the mean shear at the canopy top, since their horizontal size is of the order of h, and their vertical size of the order of $h/3$ (Finnigan 2000). The limitation of the vertical size of the domain due to computational time considerations does not allow large mesoscale structures to be resolved. This should not have noticeable consequences on the main results of this



This paper is really the low point for my JFM study. There isn't even a hint of error analysis, nor the merest description of the code aside from the mesh used. I can't see how this is acceptable scientifically!

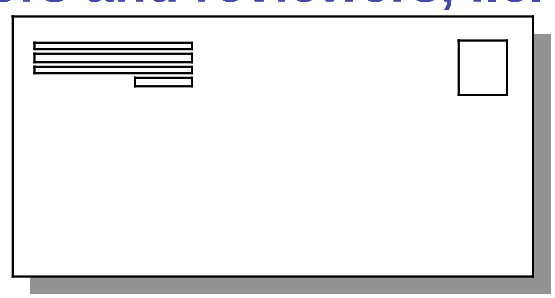


Excerpt from the editorial policy of Physical Review Letters

"Physical Review Letters, published by the American Physical Society, is charged with providing rapid publication of short reports of important fundamental research in all fields of physics. The journal should provide its diverse readership with coverage of major advances in all aspects of physics and of developments with significant consequences across subdisciplines. Letters should therefore be of broad interest."

"Mathematical and computational papers that do not have application to physics are generally not suitable for Physical Review Letters."

- **There is nothing about accuracy, validation, verification, convergence, etc…**
- **Everything is in the hands of the editors and reviewers, i.e. the experts.**



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Example 3: Physical Review Letters

PRL **102,** 224101 (2009) PHYSICAL REVIEW LETTERS week ending 5 JUNE 2009

Discrete Breathers in a Forced-Damped Array of Coupled Pendula: Modeling, Computation, and Experiment

J. Cuevas,[1] L. Q. English,[2] P. G. Kevrekidis,[3] and M. Anderson[2]

[1]*Departamento de Física Aplicada I. Escuela Universitaria Politécnica, Universidad de Sevilla. C/ Virgen de África, 7, 41011 Sevilla, Spain*

[2]*Department of Physics & Astronomy, Dickinson College, Carlisle, Pennsylvania 17013, USA*

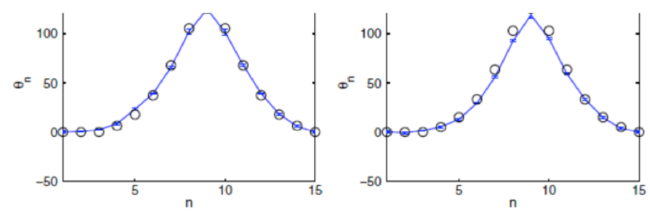
[3]*Department of Mathematics and Statistics, University of Massachusetts, Amherst, Massachusetts 01003-4515, USA*

(Received 12 February 2009; published 2 June 2009)

In this work, we present a mechanical example of an *experimental realization* of a stability reversal between on-site and intersite centered localized modes. A corresponding realization of a vanishing of the

The issues with this paper are simple. The numerical methods are not described, error is not quantified, the experimental data has unquantified error. The paper reports to put modeling, computing and experiment together yet quantified none although the comparison seems good.

represent the numerical results whereas the full lines with error bars correspond to the experimental profiles.



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PRL **102**, 217201 (2009) PHYSICAL REVIEW LETTERS week ending 29 MAY 2009

Electric Field Induced Magnetic Anisotropy in a Ferromagnet

S. J. Gamble,[1,2] Mark H. Burkhardt,[2,3] A. Kashuba,[4] Rolf Allenspach,[5] Stuart S. P. Parkin,[6] H. C. Siegmann,[1] and J. Stöhr[1,3]

[1]*PULSE Center, Stanford University, Stanford, California 94025, USA*
[2]*Department of Applied Physics, Stanford University, Stanford, California 94305, USA*
[3]*Stanford Synchrotron Radiation Lightsource, Stanford, California 94305, USA*
[4]*Bogolyubov Institute for Theoretical Physics 14-b, Metrolohichna Street, Kiev 03680, Ukraine*
[5]*IBM Research, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland*
[6]*IBM Almaden Research Center, San Jose, California 95120, USA*
(Received 8 December 2008; published 27 May 2009)

We report the first observation of a transient all electric field induced magnetic anisotropy in a thin film metallic ferromagnet. We generate the anisotropy with a strong ($\sim 10^9$ V/m) and short (70 fs) $\vec{E}$-field pulse. This field is large enough to distort the valence charge distribution in the metal, yet its duration is too brief to change the atomic positions. This pure electronic structure alteration of the sample generates a new type of transient anisotropy axis and strongly influences the magnetization dynamics. The successful creation of such an anisotropy opens the possibility for all $\vec{E}$-field induced magnetization reversal in thin metallic films—a greatly desired yet unachieved process.

This paper was highlighted by this Journal presumably because the picture looks so darn good! This seems like the the viewgraph norm personified. Again, nothing whatsoever is quantified experimentally or computationally.

of patterns (b) and (c) in Fig. 3 are $g = 2$, $K_u/K_s = 0.041$, $\gamma = 1.46$, and the intrinsic Gilbert dissipation constant $\alpha_0 = 0.017$. The spin-wave instabilities develop on a time scale $\geq$100 ps, that is long after the bunch has passed. Their inclusion accounts for the observed number of rings and their variable widths.

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Science Magazine: Editorial Policy

***SCIENCE'S* MISSION:** *Science* seeks to publish those papers that are most influential in their fields and that will significantly advance scientific understanding. Selected papers should present novel and broadly important data, syntheses, or concepts. They should merit the recognition by the scientific community and general public provided by publication in *Science*, beyond that provided by specialty journals.

CRITERIA FOR JUDGMENT

Research Articles should report a major breakthrough in a particular field. They should be in the top 20% of the papers that *Science* publishes and be of strong interdisciplinary interest or unusual interest to the specialist.

