

Computational Tools II: Explicit Simulations

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MECHANICAL & MATERIALS ENGINEERING
FOR PARTICLE ACCELERATORS AND DETECTORS

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ENGINEERING
DEPARTMENT



Outline

- More on Implicit vs. Explicit codes
- Material constitutive models
- Examples of explicit simulations for particle accelerators
 - Design & Fabrication
 - Response to accidental cases with beam
- Summary

Implicit vs Explicit codes



Implicit codes

- Unconditionally stable
- Large time steps
- Matrix inversion
- Coupled equations
- Convergence problem

Explicit codes

- Conditionally stable
- Small time steps
- «Lumped» matrix multiplication
- Uncoupled equations
- «Keep going»



- What about explicit codes drawbacks?
 - **Conditionally stable method**: instabilities if time step “too large”
 - Time step shall be sufficiently lower than a **critical time step**
 - Critical time step: minimum time step needed for a stress wave to propagate between one element and the adjacent one

$$\Delta t < \frac{L}{c} \sim L \sqrt{\frac{\rho}{E}}$$

L – element length
 c – wave propagation speed
 E – Young's modulus
 ρ – mass density

Implicit vs Explicit codes

$$\Delta t < \frac{L}{c} \sim L \sqrt{\frac{\rho}{E}}$$

Example

- 1x1x1 mm³ elements
- Material: steel (ρ 7.8 g/cm³, E 210 GPa)
- Critical time step: **0.2 μ s!**

- Even for a “standard” mesh size and material, critical time step very small!
- If the time domain of the simulated phenomenon is **very short**, this is not a huge problem:
 - **Particle beam impact on targets:** duration \sim few μ s \rightarrow **some hundreds of cycles/integration steps**
- If the simulated phenomenon is “**slow**” **transient or static**, this can be a big problem for an explicit simulation:
 - Bending oscillation of a structure with first mode 50 Hz \rightarrow duration $n * 20$ ms \rightarrow **>10⁵ cycles**
 - Quasi-static problem, duration of tens of seconds \rightarrow **>10⁸ cycles**

Implicit vs Explicit codes

Implicit

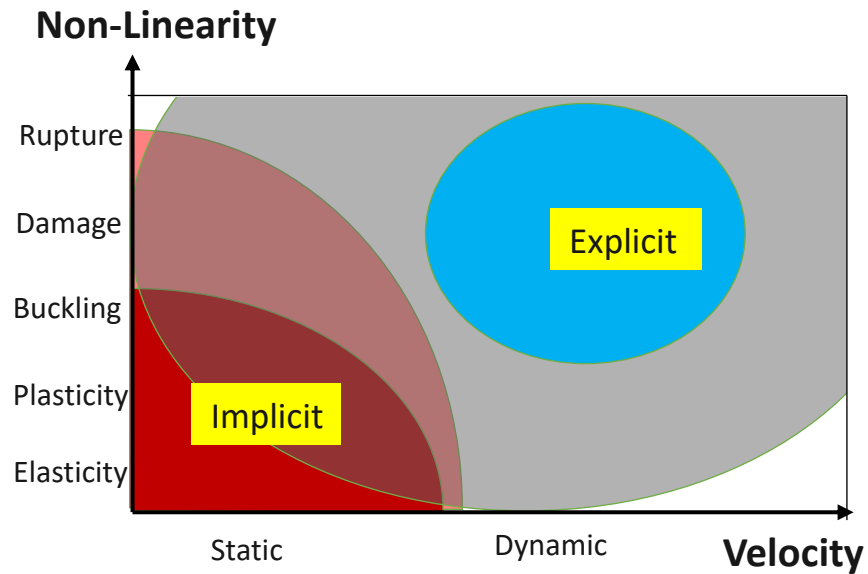
Structural dynamics/statics:

Low frequency response, vibration, static application, springback
quasi-static, boundary conditions affect the structure slowly, for low strain rates/velocity,

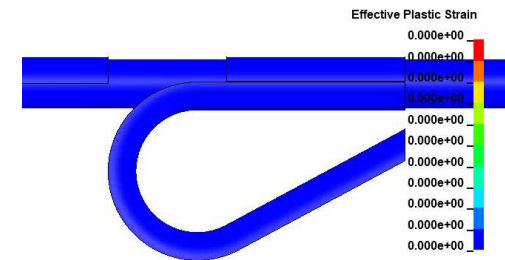
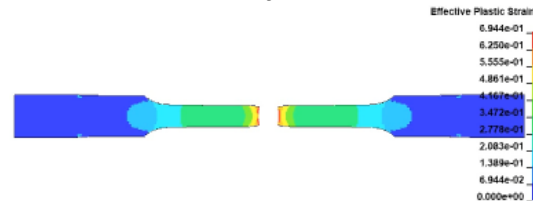
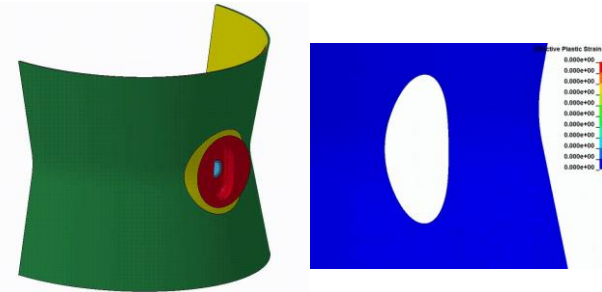
Explicit

Short time dynamics:

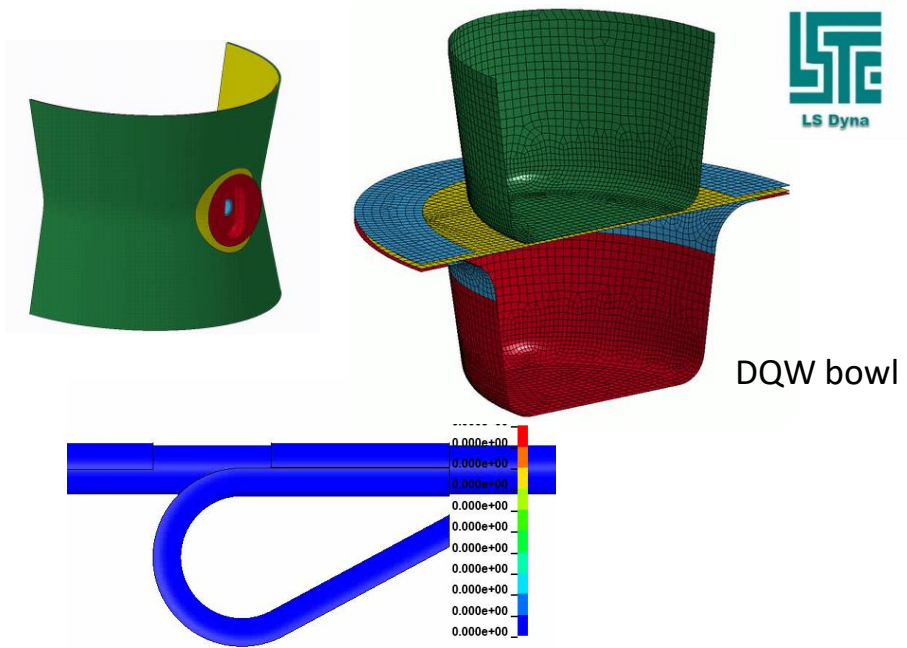
High frequency response, wave propagation
For large deformation, dynamic problems, for high strain rates/velocity, highly non-linear problems



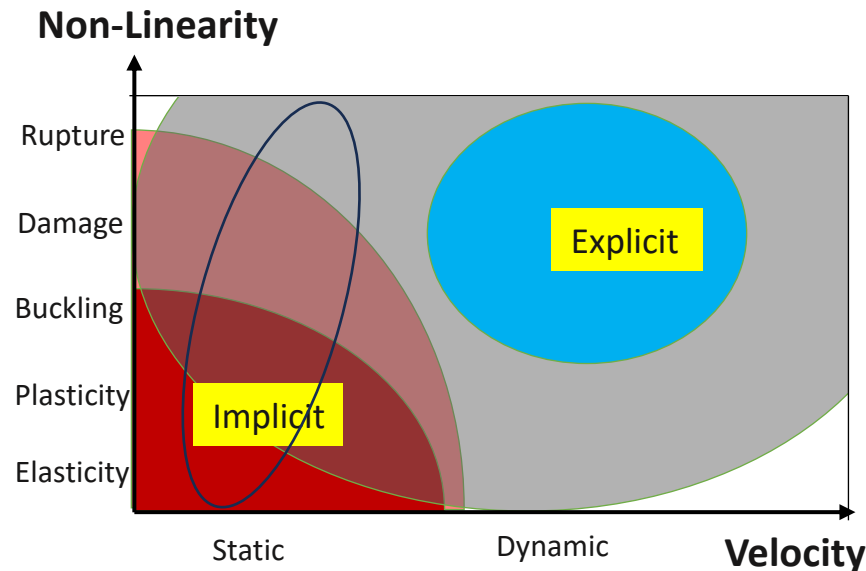
What about those?



