3rd INTERNATIONAL WORKSHOP
ON
VALIDATION OF COMPUTATIONAL MECHANICS MODELS

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The quest for truth, particularly in mechanics

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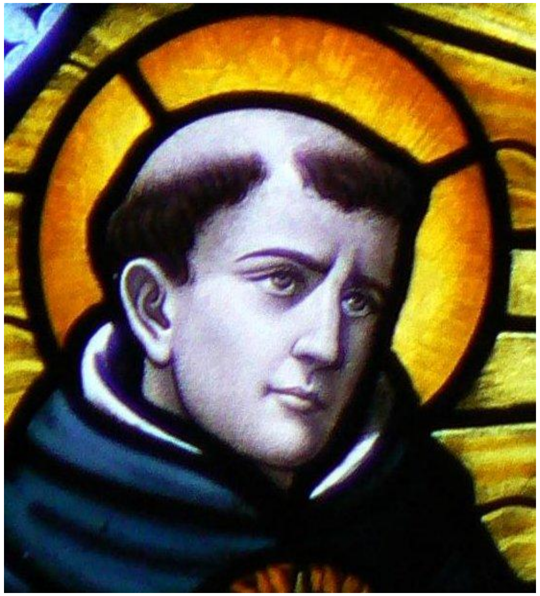
Scope of the lecture

- Agreement of reality with perception
- Theories, principles, laws and models
- Validity limits
- Terminology
- Theory vs. experiment
- Modeling the world
- The role of singularity in mathematics, physics, engineering
- Singularities in engineering models
- A few pieces of wisdom

In allotted time I will not have time to discuss all the promised items in detail.
For those who are interested I offer the full text that was published in
Estonian Journal of Engineering, December 2013, 19, 4, pp. 253 – 272.
or is available in pdf format from the author
Eng-2013-4-253-272_the_quest_as_printed.pdf

What is a 'true' approach to modeling of nature? What is truth?



Thomas Aquinas (1225 – 1274) claimed that the

the truth is an agreement of reality with perception.

Today, however, the perceived reality depends on observation tools being used.

Immanuel Kant (1724 – 1804) asked for **a clear distinction between the 'true reality' and 'perceived reality'.** Kant argues that in principle it is impossible to observe and study the world without disturbing it. His ideas are very close to Heissenberg principle of uncertainty.

When we, engineers, are modeling phenomena of Mother Nature the question of truth becomes rather irrelevant since the models we are designing, checking and using, either work or do not work to our satisfaction.

In this respect the mechanical theories, principles, laws and models, used in engineering practice, cannot be proclaimed true of false.

They are either right or wrong.

Wrong theories might appear, but not being confirmed by experiment, are quickly discarded as ether or flogiston.

Right theories are right only within the limits of their applicability.

- 1D wave equation is not able to predict stress wave pattern in a 3D body, and still is not wrong,
- Bernoulli-Navier slender beam theory 'fails' for thick beams,
- Newton's second law 'fails' for motion of bodies approaching the speed of light, and still is not wrong,
- Einstein's theory of relativity 'fails' when applied to quantum microcosmos.
- **So it is obvious that we as mechanicists rather strive for robust models with precisely specified limits of validity and not for philosophically defined categories of truth and falsehood.**

Our goals
Ability to explain and predict

- Our tools
  - Theory, principle, law , model
  - Computation
  - Experiment

Model is a purposefully simplified concept of a studied phenomenon invented with the intention to predict – what would happen if … Accepted assumptions (simplifications) specify the validity limits of the model and in this respect the model is neither true nor false. Model, regardless of being simple or complicated, is good, if it is approved by an appropriate experiment. See [Flüge, 1960].

Let‘s discuss the role of singularity in

- mathematics,
- physics,
- engineering,
- the real world.

Mathematical singularity

is a standard part of mathematics.

$$\lim_{x \to 0} \frac{1}{x} \to \infty$$

This kind of singularity could only happen in our minds, but could be grasped rather easily.

Somebody could say that this could happen on paper as well, but physically we are not able to plot the function 1/*x*, in the vicinity of *x* approaching zero.

$$f(x) = \frac{1}{x}$$

Infinity Hotel

a story attributed to David Hilbert (1862 – 1943)

- The Infinity Hotel has infinitely many rooms.
- Imagine that at a certain evening all the rooms, numbered 1, 2, 3, etc., are occupied.
- There comes a new guest to the reception asking: Do you have a room for tonight?
- No problems, says the receptionist and starts a simple procedure.
- **i = 1**
- **Until <all the guest are displaced> do**

  Move the guest from room (i) to room (i+1)

  i = i + 1
- **End of do**
- When the loop is finished, the newly arrived guest will get the room No. 1.

- Actually, any countable number of guests can be accommodated this way.
- That is the infinite number of buses, each carrying infinite number of guests.

- Logically there is no logical flaw in the story.
- Practically it is un-realizable, since its fulfillment would require the infinite time and furthermore, the infinite amount of energy would be required.

The story shows a strange character of infinity – it is not just a big number

Physical singularity
or rather
Singularity appearing in mathematical models describing physical phenomena

- is closely connected to mathematical modeling of nature.
- Examples
  - Infinite displacement, strain and stress under the point force in solid continuum mechanics,
  - infinitely fast shock wave change of pressure accompanying sonic boom in fluid mechanics,
  - Infinite stress at the crack tip in fracture mechanics,
  - within the Big Bang theory, at $t = 0$ any physical quantity as volume, pressure, temperature, energy become infinitely high.

- Generally, a singularity appearing in a model always means a serious warning concerning the range of validity of that model.
- Usually, a more general model – having a wider scope of validity – is invented removing that singularity.
- Very often there is no need to discard the older and simple model, since it might be perfectly useful in the validity range for which was conceived.

Strong views on singularity

- A singularity brings about so much arbitrariness into the theory that it actually nullify its laws …

  from A. Einstein and N. Rosen: Physical Reviews, 48, 73, 1935

- … a theory that involves singularities carries within itself the seed of its own destruction.

  from P. Bergmann in H. Woolf: Some strangeness in the Proposition, Addison Wesley, 1980.

Engineering views on singularity are not so strong

- Appearance of singularities in equations describing the behaviour of mechanical quantities in mathematical models of nature signals that the particular model in question is incomplete.
- Appearance of singularity in a model merely signals that the theory being employed has reached the limits of its validity and must be superseded by new and improved version which should replace the computed singularity by a finite measurable quantity.

Singularity in continuum

Seemingly unproblematic model of elastic continuum has embedded singularities in it. For example a point force, a frequently used tool in engineering analysis, is a forbidden entity in continuum mechanics since it leads to a singularity response – this is manifested by the fact that the displacement under the application of a point force tends towards infinity.

To a certain extent this property is retained when the continuum is treated by means of a FE model. Actually, it is smeared out by the existence of shape functions but with diminishing meshsize it is manifested by the increase of displacement under the application of a point (nodal) force.

The FE mesh made of ‘null-sized’ elements would provide the infinite displacement under the application of a nodal force as the continuum model. So making a finer and finer mesh we are representing better and better those continuum properties that are mathematically correct but physically unattainable.

This is a sort of paradigm we are used to live with. Singularity in displacement response to a point loading, Rayleigh waves and crack analysis are well-known examples both in continuum and its FE representation.

Singularities in engineering models

- Infinite speed of propagation by Newmark
- Finite element threshold
- Experiment and FEA – what is closer to reality

A modeling paradox

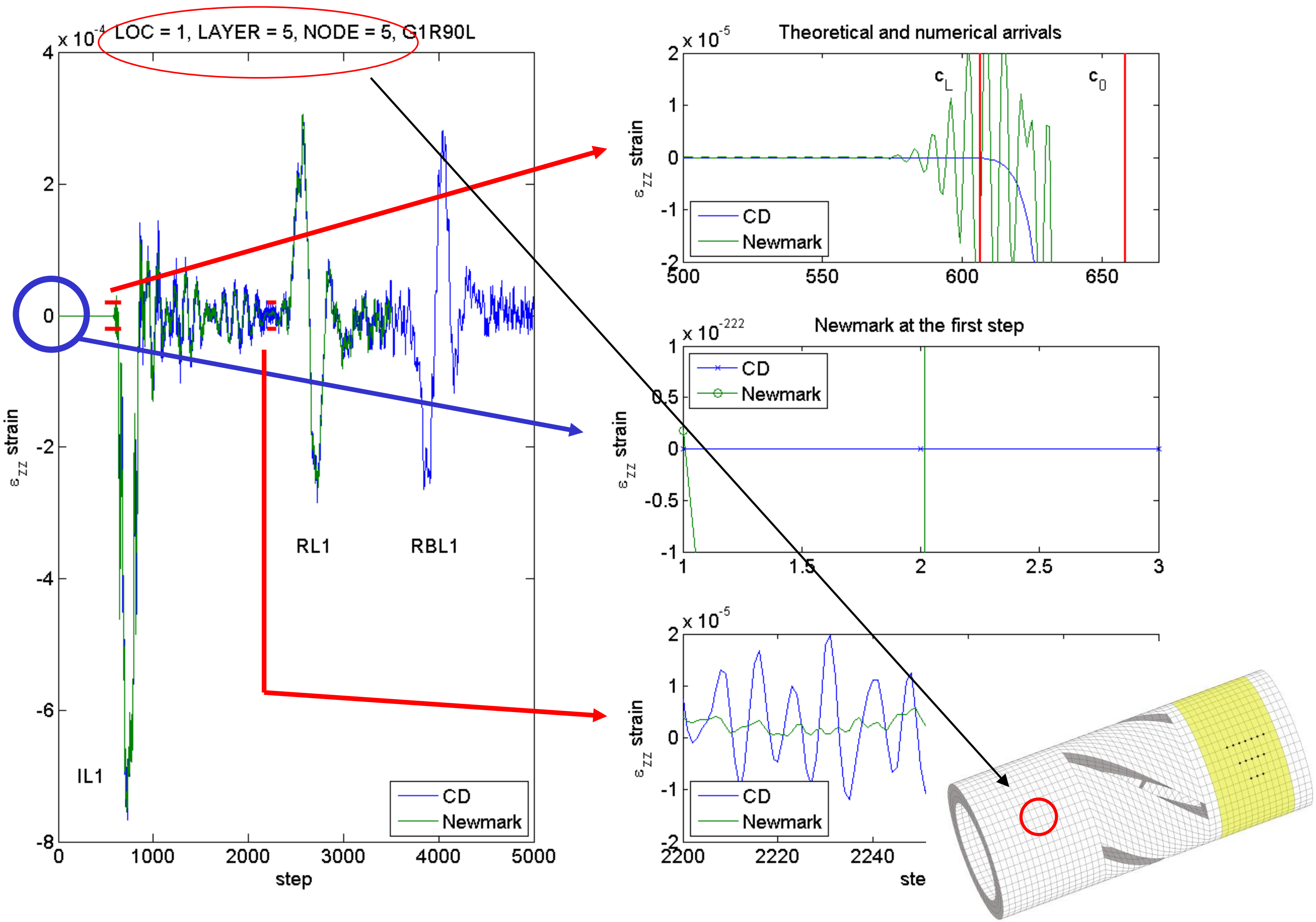
„Infinite“ speed of propagation
in FE analysis
using NM time integration operator