Technical Rigor: Evaluate whether, or to what extent, the data and methods substantiate the conclusions and interpretations. If appropriate, indicate what additional data and information are needed to validate the conclusions or support the interpretations.

Supporting Online Material. Supporting online material includes methods, text or data that is of interest only to the specialist, but that is still necessary for the integrity and excellence of the paper. It must be directly related to the conclusions of the print paper. We welcome suggestions for deletions of supporting online material or items that should be moved to supporting online material.

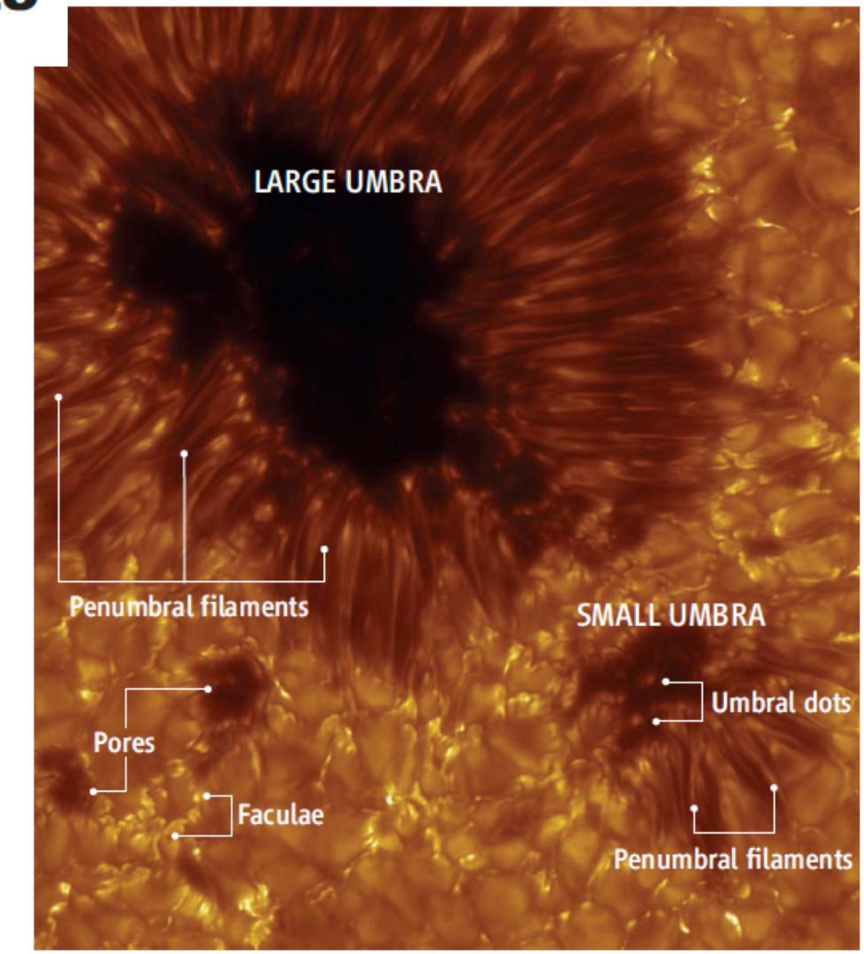
Science often has a "news" article about the research papers.

Sunspot Flows and Filaments

Göran Scharmer

In 1941, Ludwig Biermann recognized that the reduced brightness of sunspot umbrae could be due to suppression of the convective energy flux by their strong magnetic field. But this led to the problem of explaining why sunspots are not completely dark. Simulations of sunspot umbrae (*5*) demonstrate the formation of narrow plumes within which the magnetic field is expelled by overturning convection, leading to the formation of bright umbral dots.

The first 3D simulations of sunspots (*10*, *11*), although limited to azimuthally narrow slices of a sunspot, did provide consistency with several observed aspects of penumbrae. They demonstrated convection in radially aligned sheet-like structures with strongly reduced field strength and systematic (but weak) radial outflows. This led us to the conclusion that the Evershed flow is identical to the horizontal component of penumbral convection (*12*). Rempel *et al.* now present simulations of two sunspots of opposite polarities and not just thin slices of a sunspot as in the earlier simulations (*10*, *11*). They



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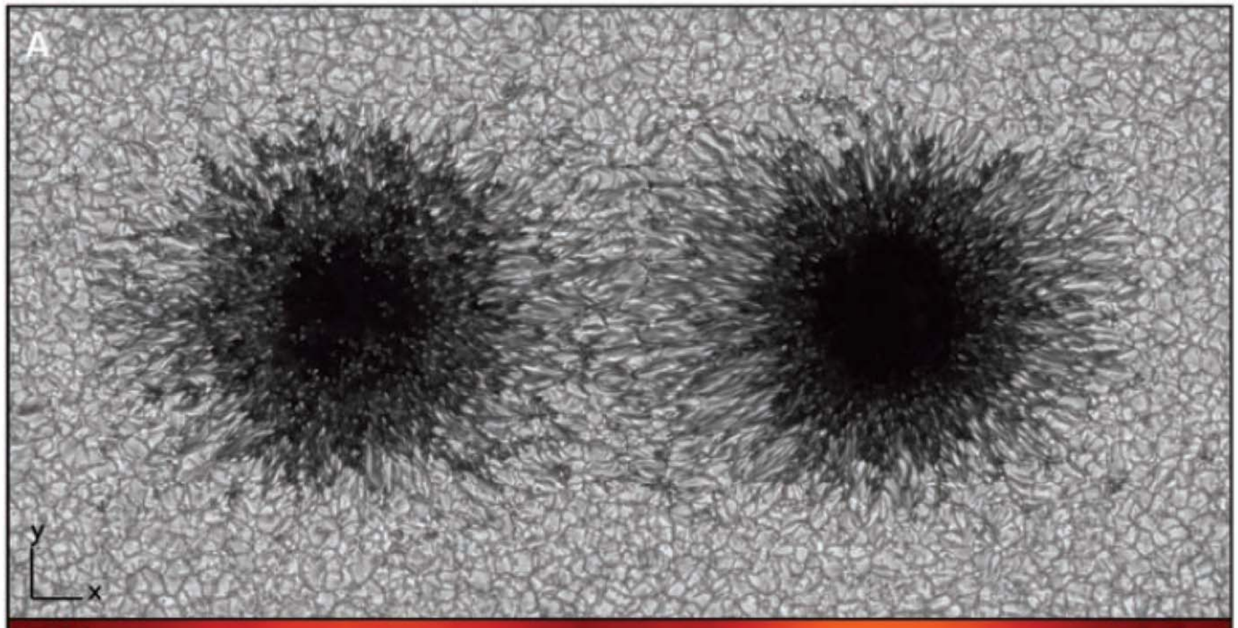
The research article in Science.