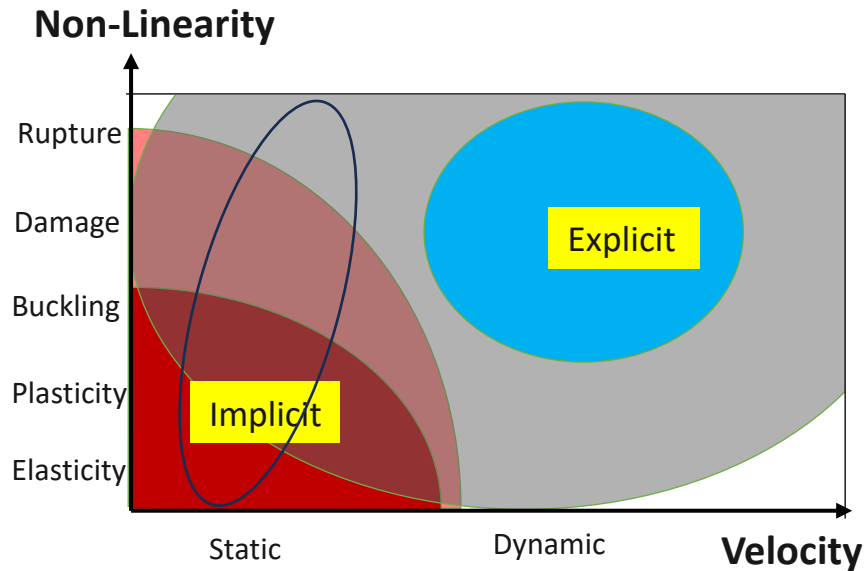
Implicit vs Explicit codes



- Simulating **fabrication processes with large plastic deformations**: slow, but with strong non-linearities!
- We are in this “blurred” region between Implicit & Explicit, no evident answer!



Implicit vs Explicit codes



- At CERN, to simulate forming, deep drawing, bending, etc. we resort to **Explicit codes**
- We need then to overcome the limitation related to the small time step / **too long computing time**



$$\Delta t < \frac{L}{c} \sim L \sqrt{\frac{\rho}{E}}$$

$$n \cdot \Delta t = t_{tot}$$

n – number of cycles, \propto *computing time*

t_{tot} – *physical phenomenon duration*

Explicit codes: dealing with long simulations

...and... increasing/optimizing the mesh size is always important!

$$\Delta t < \frac{L}{c} \sim L \sqrt{\frac{\rho}{E}}$$

Either we (artificially) increase the density \rightarrow “mass scaling”

n – number of cycles, \propto computing time

t_{tot} – physical phenomenon duration

$$n \cdot \Delta t = t_{tot}$$

Or we (artificially) decrease the phenomenon duration \rightarrow “time scaling”

Explicit codes: dealing with long simulations

How to reduce your simulation time?

Time scaling

accelerate your process duration

- Artificially increasing the tool/object velocity (higher than in real process)

But **accelerating too much** can introduce **artificial dynamic effects**. How to check it?

- Visual inspection – severe dynamic effects can be seen in the simulation graphics;
- Check if Energy Ratio=1,(Energy Ratio = total energy / (initial energy + External work)); peaks of variation should be small
- Kinetic Energy / Internal Energy should be low

Note: Parameters which depends on the velocity such strain rate should be adjusted in this case!

Mass scaling

add mass to the system to increase the time step defined by the Courant's stability criteria (critical timestep criterion)

- Artificially increasing the material density for selected parts/elements (manual method)
- Automatic mass scaling proposed by software (selective scaling: add mass only to the elements with the lowest time step)

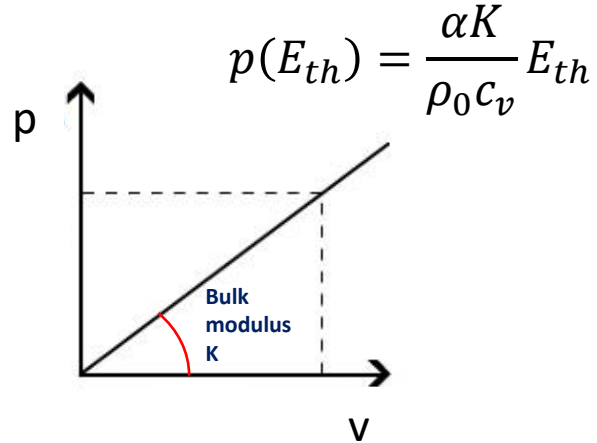
But **adding too much mass** can introduce **artificial dynamic effects**. How to check it?

- Check value of added mass
- Limit percent increase (percentage of extra mass added in relation to the system mass, less than 5%)

Material constitutive models

Implicit

Linear Equation of State



Strain-rate-independent Yield

$$\sigma = f(\varepsilon, T)$$

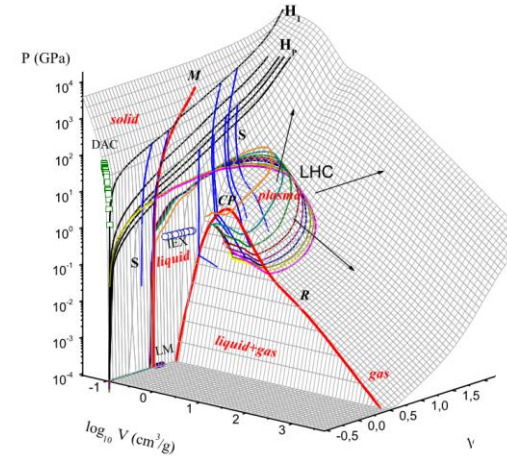
- ✓ Hollomon
- ✓ Ludwik
- ✓ Multilinear
- ✓ ...

Static Failure Strength

$$\sigma < \sigma_{ult}$$

Explicit

Polynomial and tabular Equations of State



$$p = f(\rho, E_{th}, T)$$

- ✓ Phase changes
- ✓ State transitions
- ✓ Regions

More sophisticated material models: but also more difficult to build / retrieve!

Multi-parameter Yield Models

$$\sigma = f(\varepsilon, \dot{\varepsilon}, T)$$

- ✓ Johnson-Cook
- ✓ Steinberg-Guinan
- ✓ Johnson-Holmquist
- ✓

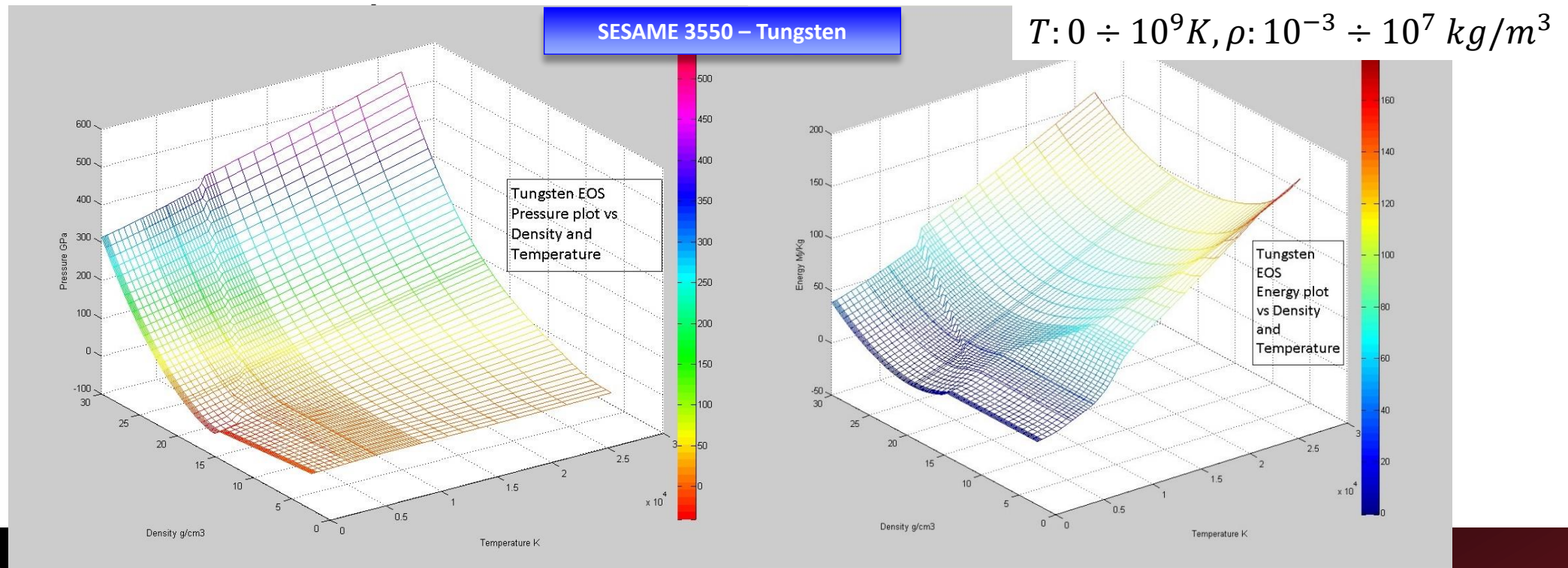
Dynamic Failure Models

Damage $D = f(\varepsilon, \dot{\varepsilon}, T, \bar{\sigma} \dots) < 1$

Spallation $p < p_s(\varepsilon, \dot{\varepsilon}, T, D, c_0, K_c, Y)$

Material constitutive models: EOS

- The EOS expresses the relation **pressure / density / energy** (or T)
- Explicit simulations often used when change of phase is involved (melting, vaporization, plasma) → need to take into account **phase transformations!**
- Most sophisticated type of equation of state: Tabular EOS. At CERN, we have access to the **most complete tabular EOS library in the world (SESAME from Los Alamos National Laboratory)**