Self-assessment
when the comparison with experiment is not available

The reliability and precision of two time integrating methods, the Newmark (NM) and central difference methods (CD) are to be assessed for a particular case. Comparison of axial strains at a certain location, obtained by both methods, is presented.
The same time integration step (1e-7 [s]) was used in both cases. For the NM method the consistent mass matrix was employed, while the diagonal mass matrix was used for the CD method.
The left-hand subplot presents the strains in the whole computed time range showing the excellent agreement of results due to both approaches. The agreement documents that the accepted space and time discretizations are suitable for this geometry and loading – the differences are minimized. Two couples of horizontal lines indicate the areas that are shown in detail the in right-hand side subplots.
In the upper right-hand subplot the positions of theoretical arrivals of 3D longitudinal () and 1D () waves are indicated by red vertical lines. The actual axial strain distributions computed by the NM and CD methods are shown as well. It is known that the computed speed of wave propagation for the CD approach with diagonal mass matrix underestimates the actual speed, while the NM approach with consistent mass matrix overestimate the actual speed. The presented results nicely show this.
What is less known is the fact, that the speed of propagating waves with NM-consistent modeling is actually ‘infinitely’ large. A brief explanation is sketched out in the following box.

Validity self-assessments for NM vs. CD, the results are method dependent.

Is this particular 'agreement' acceptable?



Computational infinite speed of wave propagation can be explained by analyzing the time marching algorithms for $\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{P}(t)$

Explicit (central differences)

Equilibrium is considered

at time t

and leads to repeated solutions of

$$\frac{1}{\Delta t^2}\mathbf{M}\mathbf{q}_{t+\Delta t} = \tilde{\mathbf{P}}_t$$

Implicit (Newmark)

$t + \Delta t$

$$\hat{\mathbf{K}}\mathbf{q}_{t+\Delta t} = \hat{\mathbf{P}}_{t+\Delta t}$$

Just after the first time step the most distant node knows that the system was loaded.

generally $\mathbf{K}, \mathbf{M}$ … banded; $\mathbf{K}^{-1}, \mathbf{M}^{-1}$ … full; $\mathbf{M}^{-1}$ is diagonal, only if $\mathbf{M}$ is diagonal

$\hat{\mathbf{K}}$ can never be diagonal … computational speed of propagation is not bounded

$$\tilde{\mathbf{P}}_t = \mathbf{P}_t - \left(\mathbf{K} - \frac{2}{\Delta t^2}\mathbf{M}\right)\mathbf{q}_t - \frac{2}{\Delta t^2}\mathbf{M}\mathbf{q}_{t-\Delta t}$$

$$\hat{\mathbf{K}} = \mathbf{K} + \frac{1}{\beta\,\Delta t^2}\mathbf{M}$$

$$\hat{\mathbf{P}}_{t+\Delta t} = \mathbf{P}_{t+\Delta t} + \mathbf{M}\left(c_1\mathbf{q}_t + c_2\dot{\mathbf{q}}_t + c_3\ddot{\mathbf{q}}_t\right)$$

Finite element threshold

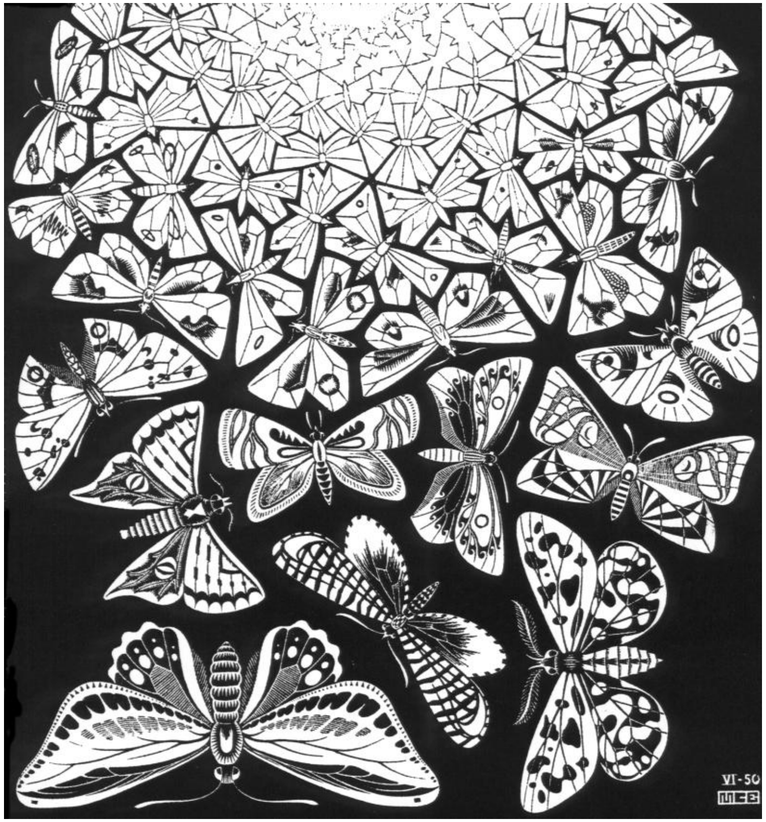
Frequency limits of continuum and of FEA

For fast transient problems as shock and impact the high frequency components of solutions are of utmost importance. In continuum, there is no upper limit of the frequency range of the response. In this respect continuum is able to deal with infinitely high frequencies. This is a sort of singularity deeply embedded in the continuum model.

As soon as we apply any of discrete methods for the approximate treatment of transient tasks in continuum mechanics, the value of upper cut-off frequency is to be known in order to 'safely' describe the frequencies of interest.

The number and range eigenmodes are limited. FE behaves as an upper-pass band filter..

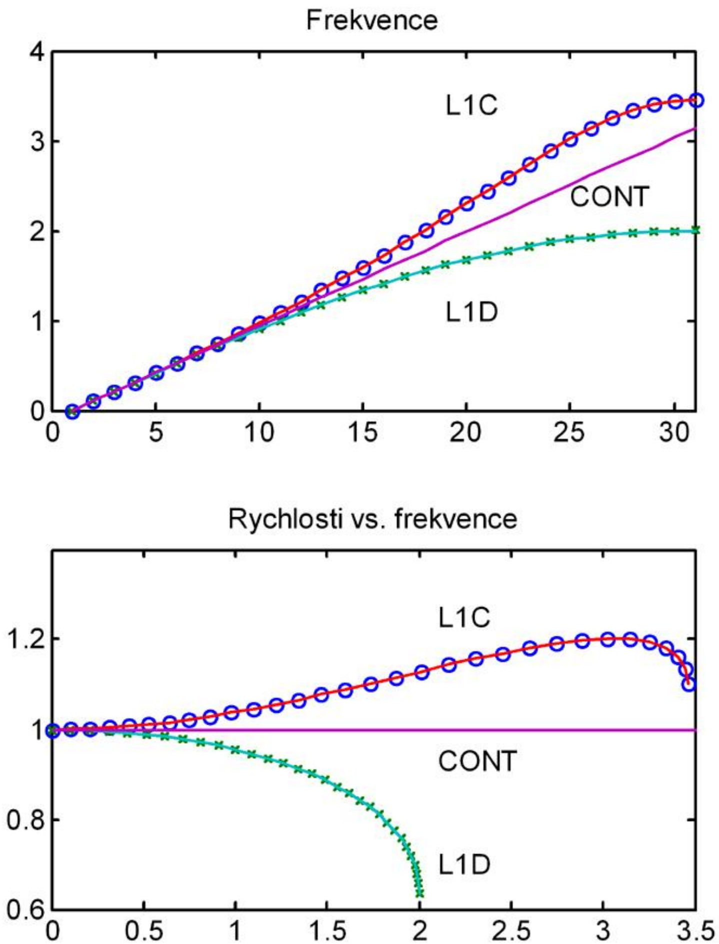
Analyzing frequency properties of discrete systems leads to the study of dispersion.

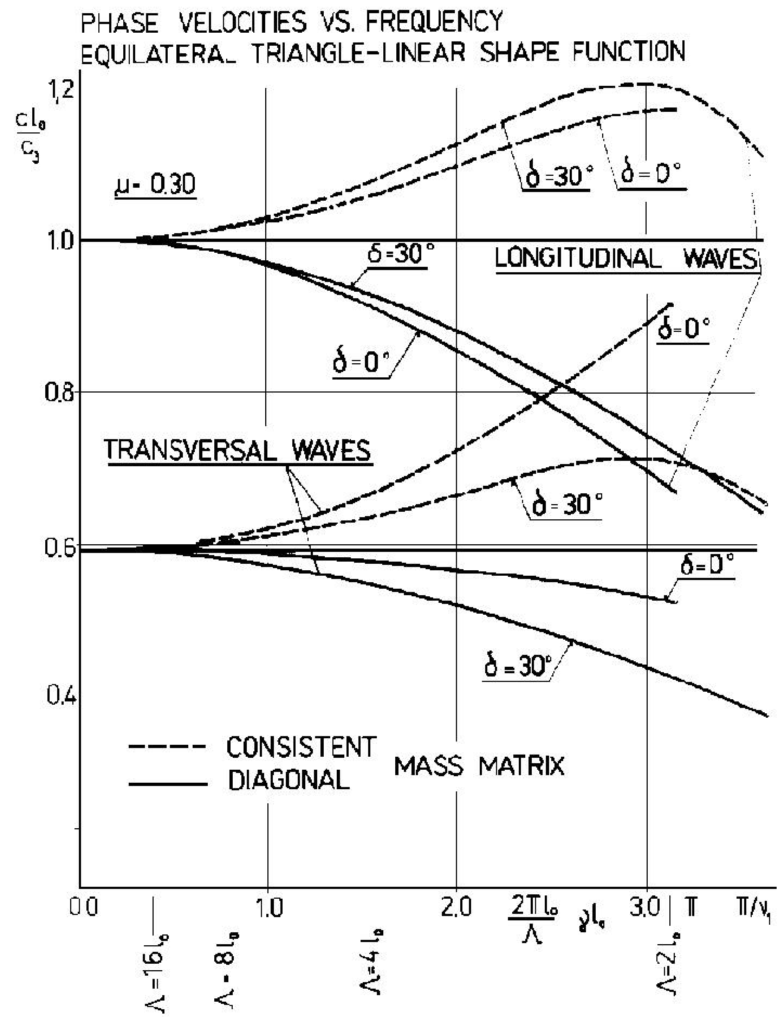


C.M. Esher
discretization

Finite dimensions of elements, instead of infinitesimal one in continuum, lead to dispersive properties of FE model