field between the spots. Our numerical box had a horizontal extension of 98 Mm by 49 Mm and a depth of 6.1 Mm. The spatial grid resolution was 32 km in the horizontal directions and 16 km in the vertical. The sunspots evolved for 3.6 hours during the simulation, which was sufficient to study the penumbral structure and dynamics; processes that evolve on longer time scales, such as moat flows, were not fully developed in this simulation. However, the surface evolution of



The strongest "evidence" is the likeness of the above picture with photographs of the actual sun. All the details and evidence of numerical quality is in supplementary material. I decided to look at it.

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umbral dots as well as inner and outer penumbrae in terms of magnetoconvection in a magnetic field with varying inclination. Furthermore, a consistent physical picture of all observational characteristics of sunspots and their surroundings is now emerging.

8. More detailed information about the physical model, the numerical code, and the simulation setup is available as supporting material on *Science* Online.

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Thank God for supplementary material!

The simulation presented here has been carried out with the *MURaM* MHD code (*1*, *2*), with modifications described in (*3*). The physics, numerics and boundary conditions are similar to earlier runs described there, the primary difference here is the far larger domain size and the initial magnetic field configuration.

We ran the simulation for the first hour of simulated time with a rather low numerical grid resolution of $96 \times 96 \times 32$ km to get past initial transients. The second hour was performed at a medium resolution of $48 \times 48 \times 24$ km and then followed by another 1.6 hours with a resolution of $32 \times 32 \times 16$ km (corresponding to $3072 \times 1536 \times 384$ grid cells). The results presented here are based on snapshots near the end of the high-resolution run and partly on temporal averages

Very disappointing! In fact new questions were raised. The references had to be examined to find any details. No V or V can be found.

3. M. Rempel, M. Schüssler, M. Knölker, *ApJ* **691**, 640 (2009).

OK, let's look at those references

There is a little, but not much in the Ap. J. paper.

Let's look at that thesis. There is no V or V.

This chapter discusses the numerical methods of the MHD code. The code used here is based on a code for general MHD applications, which was developed by T. Linde and A. Malagoli at the University of Chicago. This basic code solves the MHD equations (2.17), (2.19), (2.20), and (2.27) without radiative source term, assuming constant scalar diffusion coefficients μ, K, and η and using the

The MHD code solves the system of MHD equations on a three-dimensional equidistant cartesian grid. The spatial discretization of the equations is based on the fourth-order centered-difference scheme on a 5-point stencil. Choosing i as

The numerical solution of the system is advanced in time using an explicit fourth-

The method is described albeit not specifically. There isn't any verification at all.

separate diffusion coefficient, consisting of a shock-resolving and a hyperdiffusive part, is defined:

$$\nu_l(u) = \nu_l^{\mathrm{shk}} + \nu_l^{\mathrm{hyp}}(u). \tag{3.14}$$

$$\nu_l^{\mathrm{shk}} = \begin{cases} c_{\mathrm{shk}} \cdot \Delta x_l^2 \cdot |\nabla \cdot \mathbf{v}| & \nabla \cdot \mathbf{v} < 0 \\ 0 & \nabla \cdot \mathbf{v} \geq 0 \end{cases}. \tag{3.15}$$

$$\nu_l^{\mathrm{hyp}}(u) = c_{\mathrm{hyp}} \cdot c_{\mathrm{tot}} \cdot \Delta x_l \cdot \frac{\max_3 \Delta_l^3 u}{\max_3 \Delta_l^1 u}. \tag{3.16}$$

nature Magazine

Editorial Guidance: Writing a peer review

- **Are the claims convincing? If not, what further evidence is needed?**
- **Are there other experiments or work that would strengthen the paper further?**
- **How much would further work improve it, and how difficult would this be? Would it take a long time?**
- **Should the authors be asked to provide supplementary methods or data to accompany the paper online? (Such data might include source code for modelling studies, detailed experimental protocols or mathematical derivations.)**
- **Have they provided sufficient methodological detail that the experiments could be reproduced?**
- **Is the statistical analysis of the data sound, and does it conform to the journal's guidelines?**

The proportionality of global warming to cumulative carbon emissions

by H. Damon Matthews, Nathan P. Gillett, Peter A. Stott & Kirsten Zickfeld - Nature 459, 829-832 (11 June 2009) | doi:10.1038/nature08047

Editor's summary: To date, efforts to describe and predict the climate response to human CO2 emissions have focused on climate sensitivity: the equilibrium temperature change associated with a doubling of CO2. But recent research has suggested that this 'Charney' sensitivity, so named after the meteorologist Jule Charney who first adopted this approach in 1979, may be an incomplete representation of the full Earth system response, as it ignores changes in the carbon cycle, aerosols,

Again, the magazine has a laypersons news story plus an Editor's summary of the article. For Nature, all the numerical work that I could find was related to climate change. Its important to note that these papers are significant in terms of much larger geopolitical dynamics with massive economic consequences too.