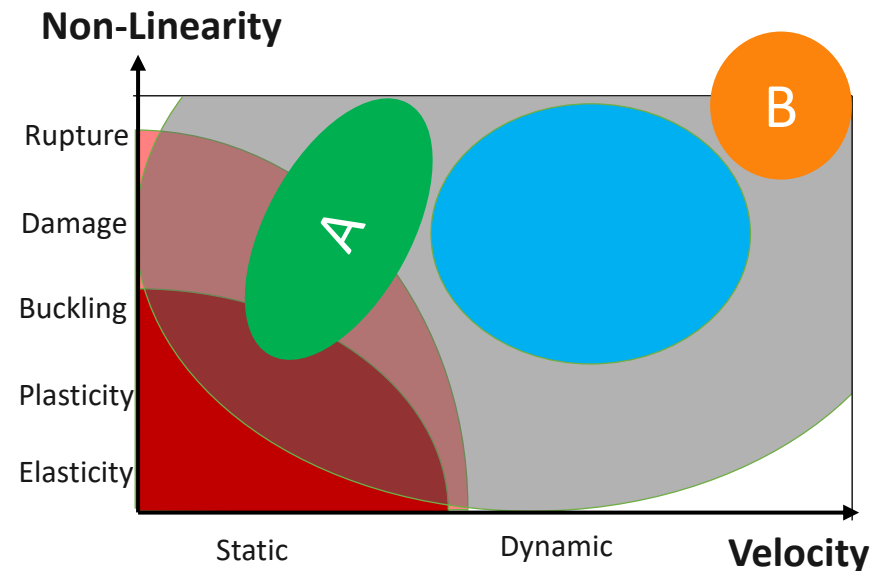
Explicit simulations at CERN

In MME, we resort to **explicit codes in two main fields**:

1. Optimization / tuning of **large-deformation manufacturing processes** (e.g. forming, deep drawing, bending, etc.), objectives:
 - Choice of the best material
 - Design of fabrication tools
 - Definition of process parameters (loading history, temperature, friction coefficients, annealing treatments, etc.)
 - Benchmarking with post-production metrology
2. Response of accelerator components to **accidental or operational beam-impacts**
 - Assess survival of the component
 - Exclude major failure of the containment (vacuum tank, cooling circuit)
 - Evaluate presence of hydrodynamic tunnelling

Explicit simulations at CERN

1. Optimization / tuning of **large-deformation manufacturing processes** (e.g. forming, deep drawing, bending, etc.) → **Region “A”** → relatively long process duration, very high non-linearities
2. Response of beam intercepting devices (BID) to **accidental or operational beam-impacts** → **Region “B”** → Very short duration, extreme non-linearities with changes of phase



Examples of Explicit simulations

Optimization / tuning of large-deformation manufacturing processes



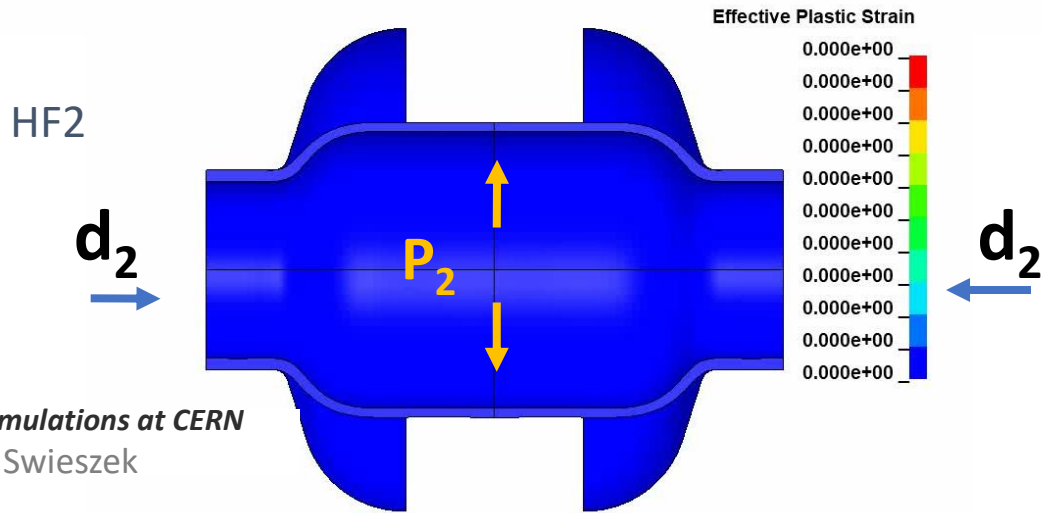
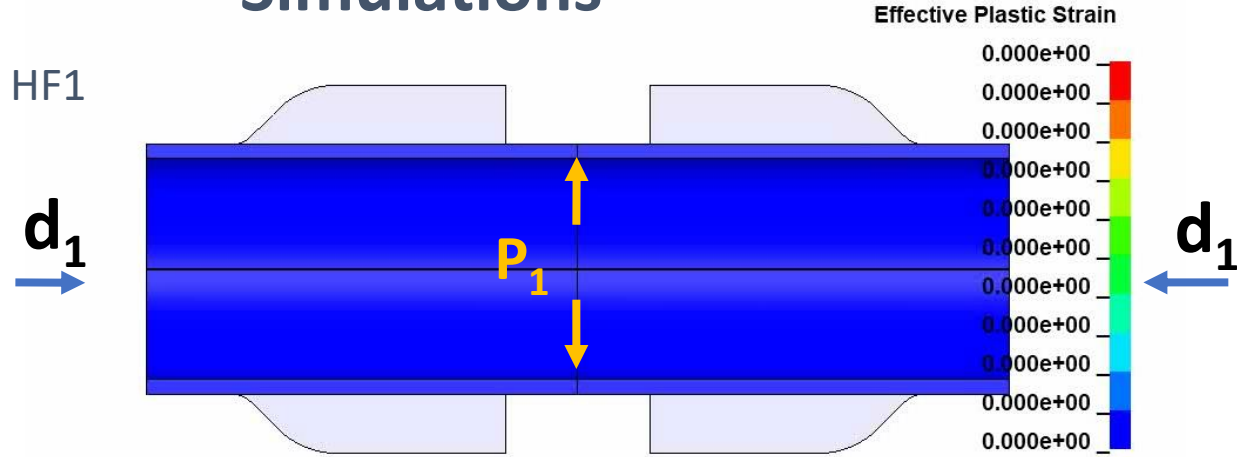
Hydroforming