Example for 1D and 2D constant strain elements





overestimated / consistent

Frequency (velocity) is ... **with** ... **mass matrix.**

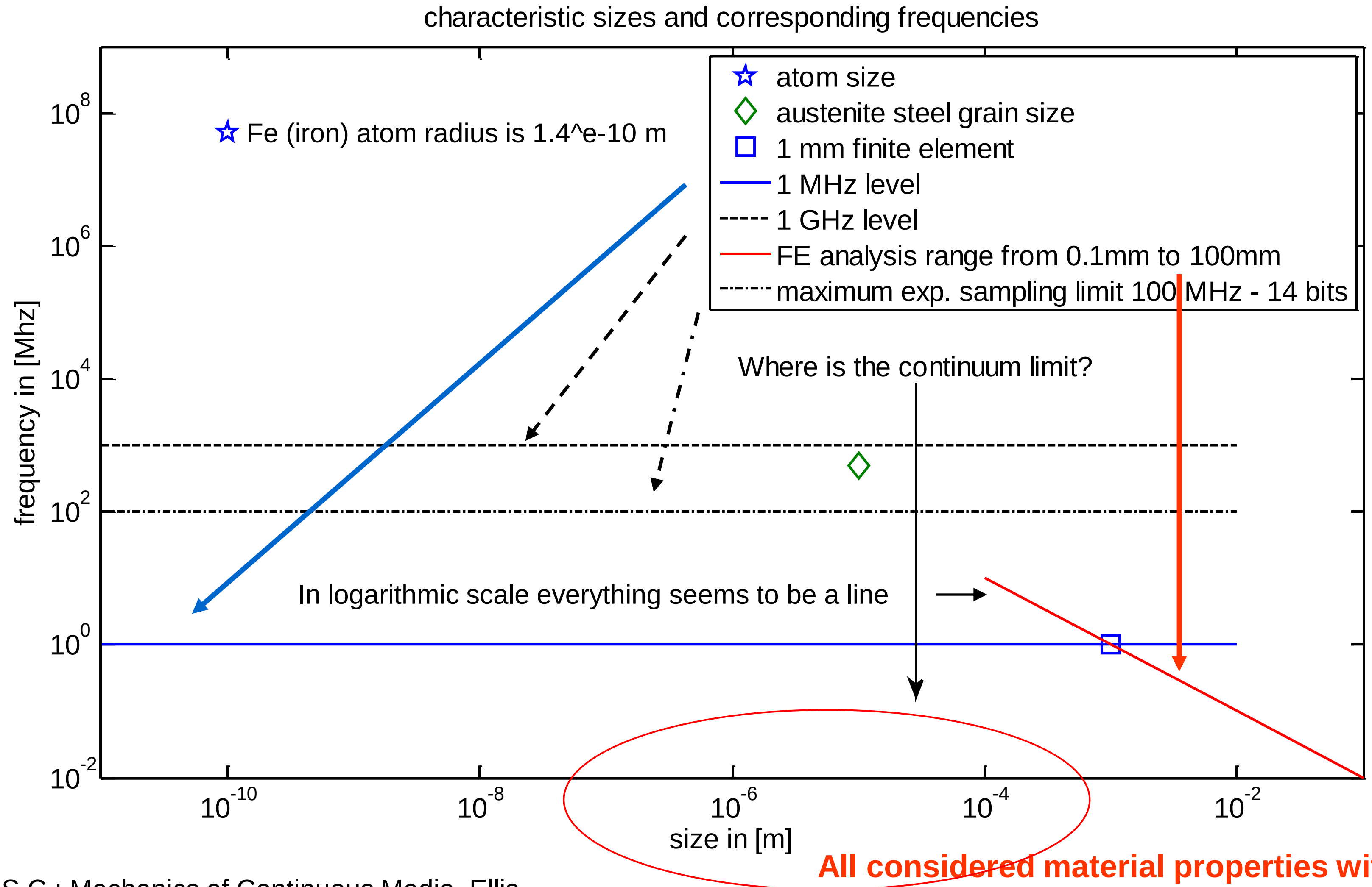
underestimated / diagonal

When looking for the upper frequency limit of a discrete approach to continuum problems, we could proceed as follows

s	• Characteristic element size
λ	• Wavelength to be registered
$\lambda = 5s$	• How many elements into the wavelength? Let's take 5
$\lambda = cT$	• Wavelength to period relation
$c = 5000$ m/s	• Wave speed in steel
$f = 1/T$	• Frequency to period relation
$f = c/(5s)$	• The five-element limit frequency

For 1 mm element we have $f = \dfrac{5000}{5\times 0.001} = 1\times 10^{6}\ \text{Hz} = 1\ \text{MHz}$

Limits of continuum, FE analysis and experiment



Hunter, S.C.: Mechanics of Continuous Media, Ellis Hornwood, Chichester, 1983

To neglect corpuscular structure of matter the specimen should be at least 10^4 times larger that the inter-atomic distance

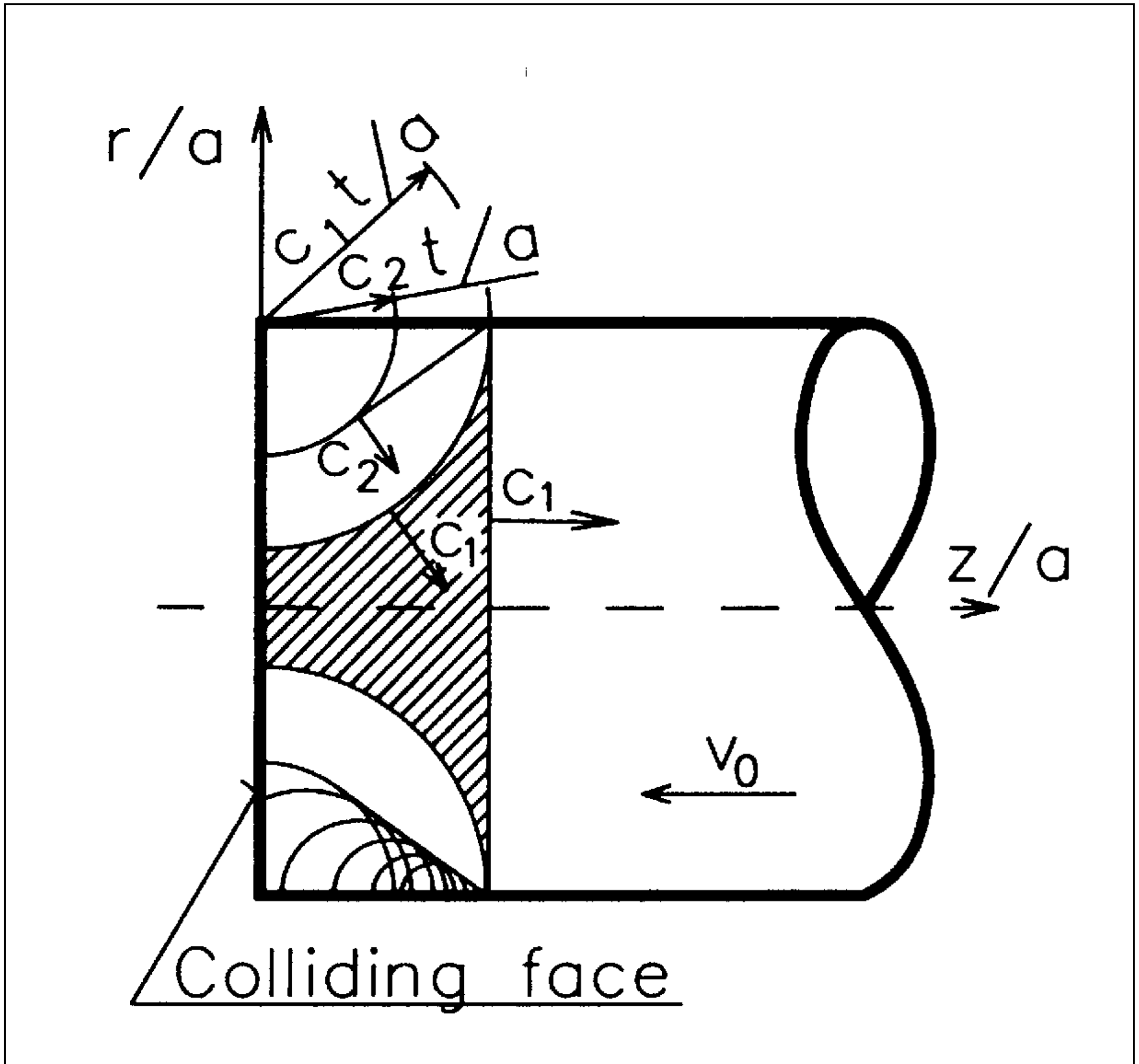
All considered material properties within the observed infinitesimal element are identical with those of a specimen of finite size

Remember that one of the definition of continuum is based on the fact that its properties are independent of the element size under consideration

Testing the robustness of impact algorithm.
Impact of two identical cylinders
Theory is always a good benchmark

Imagine what happens after two identical cylindrical bars of finite lenhgth collided.