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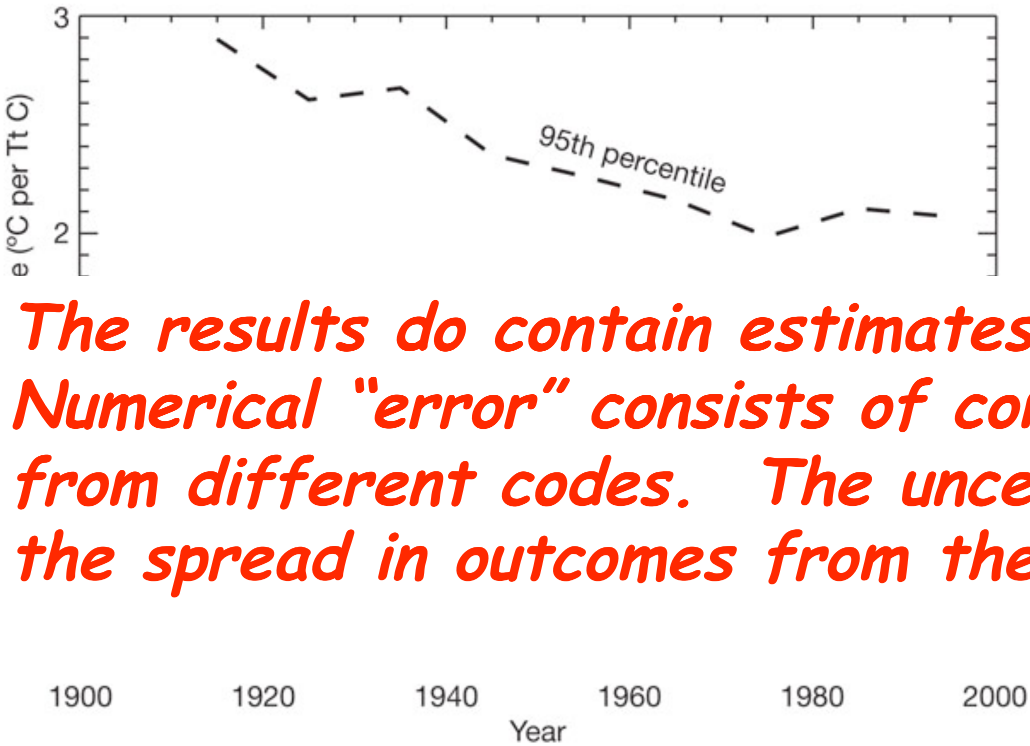
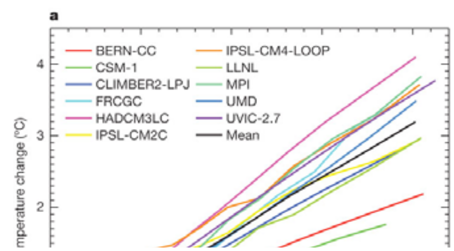
Results

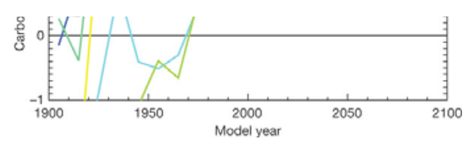
Observational estimates of CCR.

CCR estimated from the C4MIP simulations[11].





The results do contain estimates of observational errors. Numerical "error" consists of comparing the results from different codes. The uncertainty is defined as the spread in outcomes from the codes.



HD Matthews *et al. Nature* **459**, 829-832 (2009) doi:10.1038/nature08047

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Method's summary

METHODS SUMMARY

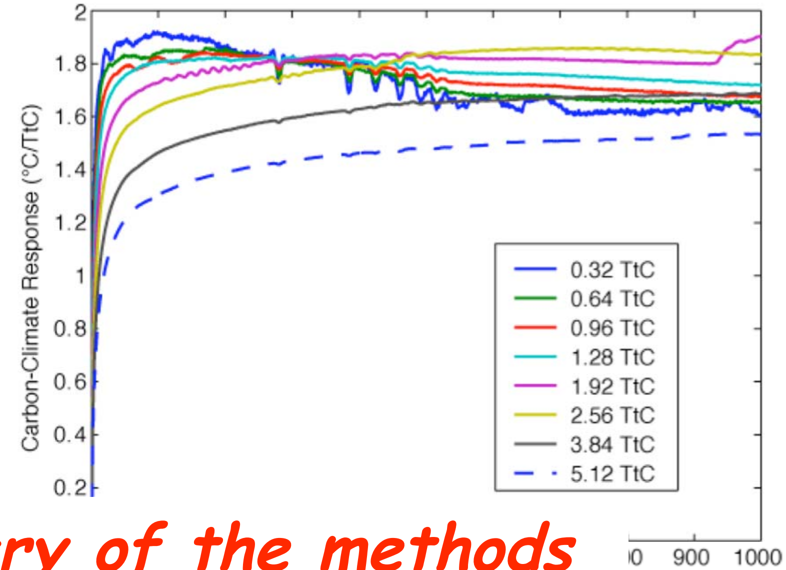
For the idealized model experiments (1% per year CO_2 increase; doubled/quadrupled CO_2) we used the UVic ESCM version 2.8 (refs 9, 18–20). The UVic ESCM is a computationally efficient coupled climate–carbon model, with interactive representations of three-dimensional ocean circulation, atmospheric energy and moisture balances, sea ice dynamics and thermodynamics, dynamic vegetation and the global carbon cycle (including land and both inorganic and organic ocean carbon). Version 2.7 of the UVic ESCM was one of the 11 participating models in C4MIP[11], in which models were driven by a common CO_2 emissions scenario and carbon sinks and atmospheric CO_2 concentrations were calculated interactively until the year 2100. From the C4MIP simulations, we estimated CCR using globally averaged temperature change and accumulated carbon emissions at the year of CO_2 doubling in each simulation.