Hydroforming

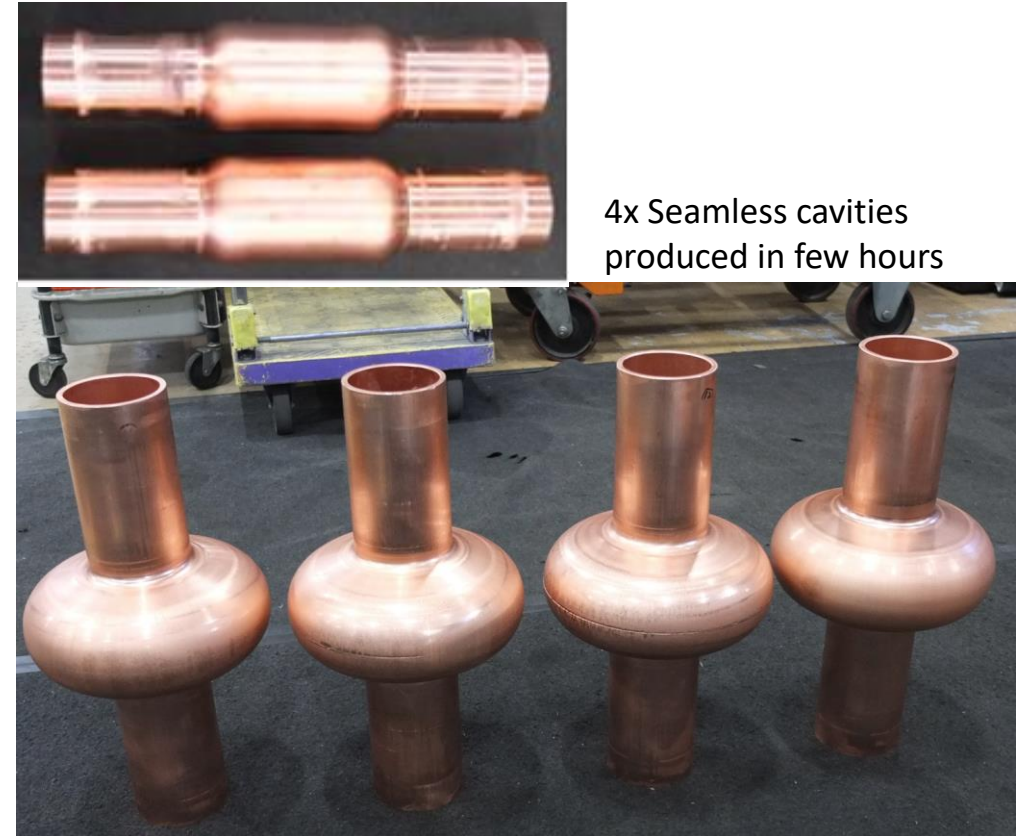


Simulations



Simulations at CERN
J. Swieszek

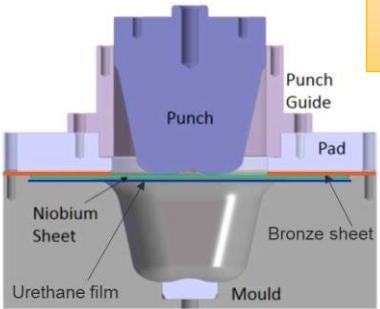
Manufacturing



Produced by KEK
M. Yamanaka, A. Yamamoto

Deep drawing

- Also used in the manufacturing of RF cavities of complex shape
- Example: superconductive RFD crab cavity for HL-LHC (niobium)

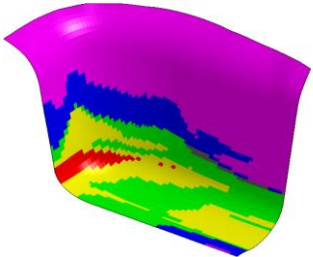


Niobium forming



Very different outcome!

- Same material specification
- Same material supplier
- 2 different material lots
- Same tooling
- Same operators
- Same forming procedure
- Same press machine



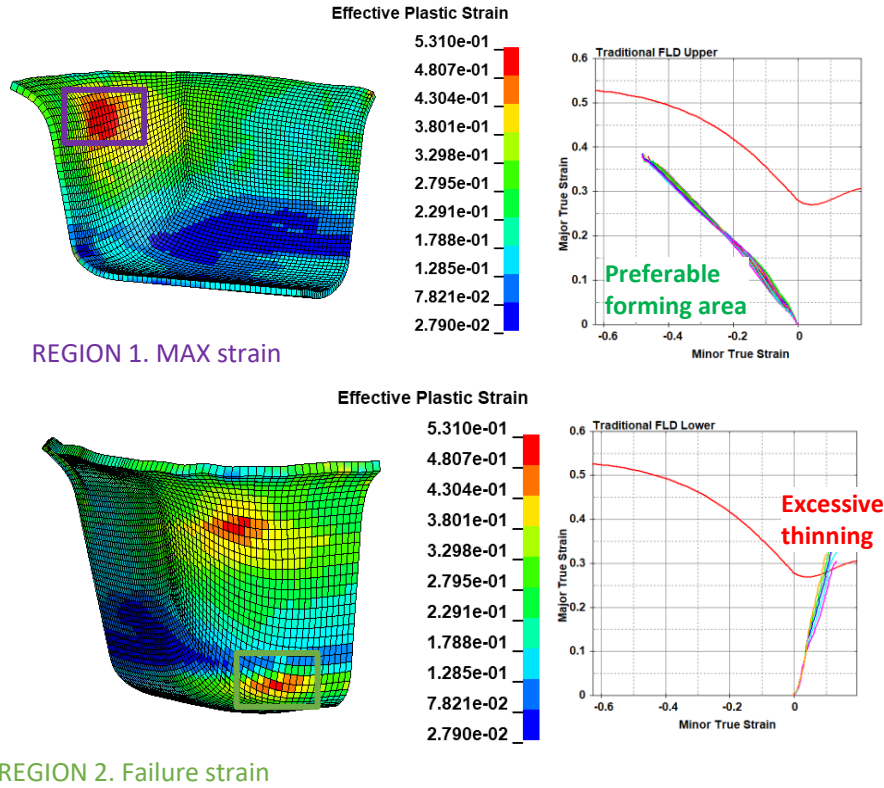
FLD Standard Formability key

| | |
|--------------------|-------------|
| Cracks | Red |
| Risk of cracks | Orange |
| Severe thinning | Yellow |
| Safe | Green |
| Inadequate stretch | Light Green |
| Wrinkling tendency | Blue |
| Wrinkles | Purple |

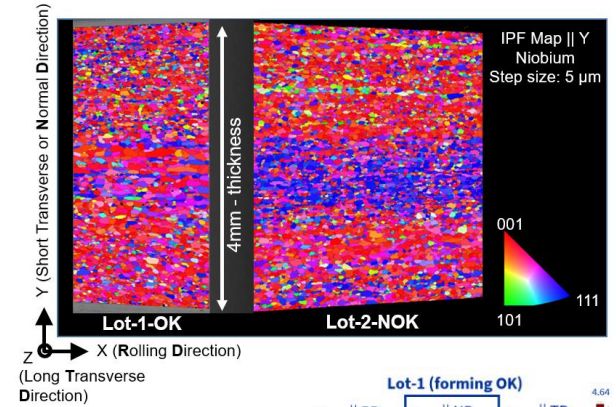
Why?

Deep drawing

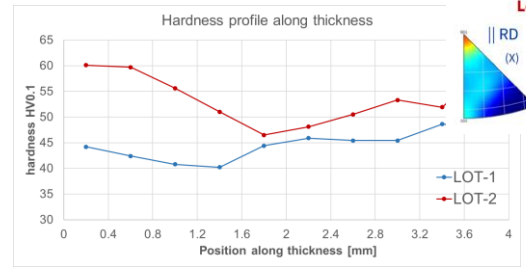
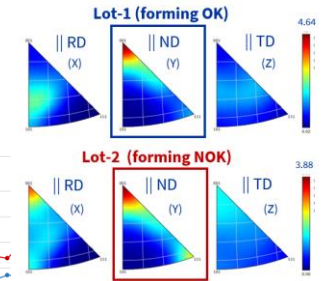
In-depth analysis of material used!
 Activities in full synergy with EN-MME Material, Metrology & NDT section



Simulations at CERN
 J. Swieszek



Crystallographic orientation and texture
 A. Gallifa Terricabras, S. Pfeiffer



Hardness profiles

R&D NIOBIUM FORMING
 Nb material model

- Anisotropy
- Strain rate sensitivity

Improved failure model

Particle beam impacts on accelerator structures



Particle beam impacts

- When a **particle beam hits an accelerator structure**, it transfers its kinetic energy to the structure under the form of heat
- We call this case “**quasi-instantaneous heating**” because the duration of the impact (ns, μ s) is very small compared to the time constants of the problem:

$$t_d <, \ll \tau_{th}, \tau_{mech}$$

$$\tau_{th} = \frac{L^2}{a} \left(a = \frac{k}{\rho c_p} \right)$$

$$\tau_{mech} = \frac{L_c}{c}$$

τ_{th} : thermal time constant

τ_{mech} : mechanical time constant

L_c : characteristic dimension of the system

a : thermal diffusivity

k : thermal conductivity

ρ : density

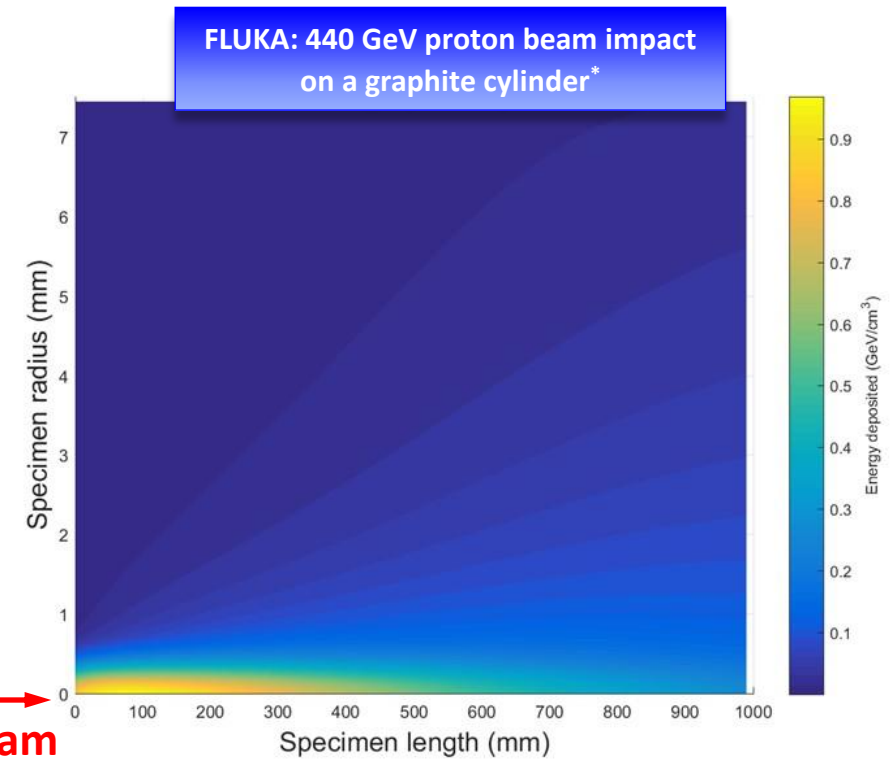
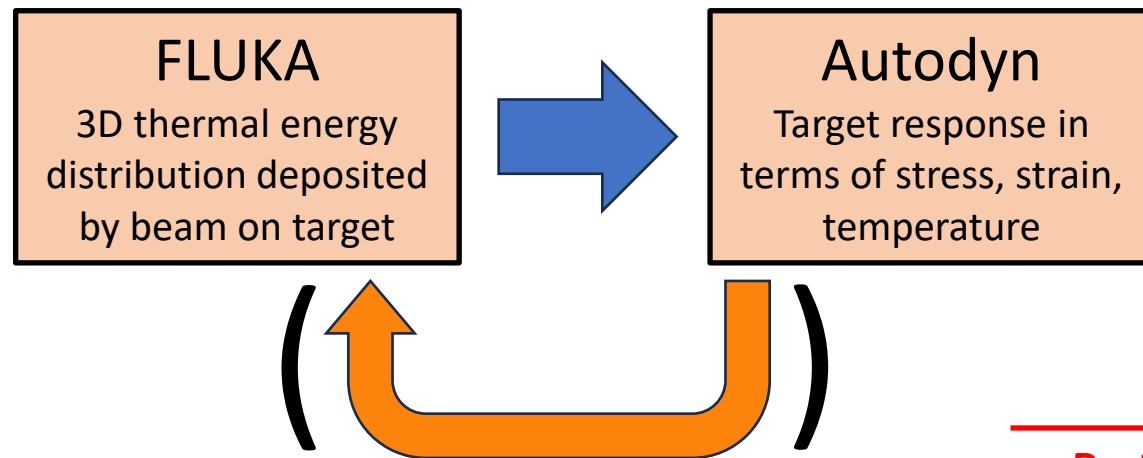
c_p : specific heat

c : wave speed (speed of sound in the elastic domain)

- Short time phenomenon, high non-linearity (melting, vaporization, fragmentation) → typical domain of **explicit codes!**
- Tool of preference for this scenario, at CERN, is **Autodyn** (self-implemented SESAME EOS, etc.)

Particle beam impacts

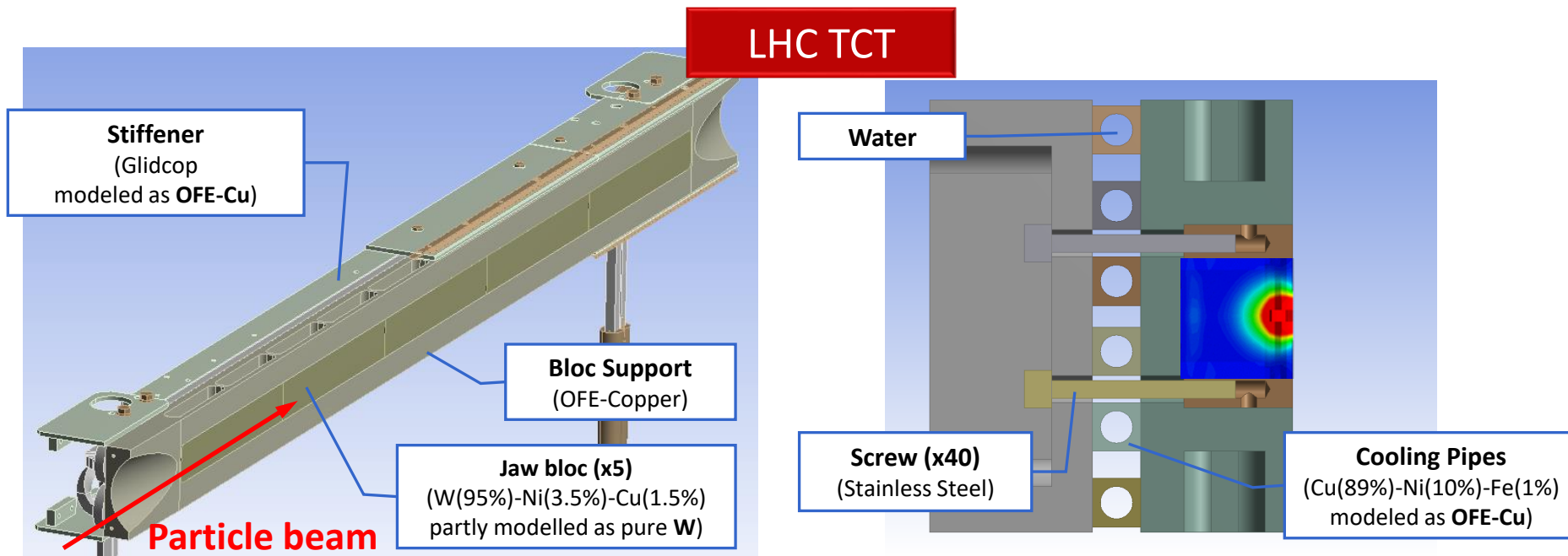
- Thermal energy deposited on the target can be evaluated through Monte-Carlo interaction and transport codes *e.g.* **GEANT4**, **MARS**, **FLUKA** (CERN, SY-STI)
- 3D energy density FLUKA maps used as an **input for the thermomechanical simulations (Autodyn, LS-Dyna)**



*Courtesy of M. Frankl, CERN, SY-STI

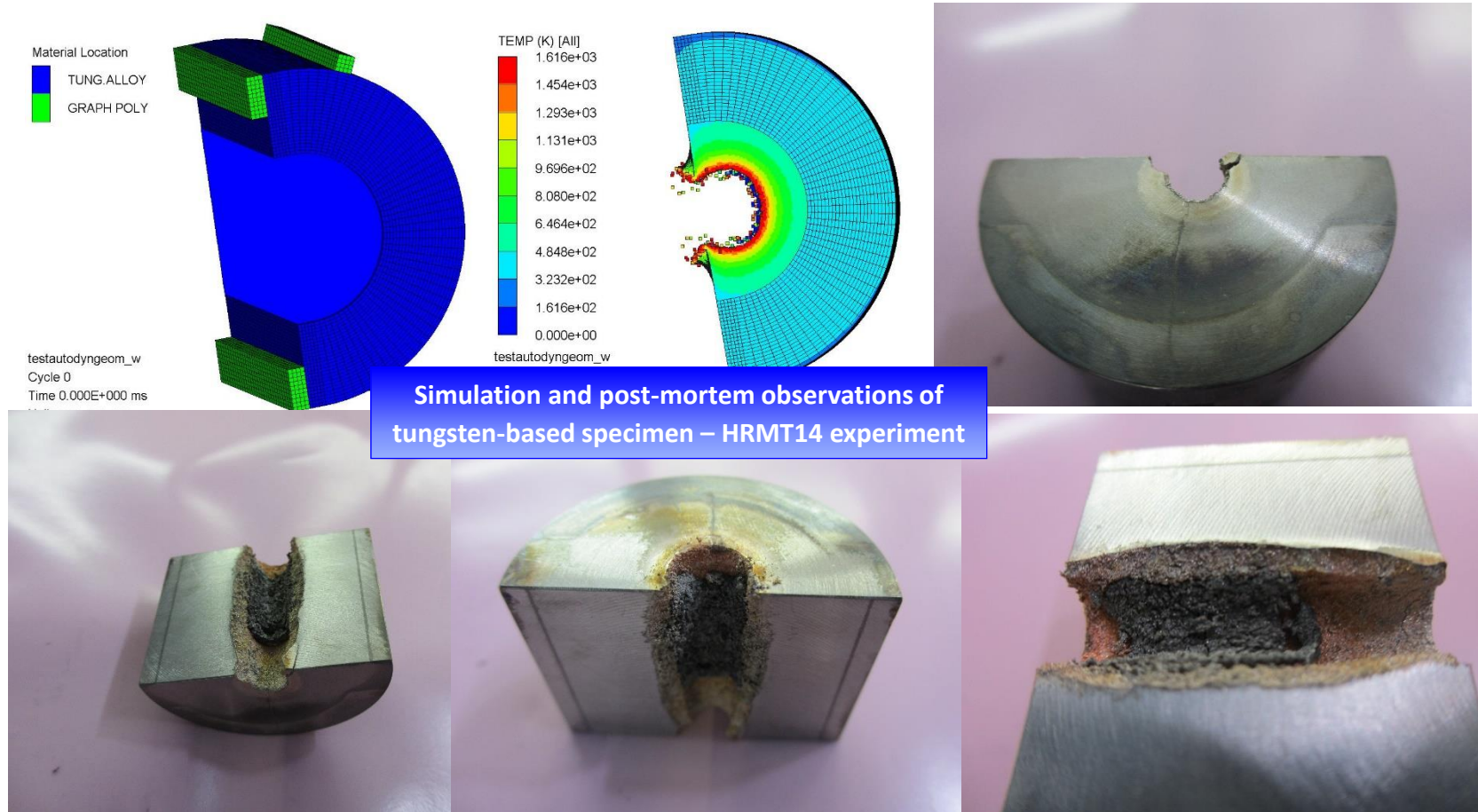
Particle beam impacts on LHC collimators