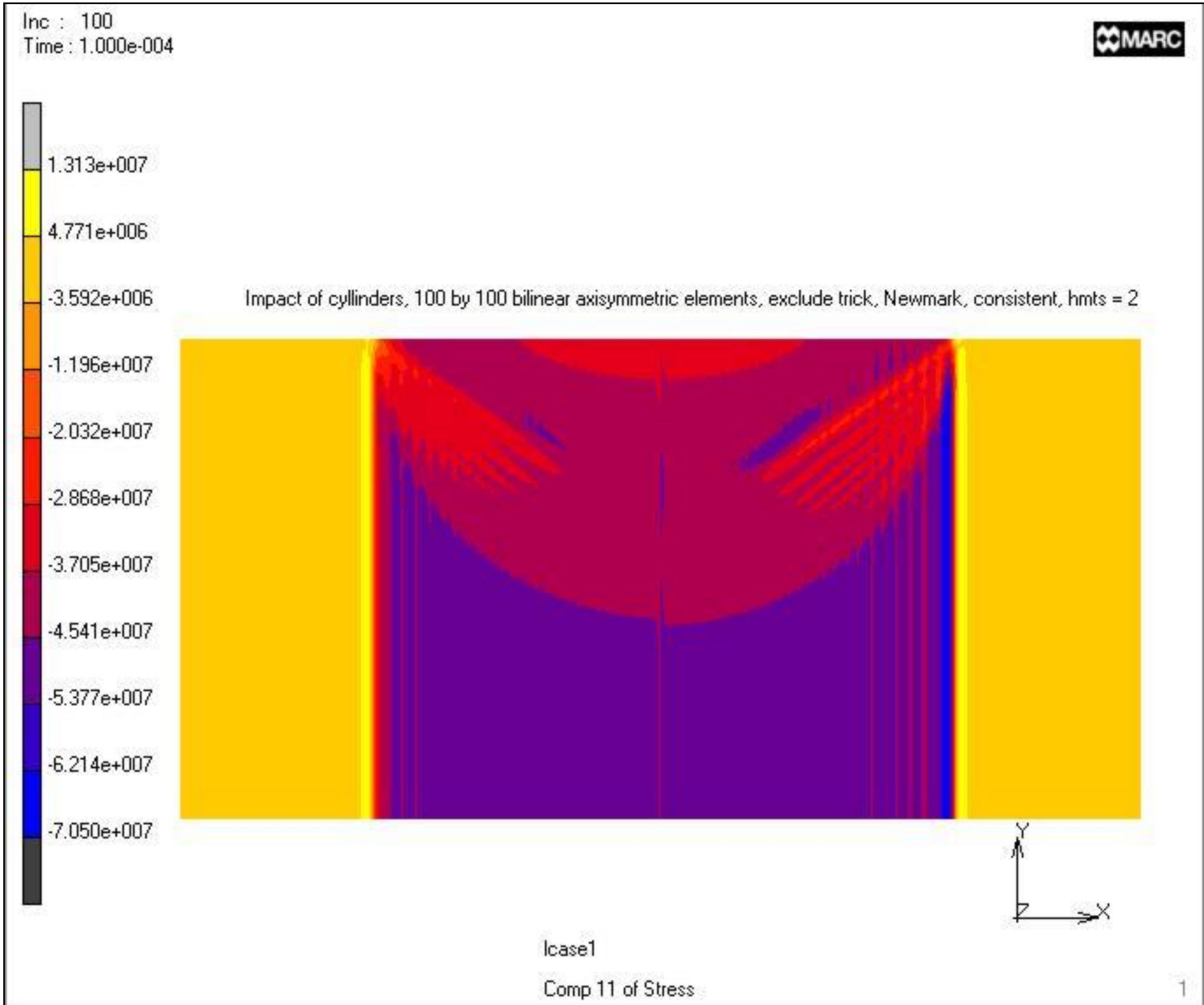
Theoretical positions of L and S wavefronts, propagating with c1 and c2 speeds, are indicated.



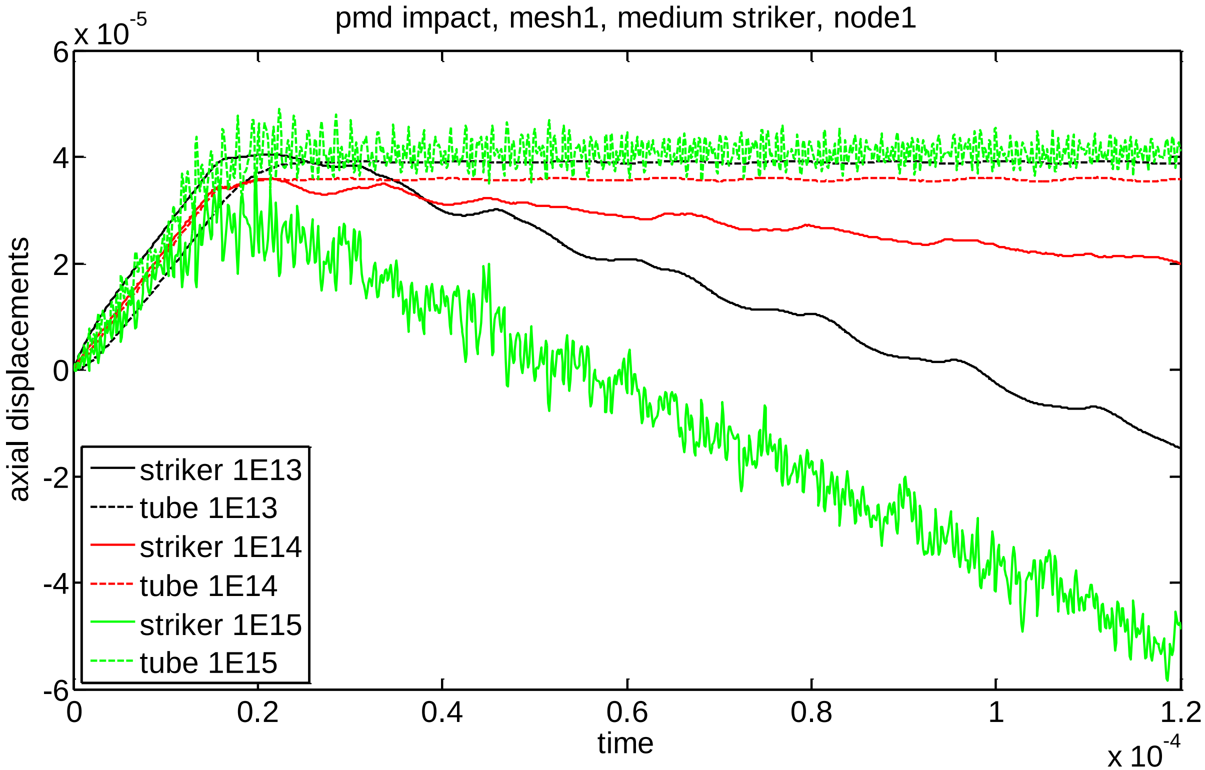
Impact of cylinders – FE analysis

Axial symmetry was employed.

Wavefronts are where they should be.



How to find a correct penalty value?
Striker (solid) and tube (dashed) were just separated



After the separation both bodies should move away with same velocities of opposite sign.

A nice test of method robustness

Striker velocity (i.e. the slope of ax. displacements vs, time) depends on the penalty value

It is evidently wrong – but is it acceptable? Furthermore, penalty consumes energy.

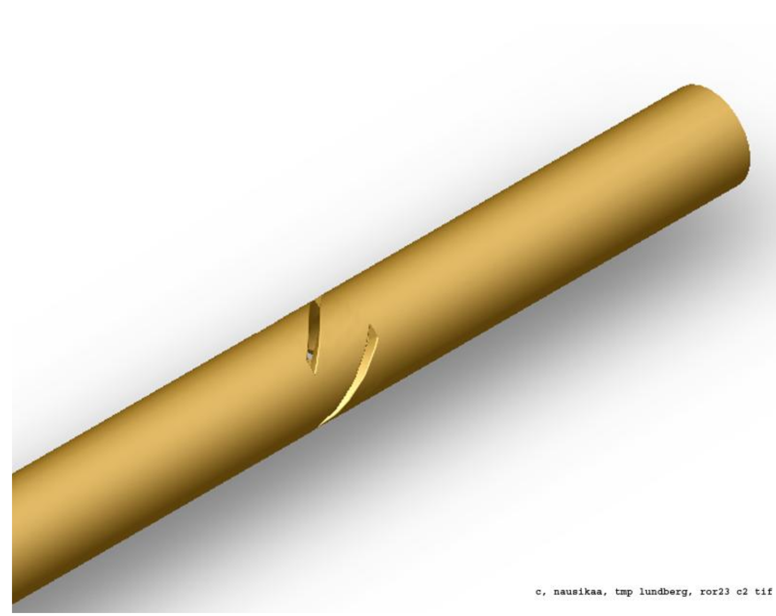
And now, from intellectual clouds to engineering reality

Impact induced stress wave energy flux

Validation of numerical and experimental approaches

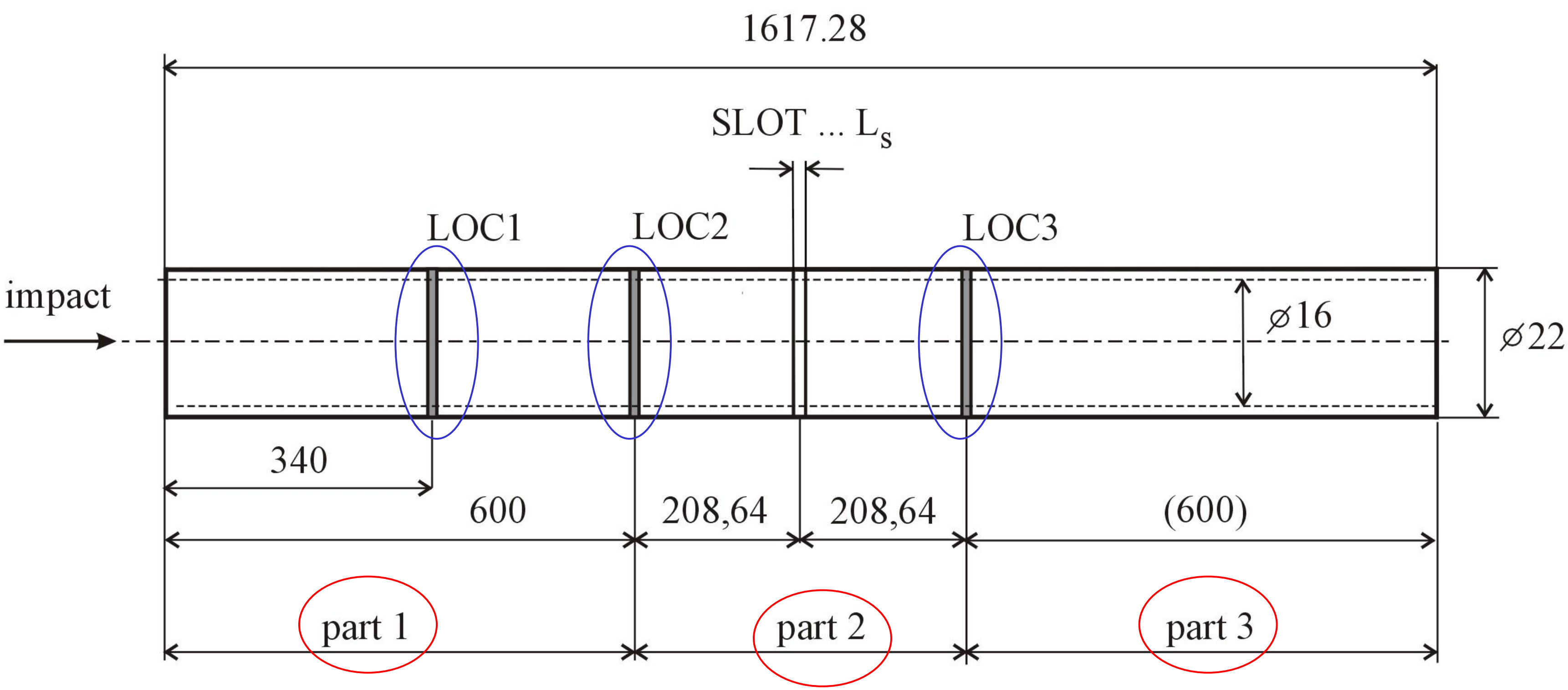
Initially motivated by a question of how much of axial input energy could be transferred into the torsional energy – people from rock drilling industry were interested.