Our observational estimate of CCR was derived using estimates of CO_2-attributable warming and cumulative CO_2 emissions for each decade of the twentieth century relative to 1900–09. We estimated CO_2-attributable warming using an

The paper also includes a summary of the methods used plus online supplementary materials.

distributed uncertainties for radiative forcings and greenhouse-gas efficacy, respectively[22]. We calculated cumulative carbon emissions from fossil fuels and land-use change[13,14,23], and assumed a one-sigma systematic uncertainty on land-use emissions of ±0.5 Pg C per year[24]. Our central estimates for CO_2-attributable warming and cumulative emissions at 1990–99 relative to 1900–09 were 0.492 °C and 0.338 Tt C, respectively. We calculated a probability density function for CCR based on the probability distributions of the constituent terms, which we used to estimate the mean and the 5th and 95th percentiles.

Full Methods and any associated references are available in the online version of the paper at www.nature.com/nature.



ted, simulated by the UVic ESCM in response to instantaneous pulse-carbon emissions from 0.32 to 5.12 TtC, followed by zero additional emissions. On timescales of 20 to 1000 years, and for emissions up to about 2 TtC, the instantaneous temperature response per unit carbon emitted is between about 1.6 and 1.9 °C/TtC.

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C4MIP?

Journal of Climate Article: Volume 19, Issue 14 (July 2006) pp. 3337–3353
Climate–Carbon Cycle Feedback Analysis: Results from the C4MIP Model Intercomparison

P. Friedlingstein, L. Bopp, P. Rayner P. Cox R. Betts, C. Jones W. von Bloh, V. Brovkin P. Cadule, S. Doney, M. Eby, H. D. Matthews, A. J. Weaver, I. Fung J. John, G. Bala, F. Joos K. Strassmann, T. Kato, M. Kawamiya, C. Yoshikawa, W. Knorr, K. Lindsay, H. D. Matthews, T. Raddatz and C. Reick, E. Roeckner, K.-G. Schnitzler, R. Schnur, and N. Zeng,

Models	Atmosphere	Ocean	Land carbon	DGVM	Ocean carbon	References
HadCM3LC	HADCM3 2.5° × 3.75°, L19	2.5° × 3.75°, L20 flux adjustment	MOSES/TRIFFID	Yes	HadOCC	Cox et al. (2000)
IPSL-CM2C	LMD5 64 × 50, L19 (5° × 4°)	OPA-7, 2° × 2°, L31 no flux adjustment	SLAVE	No	NPZD	Dufresne et al. (2002)
IPSL-CM4-LOOP	LMDZ-4 96 × 72, L19 (3° × 3)	ORCA2, 2° × 2°, L31, no flux adjustment	ORCHIDEE	Not here	PISCES	Marti et al. (2005) Krinner et al. (2005) Aumont et al. (2003)
CSM-1	CCM3 T31, L18	NCOM 3.6 ° lon 0.8–1.8 ° lat	LSM, CASA	No	OCMIP-biotic	Doney et al. (2006); Fung et al. (2005)
MPI	ECHAM5, T63, L31	MPI-OM, 1.5 °, L40, no flux adjustment	JSBACH	No	HAMOCC5	Raddatz et al. (2005, unpublished manuscript)
LLNL	CCM3, 2.8° × 2.8°, L18	POP 0.6 ° × 0.6 °, L40	IBIS, flux adjustment	Yes	OCMIP	Thompson et al. (2004)
FRCGC	CCSR/NIES/FRCGC T42(2.8° × 2.8°), L20	COCO No flux adjustment, (0.5°–1.4°) × 1.4°, L20	Sim-CYCLE	No	NPZD	
UMD	QTCM 5.6° × 3.7°	Slab mixed layer, 5.6° × 3.7°	VEGAS	Yes	Three-box model	Zeng et al. (2004)
UVic-2.7	EMBM 1.8° × 3.6°	Mom 2.2, 1.8° × 3.6°, L19, no flux adjustment	MOSES/TRIFFID	Yes	OCMIP Abiotic	Meissner et al. (2003) Matthews et al. (2005a)
CLIMBER2-LPJ	2.5-D, 10° × 51° statistical-dynamical	Zonally averaged, 2.5°lat, 3 basins	LPJ	Yes	NPZD	Brovkin et al. (2004) Sitch et al. (2005)
BERN-CC	EBM 2.5° × 3.75°	HILDA box-diffusion model	LPJ	Yes	Perturbation approach	Joos et al. (2001) Gerber et al. (2003)

“The plural of 'anecdote' is not ‘evidence’.”
Alan Leshner, publisher of <u>Science</u>

“...what can be asserted without evidence can also be dismissed without evidence.”

by Chirstopher Hitchens

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Excerpt from the editorial policy of JFE

"Journal of Fluids Engineering disseminates technical information in fluid mechanics of interest to researchers and designers in mechanical engineering. *The majority of papers present original analytical, numerical or experimental results and physical interpretation of lasting scientific value*. Other papers are devoted to the review of recent contributions to a topic, or the description of the methodology and/or the physical significance of an area that has recently matured."

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Excerpt from the editorial policy of JFE (i.e. the fine print)

“Although no standard method for evaluating numerical uncertainty is currently accepted by the CFD community, there are numerous methods and techniques available to the user to accomplish this task. The following is a list of guidelines, enumerating the criteria to be considered for archival publication of computational results in the *Journal of Fluids Engineering*.”

Then 10 different means of achieving this end are discussed, and a seven page article on the topic.

Excerpt from the editorial policy of JFE (digging even deeper, more fine print!)

"An uncertainty analysis of experimental measurements is necessary for the results to be used to their fullest value. Authors submitting papers for publication to this Journal are expected to describe the uncertainties in their experimental measurements and in the results calculated from those measurements and unsteadiness."

- *The numerical treatment of uncertainty follows directly from the need to assess the experimental uncertainty.*
- This gives a sense of the difference in communities.