- **LHC collimators:** objects intercepting the external halo of the circulating proton beam (steady state load)
- **In accidental cases:** direct beam impact on the collimator absorber!
- Most critical case is on **tertiary collimators** (tungsten-based, dense absorber)



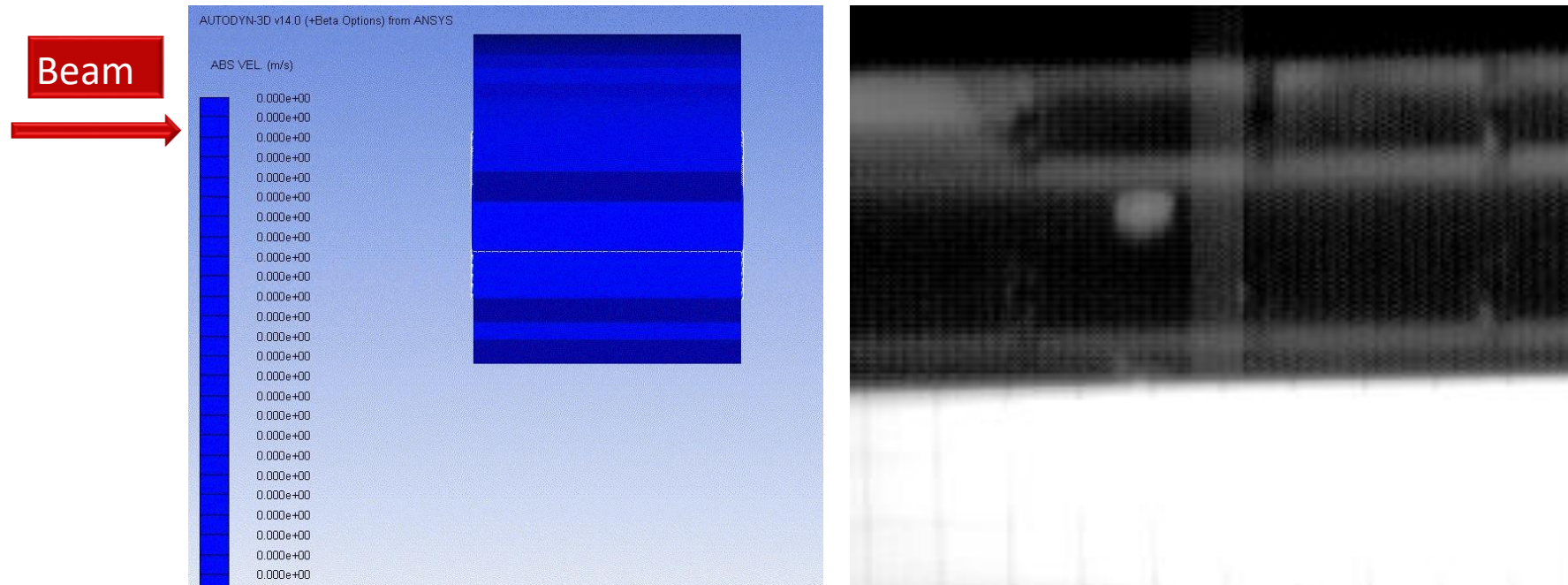
Particle beam impacts on LHC collimators: material testing

- Materials can be tested in these conditions at CERN: **HiRadMat facility**



Particle beam impacts on LHC collimators: material testing

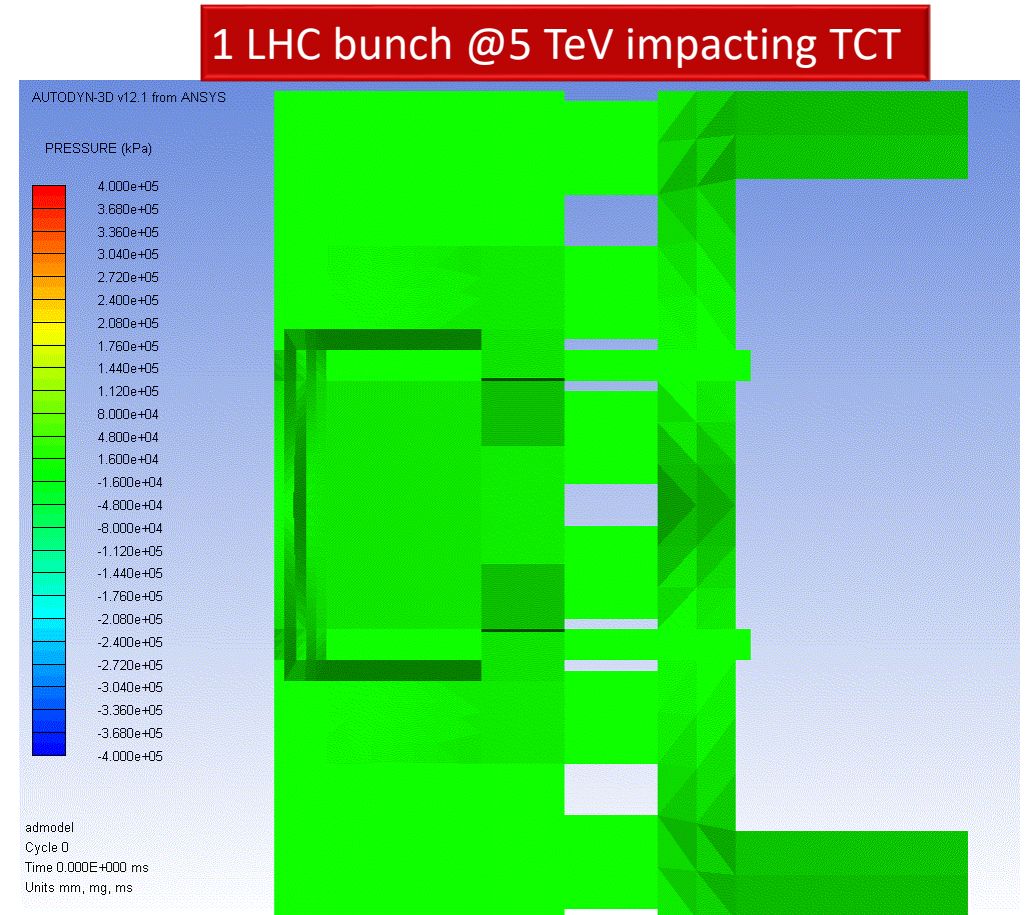
- Materials can be tested in these conditions at CERN: **HiRadMat facility**