Stress wave energy flux through the spiral slot of a tube induced by axial impact



Tube with a spiral slot – its dimensions in [mm]

and three surface locations of interest



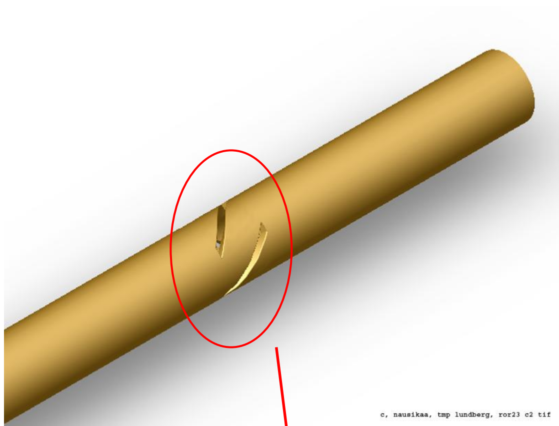
Notice that three body parts are considered for FE analysis

NOT TO SCALE

Two types of spiral slots, i.e **L90** and **2L180**, were considered

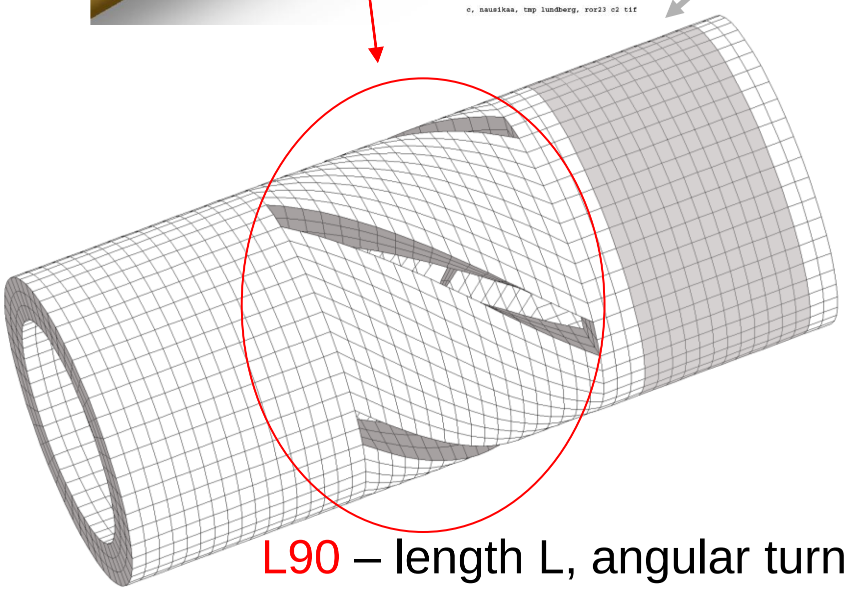
The coarse mesh and dimensions of a typical **surface 'location'** are depicted

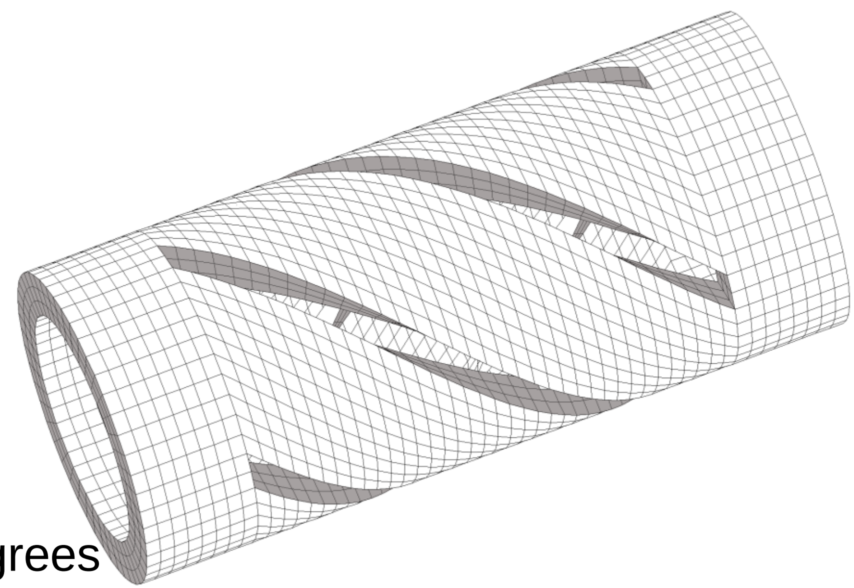
Only a middle part of the mesh assembly is depicted



Later, we will talk about quantities distributed at the unfold surface (gray shaded area)

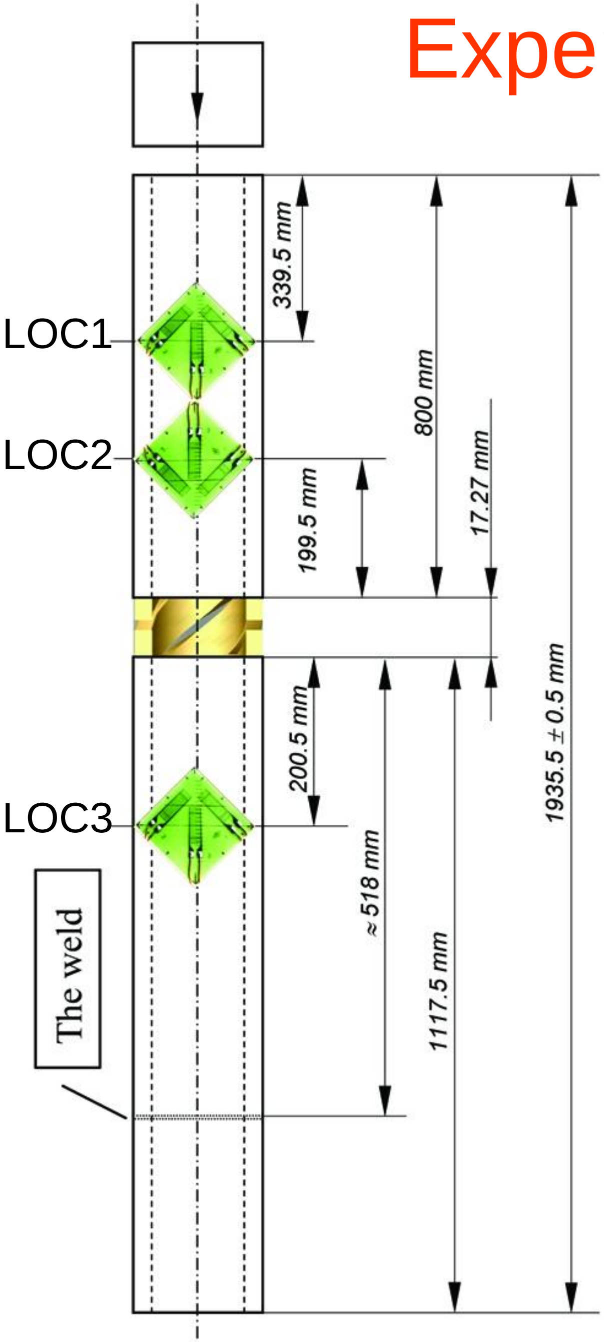
2L180 – length 2L, angular turn 180 degrees





L90 – length L, angular turn 90 degrees

Experimental considerations



There are three axial strain signals associated with the longitudinal energy constituents

IL	incident longitudinal,
RL	reflected longitudinal,
TL	transmitted longitudinal,

and two shear signals associated with torsional reflected and transmitted energy constituents.

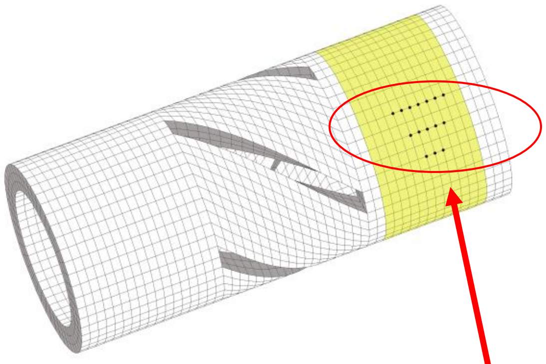
RT	reflected torsional,
TT	transmitted torsional.