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Excerpt from the editorial policy of JFE

"*The Journal of Fluids Engineering* ***will not*** *consider any paper reporting the numerical solution of a fluids engineering problem* ***that fails to address the task of systematic truncation error testing and accuracy estimation.*** *Authors should address the following criteria for assessing numerical uncertainty.* "

The differences in approach are substantial.

Other journals in each field have similar statements.

Example from JFE

Assessment of Large-Eddy Simulation of Internal Separated Flow

Marco Hahn[1]
e-mail: m.hahn@cranfield.ac.uk

Dimitris Drikakis

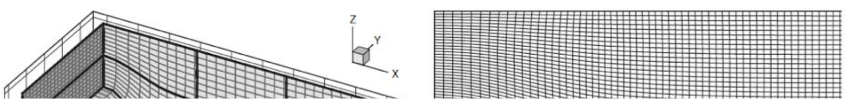
Department of Aerospace Sciences,
Fluid Mechanics and Computational Science Group,
Cranfield University,
Bedfordshire MK43 0AL, UK

This paper presents a systematic numerical investigation of different implicit large-eddy simulations (LESs) for massively separated flows. Three numerical schemes, a third-order accurate monotonic upwind scheme for scalar conservation laws (MUSCL) scheme, a fifth-order accurate MUSCL scheme, and a ninth-order accurate weighted essentially non-oscillatory (WENO) method, are tested in the context of separation from a gently curved surface. The case considered here is a simple wall-bounded flow that consists of a channel with a hill-type curvature on the lower wall. The separation and reattachment locations, velocity, and Reynolds stress profiles are presented and compared against solutions from classical LES simulations.
[DOI: 10.1115/1.3130243]

Journal of Fluids Engineering **Copyright © 2009 by ASME** JULY 2009, Vol. 131 / **07120**

The numerical investigation of high-resolution methods for large-eddy simulation has been carried out using three different computational grids. The computational domain representing the constricted channel extents $9h$ and $4.5h$, and between $2h$ and $3.035h$ in x-, y-, and z-direction, also referred to as streamwise, cross-stream, and vertical directions, respectively. Here, h is the height of the hill-type shape at the lower wall. A H-H-type topology was chosen (Fig. 1(*a*)) and no-slip boundary conditions are applied at the top and bottom walls of the channel, while periodicity was assumed in the streamwise and cross-stream directions.

Three different grid resolutions have been investigated here: (i) a highly under-resolved grid, referred to as "coarse," comprising approximately 0.65×10^6 relative uniformly distributed points; (ii) a modified version of the coarse grid with an identical number of points, referred to as "modified," featuring a finer clustering near the top and bottom walls of the channel; and (iii) a moderately finer grid consisting of 1.03×10^6 points, referred to as "medium," where the refinement mainly affects the distribution around the hill crest and a slightly better resolution near the bottom wall is achieved; see Figs. 1(*b*)–1(*d*). The coarse and medium grids are basically identical to the ones used in previous wall-modeled LES [9]. The characteristic parameters for all three grids, including z^+



Wow! What a difference. Three grids and some degree of quantification. Much more than other papers, but still not enough.

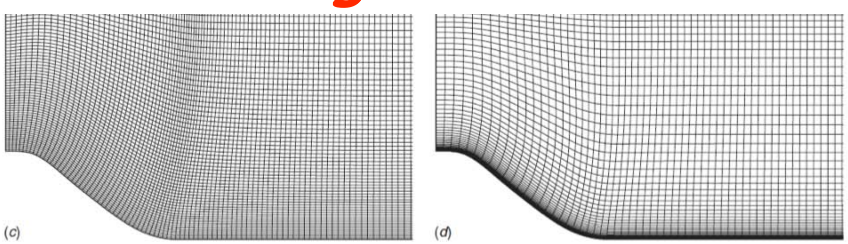
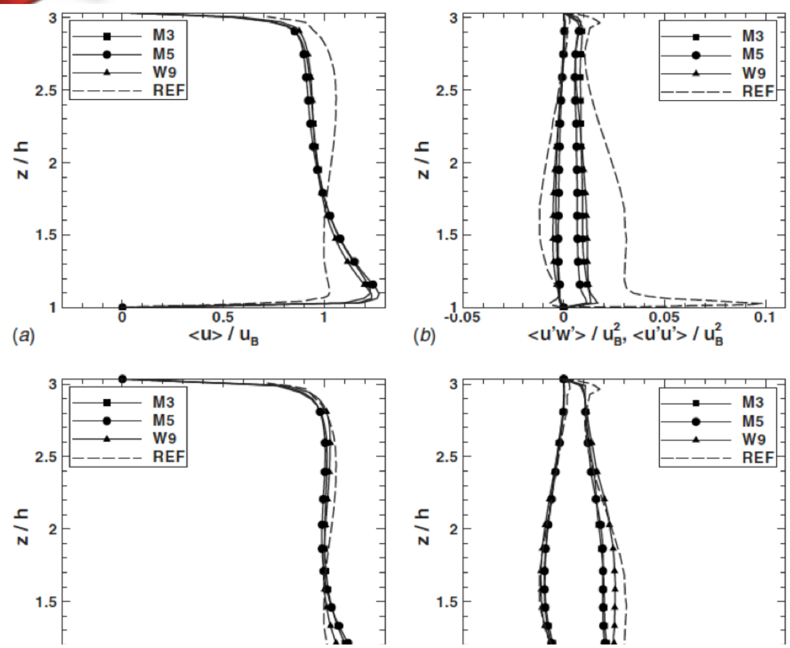