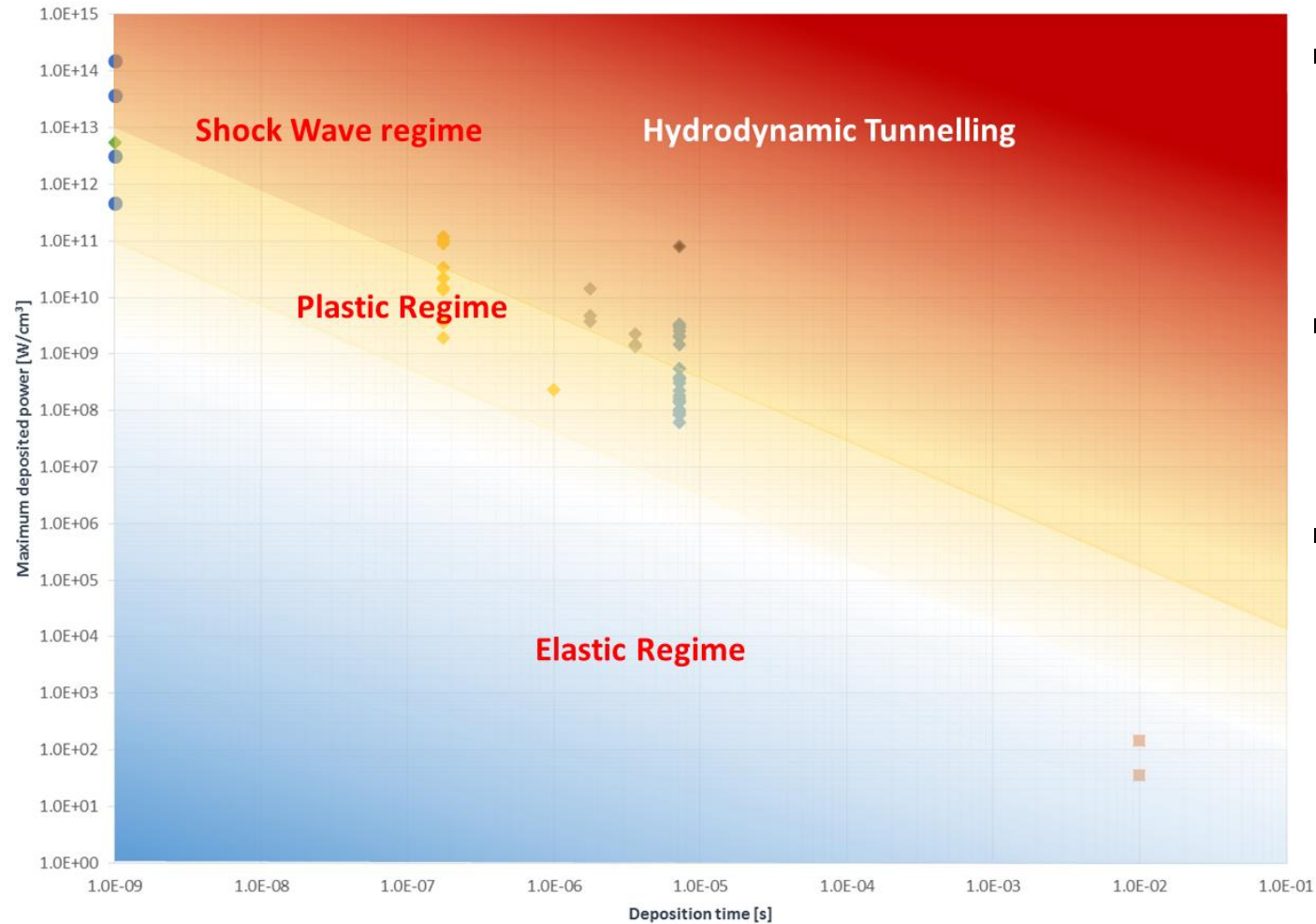
- Maximum fragment velocity:
 - Numerical 316 m/s
 - Experimental 275 m/s

Particle beam impacts on LHC collimators

- What is the point in simulating so extreme accidental scenarios?
- Reason: we can accept failure of the absorber and replace the collimator. But **we cannot accept major failure possibly jeopardizing the close-by environment** (full vacuum sector or even outside of the tank)
- Design must ensure:
 - Resistance of the **cooling circuit**
 - Resistance of the **vacuum containment** (absorber fragments are like hot bullets!)



Particle beam impacts with hydrodynamic tunnelling



- Depending on the energy and densities, a device impacted by the particle beam will undergo **different regimes**
- Most complex to study / simulate is the **hydrodynamic tunnelling regime**
- **What's that?**

• A. Bertarelli (2016). *Beam-induced damage mechanisms and their calculation*. CERN Yellow Reports, v. 2, p. 159, Jan. 2016. ISSN 00078328.

Particle beam impacts with hydrodynamic tunnelling

- We said, for beam impacts →

$$t_d <, \ll \tau_{th}, \tau_{mech}$$

- With FLUKA, the simulation starts from a component with density ρ_0

- At the impact spot: instantaneous temperature and density change

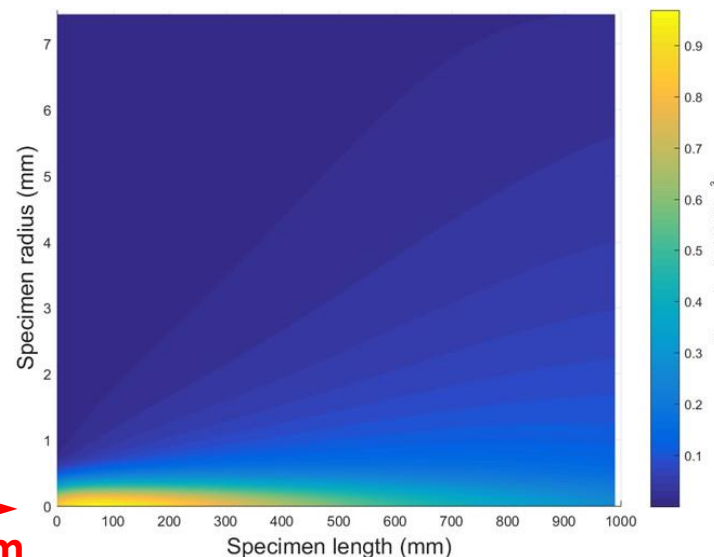
- However, as soon as the target remains solid, the density change is small →

$$\rho(t) \sim \rho_0$$

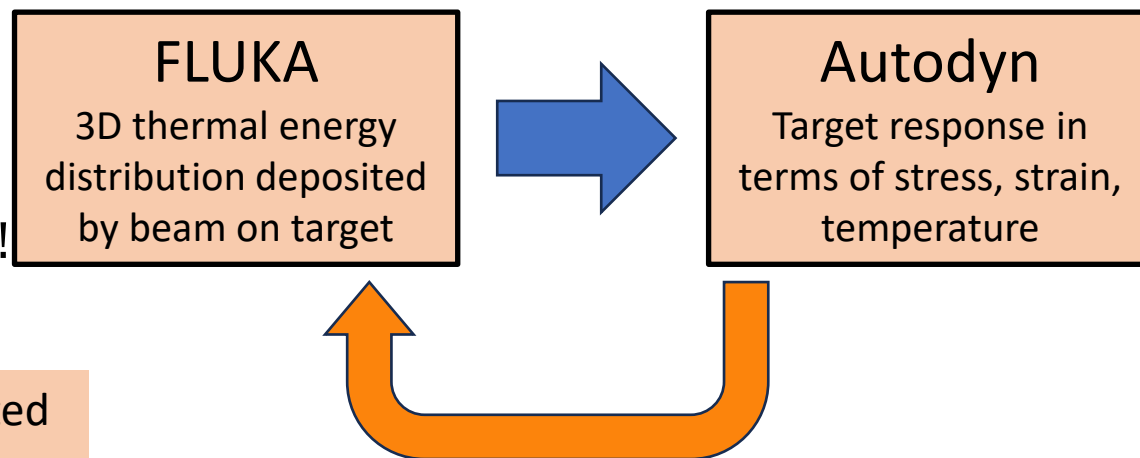
- At a certain time of the impact τ_{tu} , change of phase occurs. There →

$$\rho \tau_{tu} <, \ll \rho_0 !$$

*Courtesy of M. Frankl, CERN, SY-STI



Particle beam

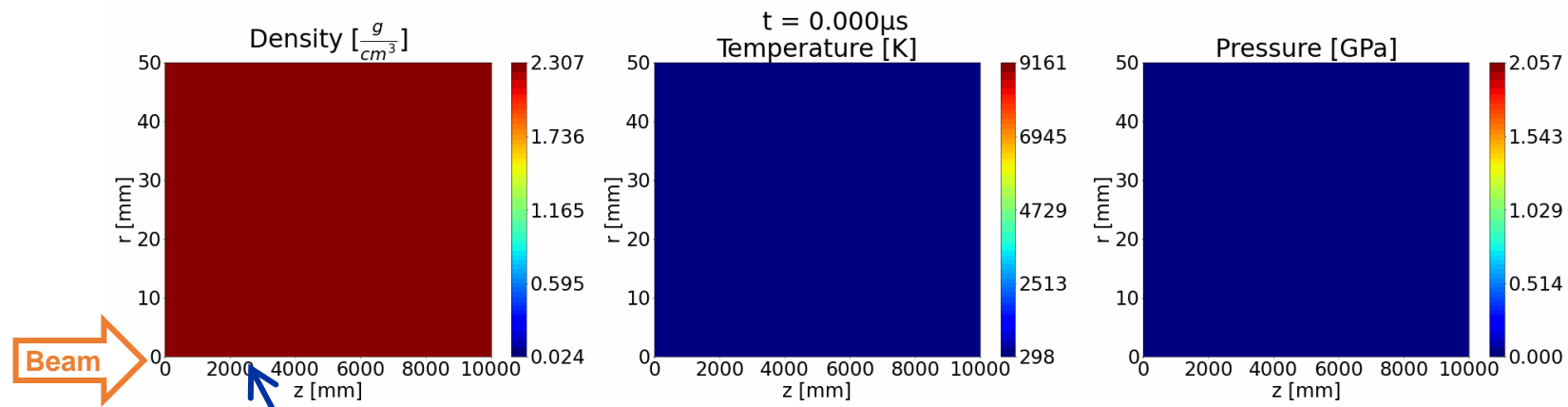


If $t_d > \tau_{tu}$ → the FLUKA map needs to be updated with the new target density distribution