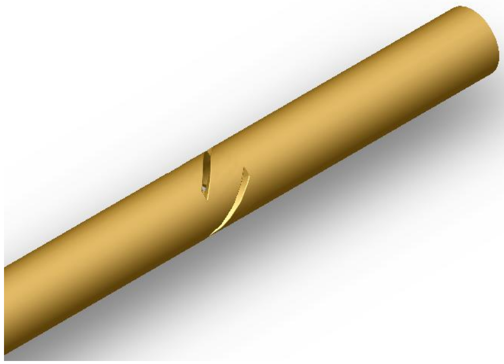
Experimental energy evaluation is based on 1D theory

$$T_{\mathrm{L}} = \frac{1}{Z}\int_{t_1}^{t_2} N^2 \,\mathrm{d}t = AEc_0 \int_{t_1}^{t_2} \varepsilon_{\mathrm{L}}^2 \,\mathrm{d}t$$

$$T_{\mathrm{T}} = \frac{1}{Z_{\mathrm{T}}}\int_{t_1}^{t_2} M^2 \,\mathrm{d}t = 4Gkc_{\mathrm{T}} / b^2 \int_{t_1}^{t_2} \varepsilon_{\mathrm{T}}^2 \,\mathrm{d}t$$

Experiment relies on surface strains only – they are considered to be uniformly distributed across the whole cross sectional surface





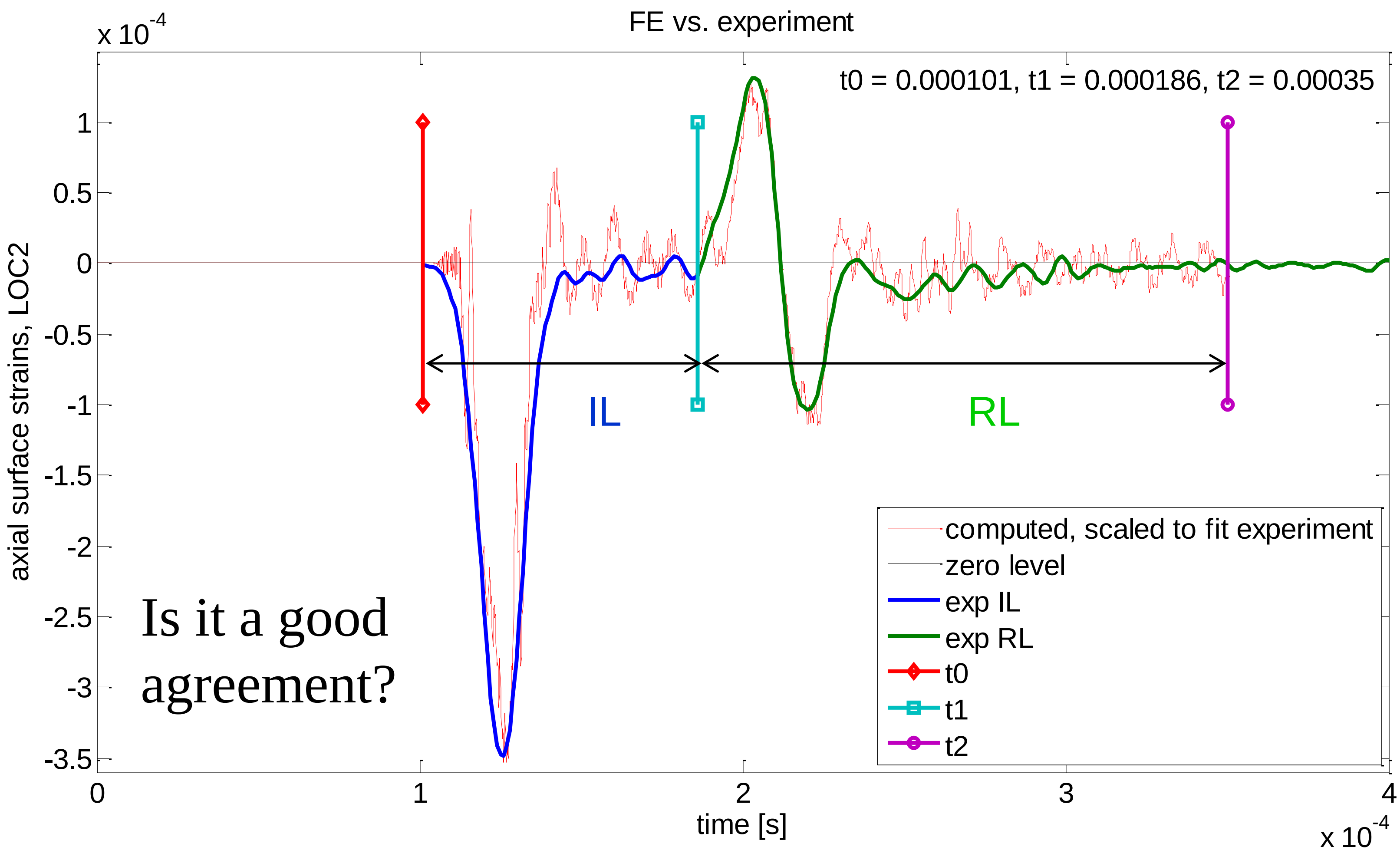
Thinking about good and bad agreements of surface strains obtained by means of experiment and FE analysis

L90

Example: Surface axial strains at LOC 2 – FE vs. experiment

One experimental signal has to be attributed to two (IL and RL) strains

Do IL (Incident Longitudinal) and RL (ReflectedLongidudinal) signals overlap or not?



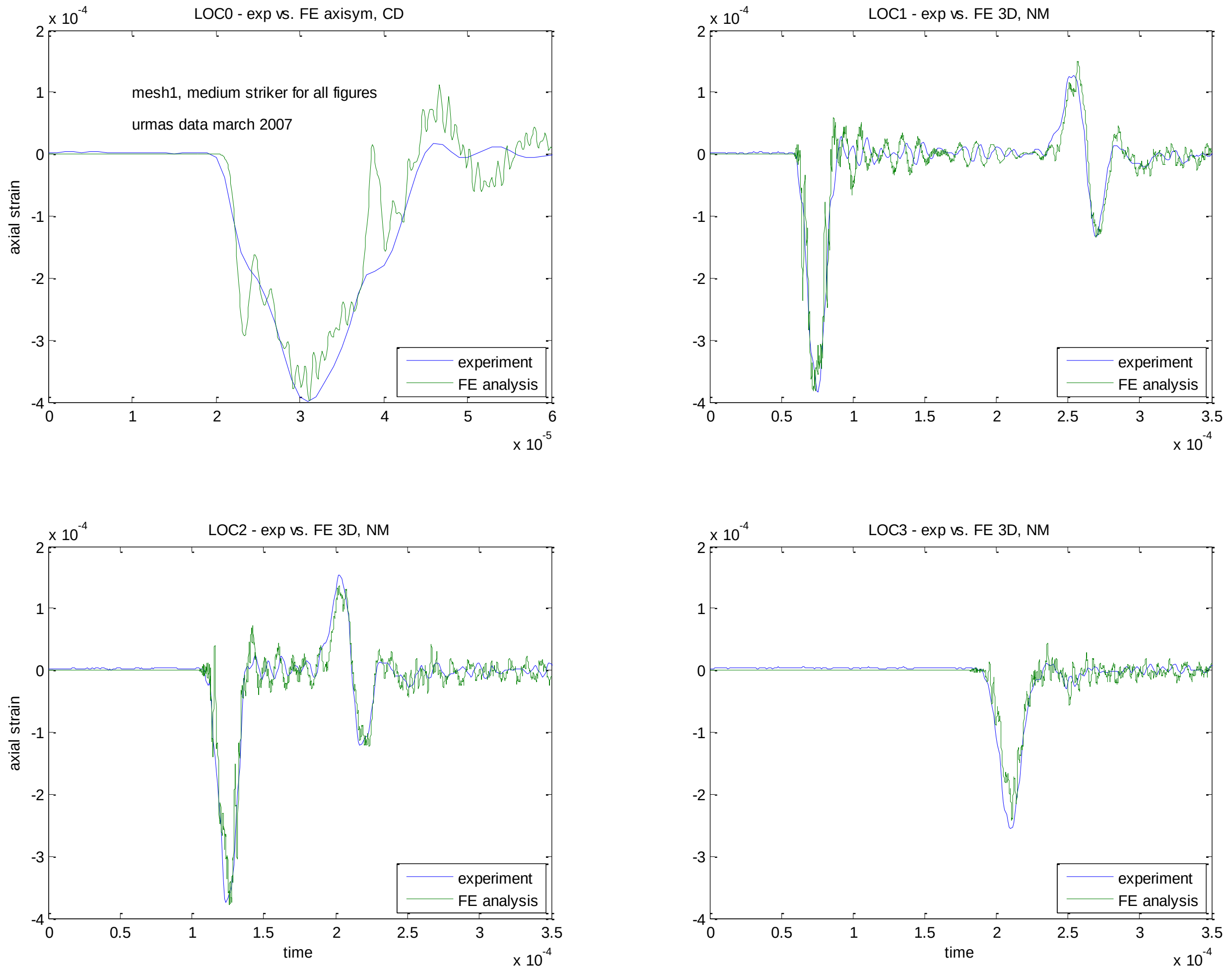
Raw comparison – no tricks

The cut-off frequency of experimental setup had the value of

0.1 MHz

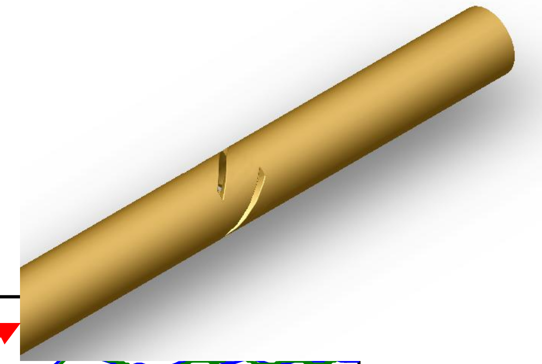
The Nyquist frequency for the FE analysis, based on the integration timestep – which is a sort of sampling interval – is