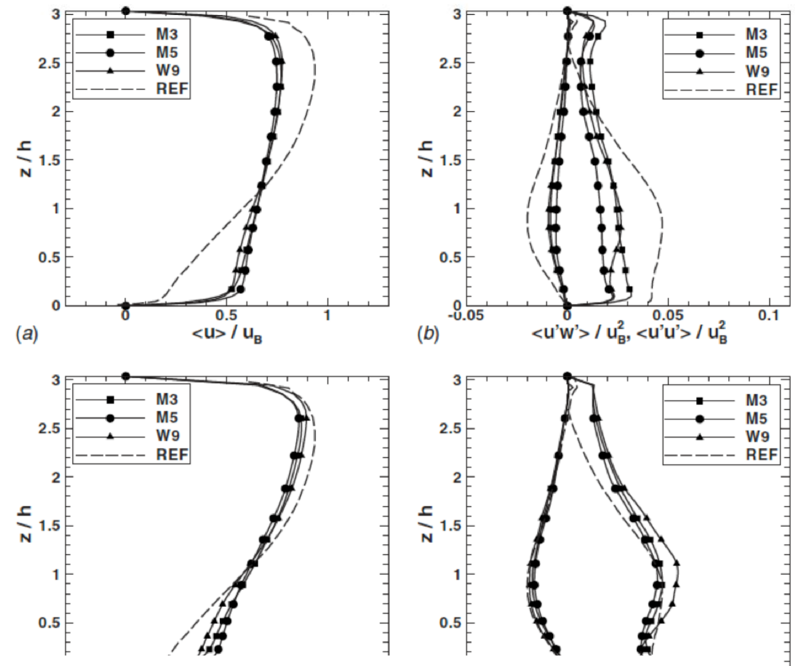
Fig. 1 The computational H-H-type grid topology and the three different grids employed in the simulations of the hill flow

Table 1 Characteristic parameters for the three grids employed here and for the highly resolved reference LES

Grid	$N_x\times N_y\times N_z$	Size	$\Delta x/h$	$\Delta y/h$	$\Delta z/h$	z^+_{min}	z^+_{max}
Coarse	$112\times91\times64$	0.65×10^6	0.08	0.049	0.032	≈7	≈14
Modified	$112\times91\times64$	0.65×10^6	0.08	0.049	0.0047	≈1	≈3
Medium	$176\times91\times64$	1.03×10^6	0.04	0.049	0.02	≈4	≈9
Reference	$196\times186\times128$	4.67×10^6	0.032	0.024	0.0033	≈0.5	≈1

Example from JFE





No experimental data, and the reference solution has no quantification of its quality.

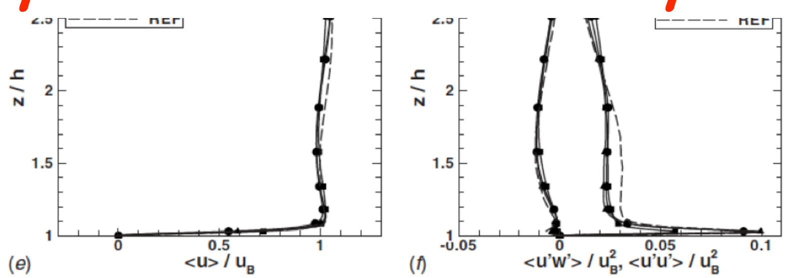


Fig. 3 Comparison of the averaged streamwise velocity and Reynolds stresses near the hill crest at $x/h=0.05$ as obtained by different high-resolution methods on the coarse, medium and modified grids with the reference LES

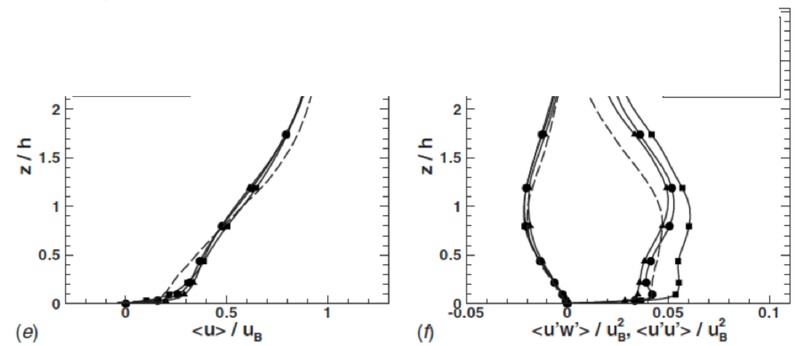


Fig. 5 Comparison of the averaged streamwise velocity and Reynolds stresses after reattachment at $x/h=6$ as obtained by different high-resolution methods on the coarse, medium and modified grids with the reference LES

Example from J. Appl. Mech.

Jeong-Hoon Song[1]
Postdoctoral Fellow
e-mail: j-song2@northwestern.edu

Ted Belytschko
Walter P. Murphy Professor
McCormick Professor

Theoretical and Applied Mechanics,
Northwestern University,
Evanston, IL 60208-3111

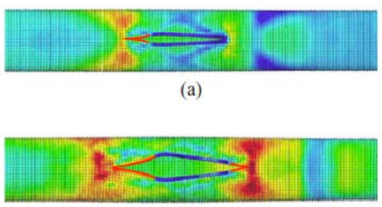
Dynamic Fracture of Shells Subjected to Impulsive Loads

A finite element method for the simulation of dynamic cracks in thin shells and its applications to quasibrittle fracture problem are presented. Discontinuities in the translational and angular velocity fields are introduced to model cracks by the extended finite element method. The proposed method is implemented for the Belytschko–Lin–Tsay shell element, which has high computational efficiency because of its use of a one-point integration scheme. Comparisons with elastoplastic crack propagation experiments involving quasibrittle fracture show that the method is able to reproduce experimental fracture patterns quite well. [DOI: 10.1115/1.3129711]

Journal of Applied Mechanics **Copyright © 2009 by ASME** SEPTEMBER 2009, Vol. 76 / **051301-1**

For the numerical simulation, we discretized the right segment of the cylinder length of the 91.40 cm with 54,382 four-node quadrilateral shell elements ($h_e \simeq 0.90$ mm); see Figs. 8(*b*) and 8(*c*). The shell material is aluminum 6061-T6 and we modeled it with J_2-plasticity, density $\rho = 2780.0$ kg/m^3, Young's modulus $E = 69.0$ GPa, Poisson's ratio $\nu = 0.30$, and yield stress $\sigma_y = 275.0$ MPa. We used linear hardening with constant slope $h_p = 640.0$ MPa. The cohesive fracture energy $G_f = 19.0$ kJ/m^2 is treated in terms of a cohesive law (the assigned fracture energy is based on Refs. [26–28]).

In order to induce unsymmetrical crack propagation with an axisymmetric shell structure and loading, we introduced a small scatter in the yield strength of bulk material. The yield strength at every material point is perturbed by factors ranging from −5.0% to 5.0%: The perturbation factor is obtained from a log-normal



(a)

(a)

(a)

No editorial statement on numerical simulation accuarary. The example is chosen from a number of experiments presumably because the end products looked so much alike. Really nothing else is done to quantify the errors.

F
p
=
n

Computations were made for two of the Chao and Shepherd [16] experiments of explosively loaded pipes. The finite element model was simply loaded by the pressure time history of the detonation traveling wave; fluid-structure interaction effects were not considered. Nevertheless, the computations reproduce many of the salient features of each experiment and differences in crack paths between two experiments.

"A computer lets you make more mistakes faster than any invention in human history — with the possible exceptions of handguns and tequila."

Mitch Ratliffe, Technology Review, April, 1992

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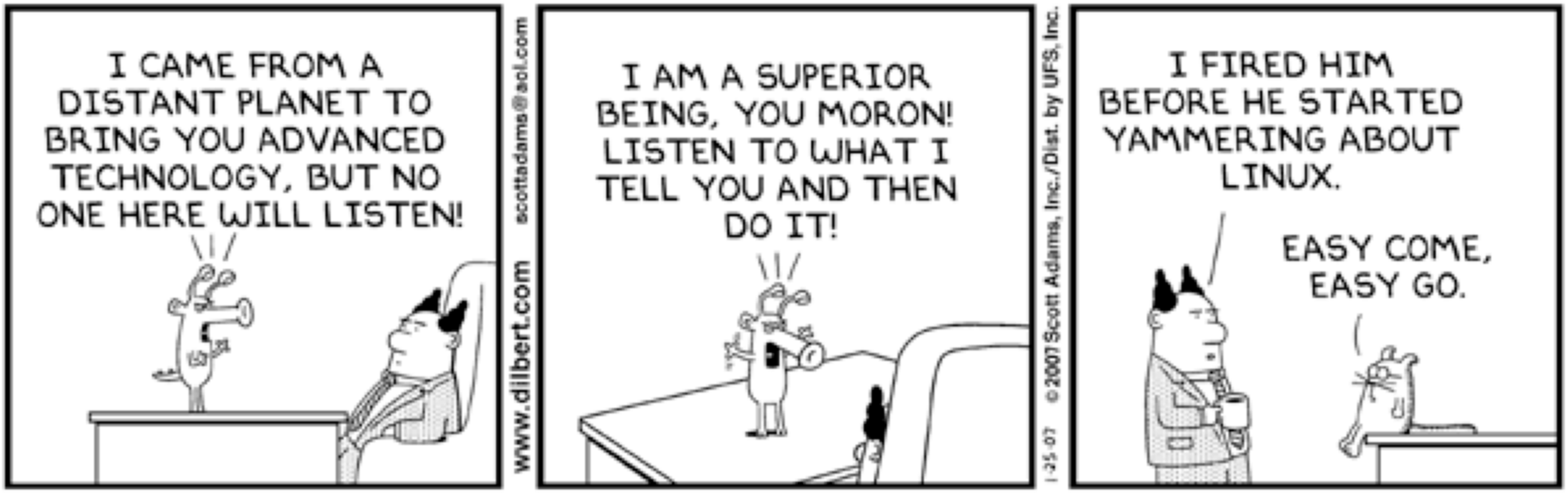
"Dilbert isn't a comic strip, it's a documentary" – Paul Dubois



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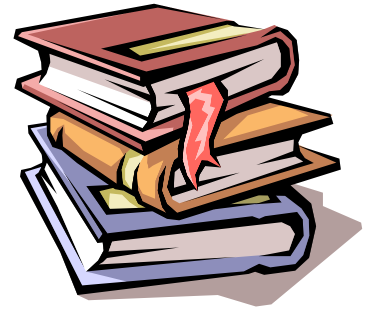
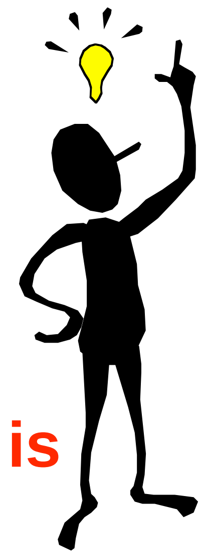
A new proposed definition for Verification



Verification is the process of determining that a model is implemented correctly and estimating its numerical errors.



- **The benefit of this definition is subtle**
  - **The correctness of a model's implementation is central**
  - **The fact that even a correct model has numerical error is defined and that these errors should be estimated.**

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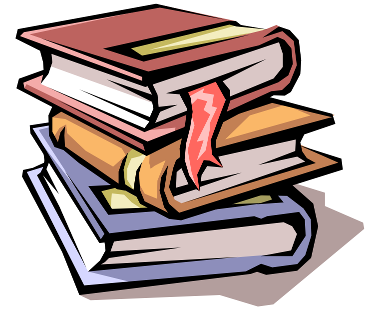
A new proposed definition for Validation



Validation is the process of assessing the quality of modeling a physical process and the magnitude of error associated with the simulation (inc. numerical error, verification).

- **The benefit of this definition is subtle**
  - **The appropriateness of a model for a physical circumstance is central.**
  - **The fact that even an appropriate model has errors (uncertainty) is defined.**
  - **This process must include model verification as a key part of the complete validation.**