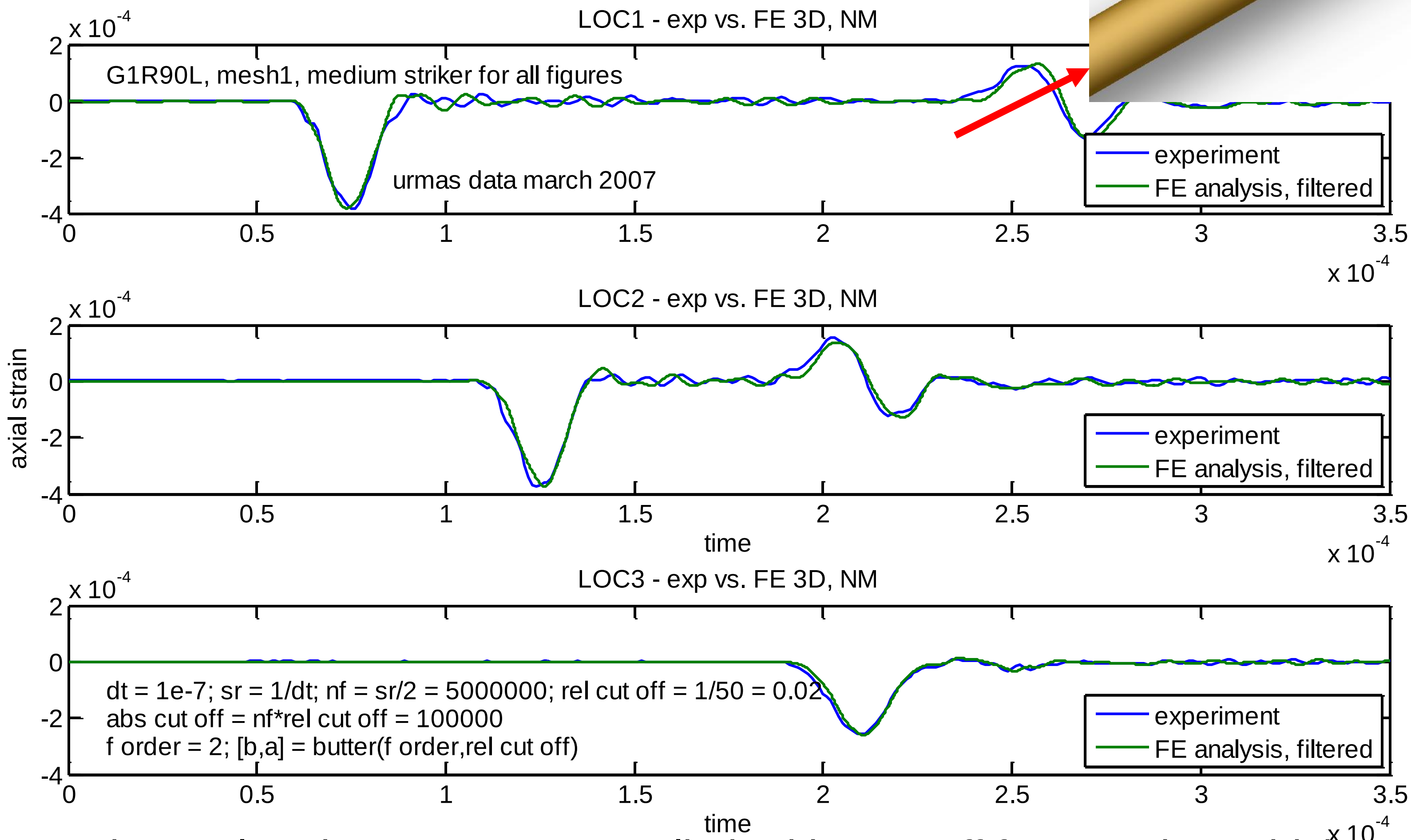
0.5 MHz



Is it a bad or good agreement? Is experiment or FEA closer to reality? Where is the truth? Experimental people often say to FE analysts: All your high frequency components are just a numerical noise.

A ‘better agreement’ of experimental and FE results





Experimental and FE treatment are limited by cut-off frequencies, which are generally different – in this case the filter applied on FE results has the same frequency limit as raw experimental data.

L90

Is it a dirty trick or not?

But can all high-frequency components be attributed to numerical noise?

When experimental and FE results are compared two questions should be considered

First. What are the experimental limits?

- Only axial and shear strains are measured – radial ones are not,
- 1D wave theory is used, so the values of measured surface quantities (displacements, strains, velocities) are attributed to the whole cross-sectional area,
- a smaller frequency sampling rate.

Second. What are the FEA limits?

FFT frequency analysis of signals in FEA is a tools that might indicate what are FEA frequency limits

Let's concentrate on the frequency analysis analysis of the loading pulse and of axial and radial displacements obtained in the outer corner node of location C by means of NM and CD operators for the mesh1. The normalized power spectra are plotted in the range from 0 to Nyquist frequency together with the power spectrum of the loading pulse.

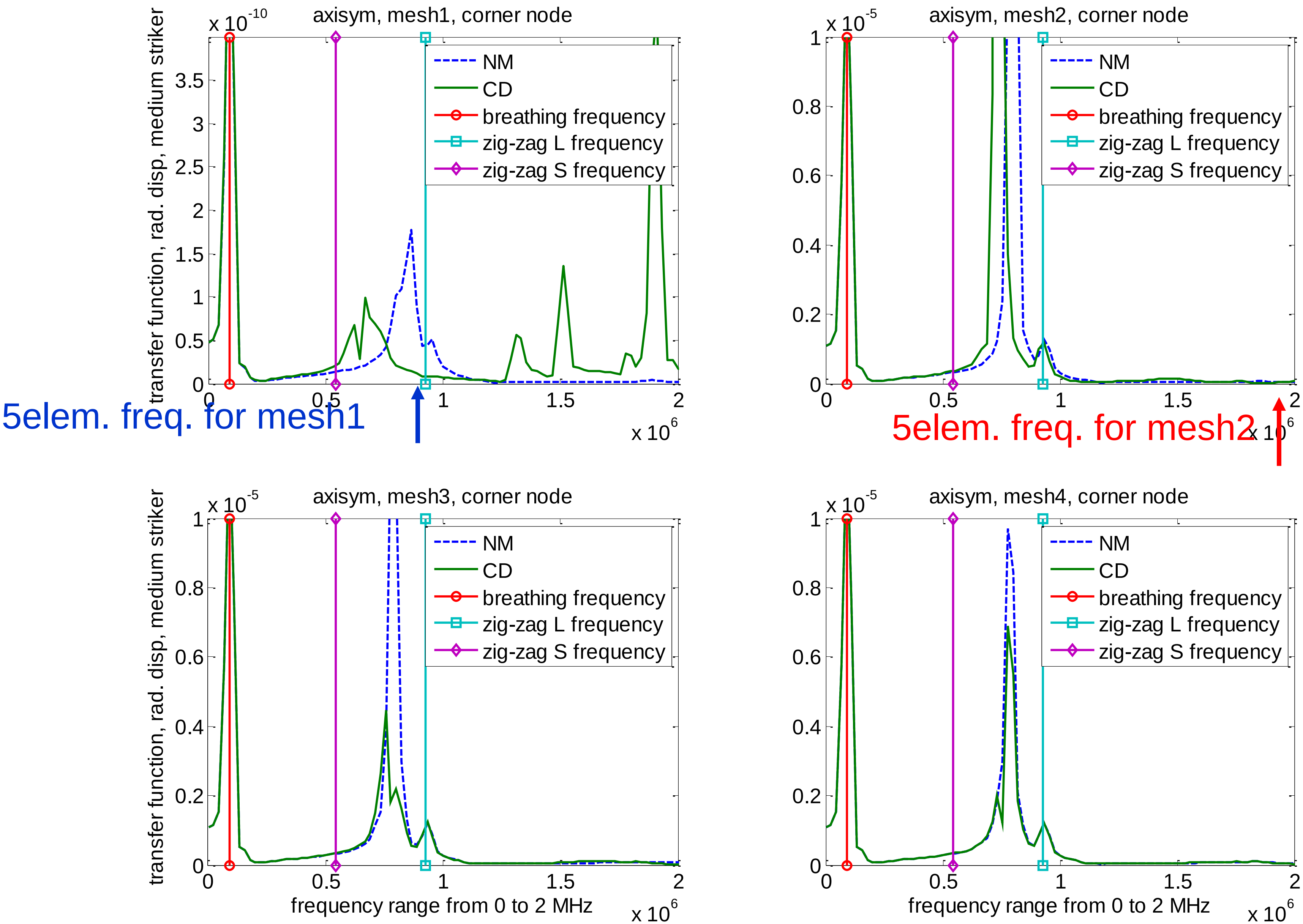
	timestep [s]	**sampling rate** [MHz]	**Nyquist frequency** [MHz]	**meshsize**[mm]
mesh1	1e-7	10	5	1
mesh2	1e-7/2	20	10	1/2
mesh3	1e-7/4	40	20	1/4
mesh4	1e-7/8	80	40	1/8

FE vs. experiment

- The experiment, as conceived in this case, could not ‘catch’ the ‘actual’ frequency components higher than its upper frequency limit.
- In this case the upper frequency limit of FE analysis is substantially higher, so the FE spectrum is longer.
- A question arises what is the range of computed frequencies which are ‘correct’, especially in view of the fact that the FE transfer spectrum is method dependent. Notice the differences for NM and CD treatment.
- Since an experiment with a finer time and frequency resolution is not available, the FE analysis should help itself to answer the question. Self-assessment by mesh- and timestep refinement could help.

Remember the Richardson method, known from quadrature analysis, where the subsequent halving the integration increment is used for the quadrature error estimation.

FEA validity **self-assessments**, **Mesh- and timestep refinement,**
Transfer functions of four meshes are compared –
subsequent mesh is always twice as fine as the previous one

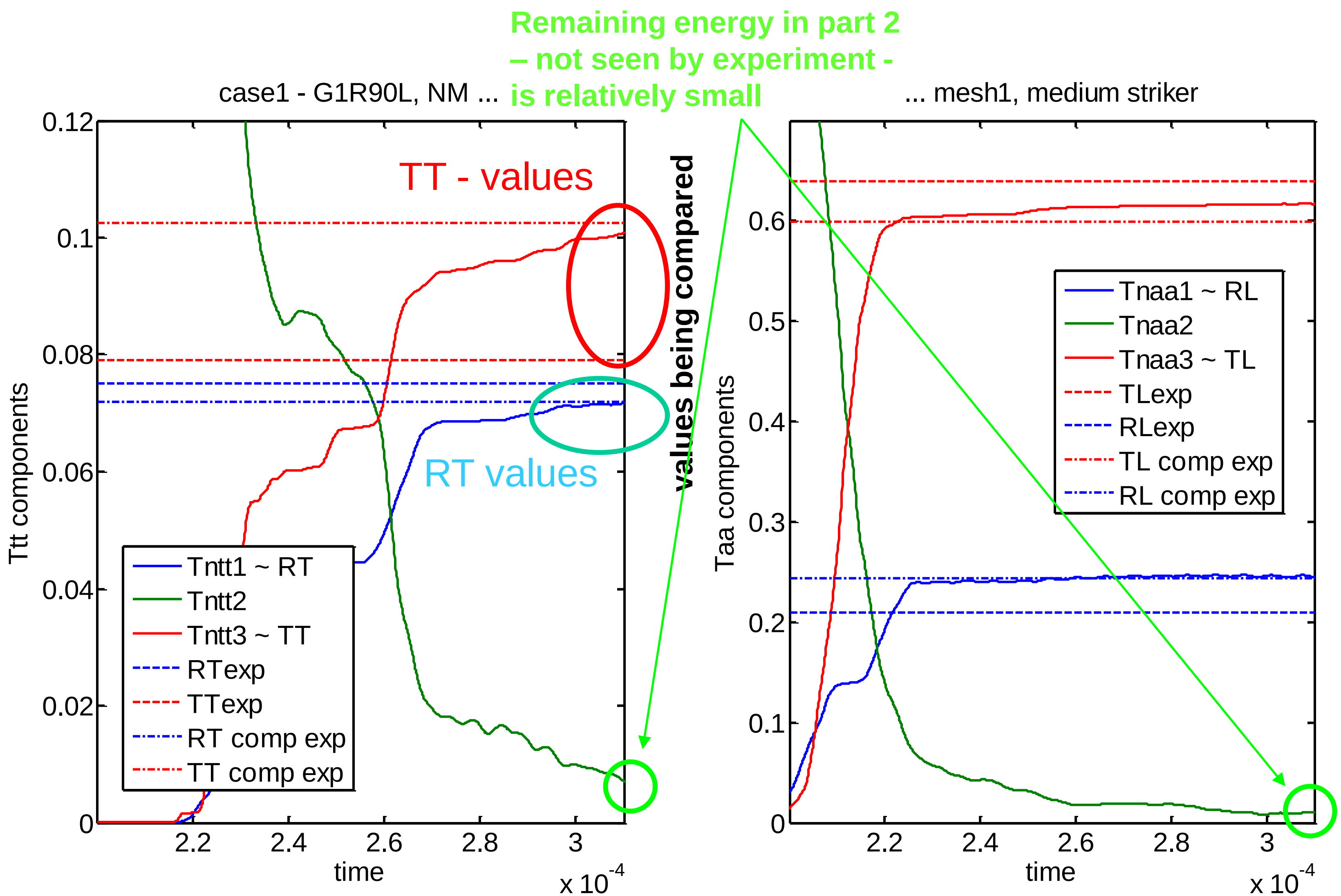


Conclusions to spiral slot treatment by FEA

- As far as the mesh- and timestep-refinement is concerned, one can draw the following conclusions
- A distinct indication of the breathing and zig-zag frequencies,
- the ‘convergence’ of CD and NM responses,
- subsequent disappearance of ‘false’ CD responses,
- ‘false’ CD frequency peaks do not have their counterparts in NM responses.

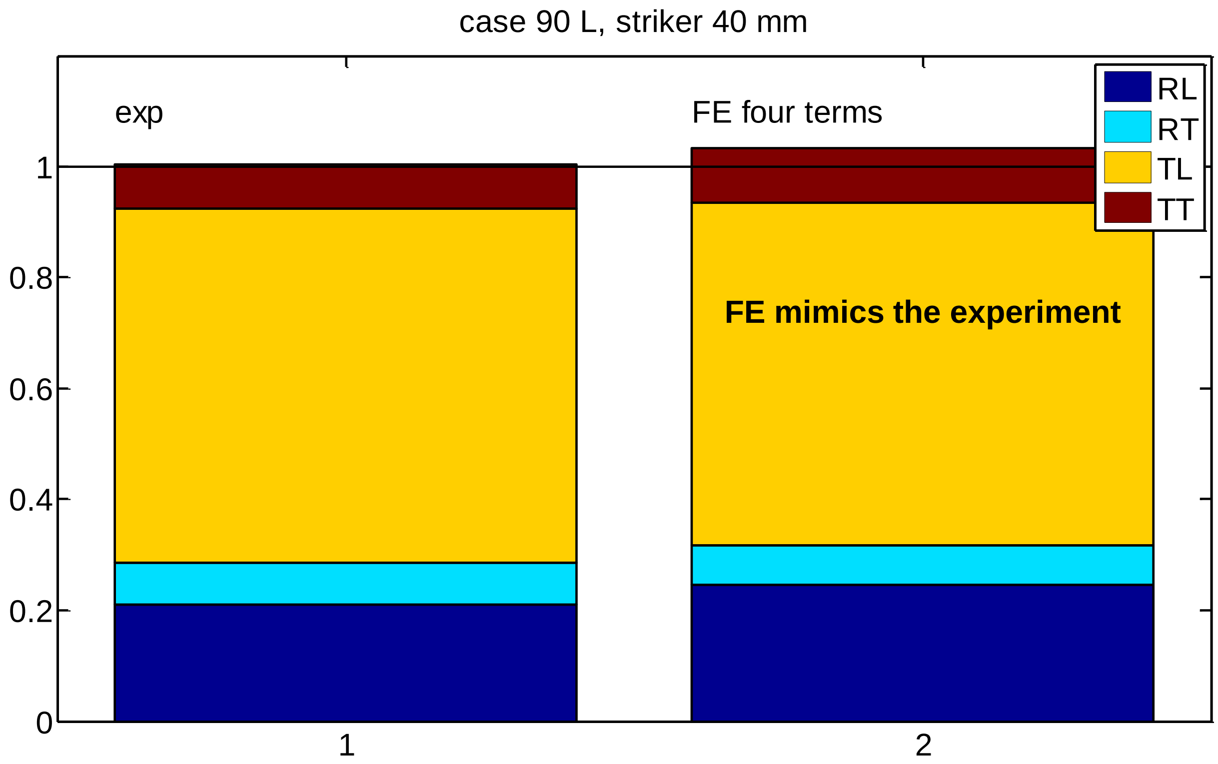
Exp. vs. FE for L90 – three kinds of data are presented and compared

1. experiment based on surface strains … RTexp, TTexp and TLexp, RLexp – **constant values**
2. full 3D finite element treatment … Tntt1 to Tntt3 and Tnaa1 to Tnaa3 – **functions of time**
3. numerical experiment based on computed surface strains … RT_comp_exp, TT_comp_exp and TL_com_exp, RL_comp_exp – **constant values**



Partial energy checksum

Energies from experiment are compared with those computed from four selected surface strains



L90

Experimental energy is not conserved due to the fact that

(i) surface strains are attributed to the whole cross sectional area and

(ii) the remains of energy in other parts of the body are not seen

A few quotations from literature

- Scientists like to show that things held to be impossible are in fact entirely possible.
- Philosophers are more inclined to demonstrate that things widely regarded as perfectly feasible are in fact impossible.

- **The role of doubts is far from negative.**

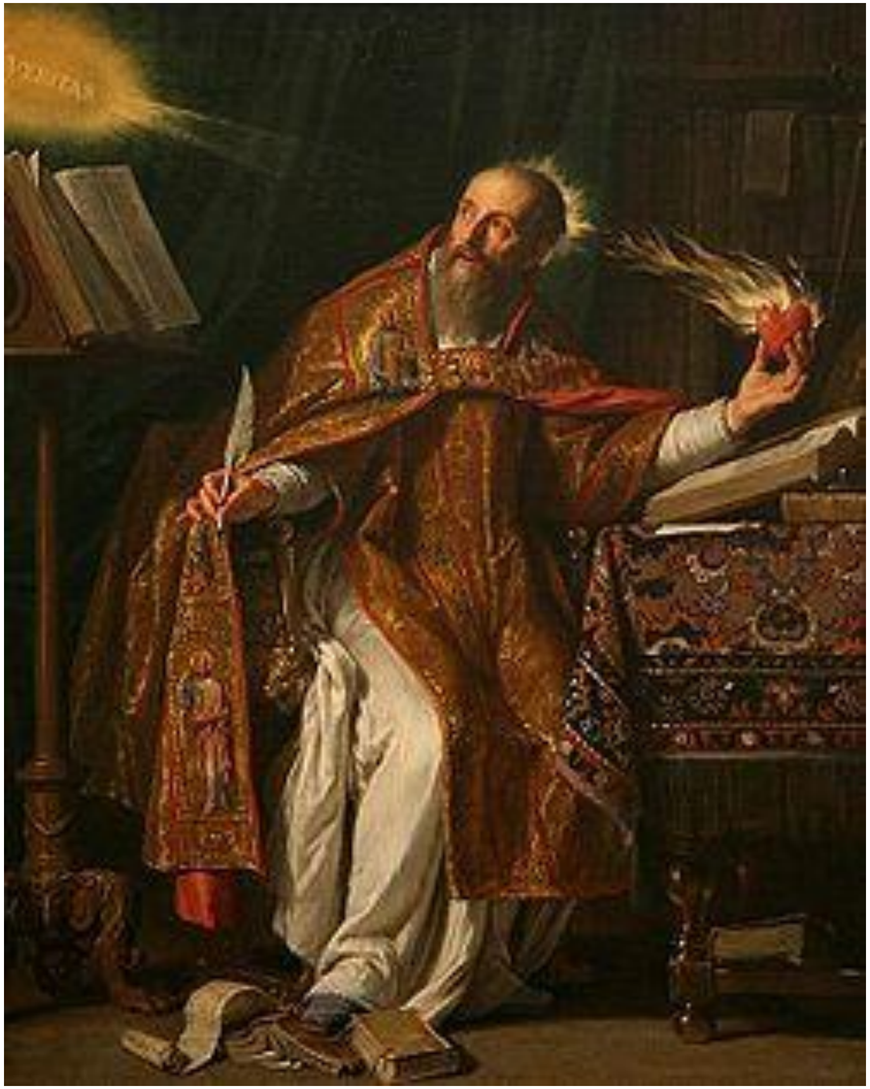
John D. Barrow Impossibility, The Limits of Science and the Science of Limits

A cheep wisdom instead of conclusions

Reaching satisfactory precision, reliability and robustness of experimental and numerical methods is a never-ending but still a worth pursuing task.

Comparing results obtained by experimental and numerical analysis allows shedding light on the accuracy of the measurement and

Comparing these results allows to ponder about the range of applicability of both approaches since none of them has built-in self-limiting features.



Augustine of Hippo

also known as **St. Augustine** November 13, 354 – August 28, 430

Notice the pen and the burning heart

Wishing you a burning heart and sharply pointed pen,

needed for writing grant proposals,

I thank you for your attention

In Book 11 of St. Augustine's Confessions,
he ruminates on the nature of time, asking,

What then is time? If no one asks me, I know:
If I wish to explain it to one that asketh, I know not.

Quid est ergo tempus?
Si nemo ex me quaerat, scio; si quaerenti explicare velim, nescio.

http://www9.georgetown.edu/faculty/jod/latinconf/11.html

If you know that ‘scio’ is ‘I know’ and ‘nescio’ is ‘I do not know’ and if you will be able to sell it during the coffee break to your colleagues you will get a flavour of an expert having a sort of classical education.