Particle beam impacts with hydrodynamic tunnelling

In a nutshell

- **Hydrodynamic tunnelling:** the impacting beam penetrates deeper and deeper into the target, as the density of the impact region depletes over time
- If FLUKA map is not updated over time → strong underestimation of the beam penetration into the target → **could be a problem for beam dumps!**
- **Example: full HL-LHC beam impact on graphite target ($t_d > 70 \mu\text{s}$)**



Density depleting to zero at the axis.

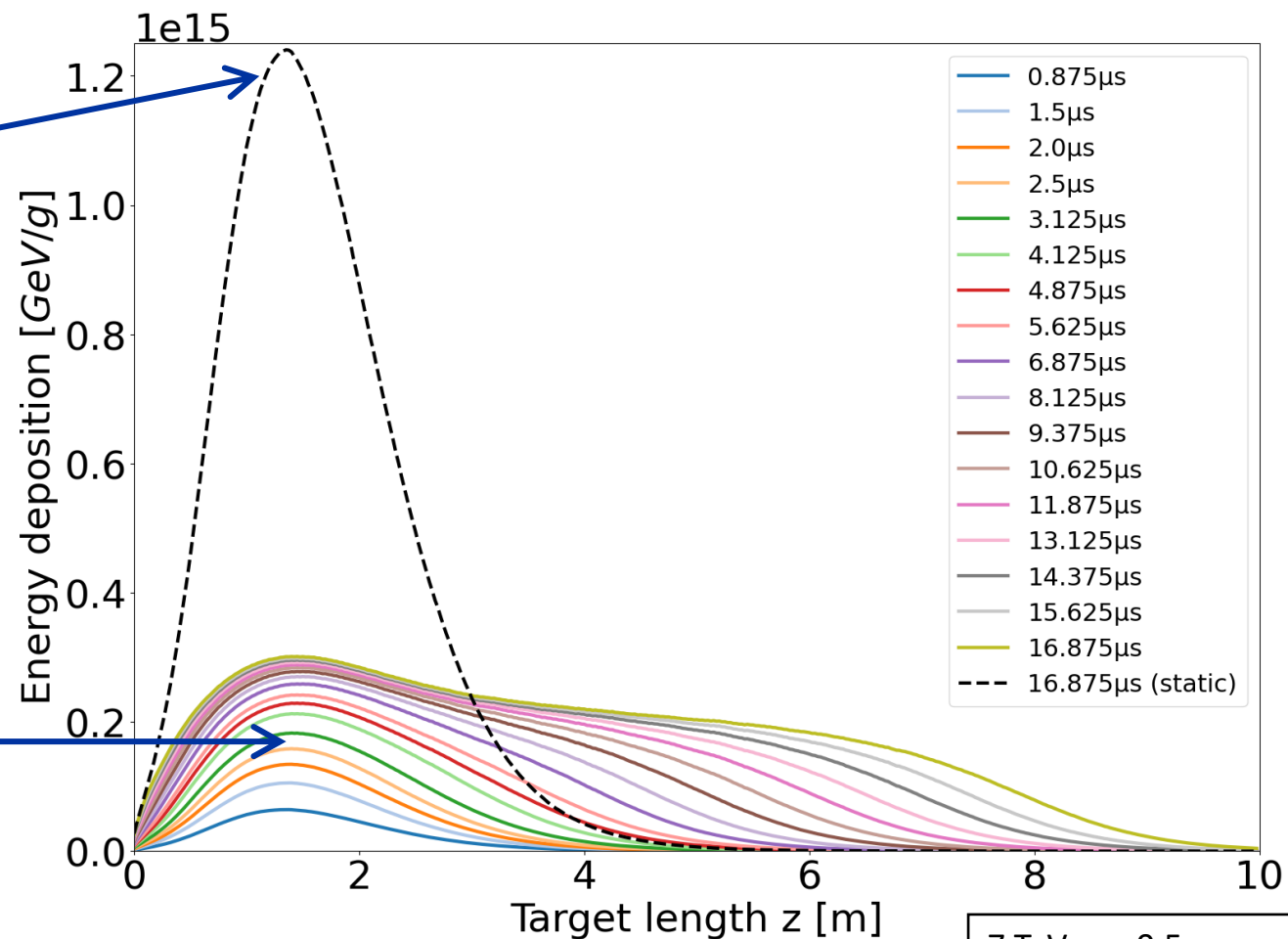
Courtesy of I. Hjelle (CERN, TE-MPE)
& A. Piccini (CERN, EN-MME)

Particle beam impacts with hydrodynamic tunnelling

No FLUKA/Autodyn coupling: beam penetration after 70 μs into target = $\sim 5\text{m}$

FLUKA/Autodyn coupling: beam penetration into target after 17 μs \rightarrow $\sim 10\text{m}$ (and after 70 μs \rightarrow $\sim 30\text{m}$!)

Tunnelling!



7 TeV, $\sigma = 0.5$ mm,
 2.2×10^{11} ppb

Computational Tools II - Summary

- At CERN, and especially in the phase of designing particle accelerator components, we **most often resort to implicit tools such as ANSYS.**
- Explicit codes usually offer a wider range of material models and possibilities for **non-linear calculations.**
- However, **defining / obtaining such models is a complex and laborious exercise.** For this reason, explicit tools are not the 1st choice at CERN.
- Specific fields that require to us the use of explicit tools such as **LS-Dyna and Autodyn** are:
 - **Large-deformation processes**, e.g. manufacturing by forming and bending
 - Accidental (or operational) **particle beam impacts on accelerator devices**
- Given the complexity of explicit simulations and material models, for this type of studies **extensive experimental testing and benchmarking** is of paramount importance.

Bibliography

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- J. A. Zukas (2004). “Introduction to hydrocodes”. Studies in applied mechanics, Elsevier, ISBN 0080443486.
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Symbols (1/2)

- Δt : integration time step [s]
- L : characteristic length [m]
- c : wave propagation speed [m/s]
- ρ : density [kg/m³]
- E : Young modulus [Pa]
- n : number of integration cycles/steps[–]
- t_{tot} : total duration of the real process [s]
- p : pressure [Pa]
- E_{th} : thermal energy [J]
- α : thermal expansion coefficient [K⁻¹]
- K : Bulk modulus [Pa]
- c_p, c_v : specific heat at constant pressure or volume [J/(kg · K)]
- ε : strain [–]
- $\dot{\varepsilon}$: strain rate [s⁻¹]
- T : temperature [K]
- σ : stress [Pa]
- σ_{ult} : material ultimate strength [Pa]
- D : damage function [–]
- $\bar{\sigma}$: hydrostatic stress [Pa]

Symbols (2/2)

- p_s : spallation pressure [Pa]
- c_0 : sound speed [m/s]
- K_c : fracture toughness [$MPa \cdot \sqrt{m}$]
- Y : material yield strength in uniaxial strain state [Pa]
- τ_{th} : thermal time constant [s]
- τ_{mech} : mechanical time constant [s]
- a : thermal diffusivity [m^2/s]
- k : thermal conductivity [$W/(m \cdot K)$]
- t_d : beam impact duration [s]
- τ_{tu} : time at which change of phase occurs [s]

Thanks for your attention!

And thanks to the many contributors:

In random order and for sure forgetting someone A Piccini, J. Swieszek, G. Coladonato, T. Guillen-Hernandez, A. Bertarelli, L. Dassa, T. Sahner, M. Timmins, M. Guinchard, M. Scapin, M. Frankl, I. Helle, C. Wesner, A. Lechner, I. Lamas, O. Aberle, S. Redaelli, I. Tabian, N. Vejinovic, K. Artoos, A. Dallochio, B. Riffaud, L. Zuccalli, L. Gentini, L. Piacentini, I. Aviles, A. Gallifa, A. Amorim, A. Yamamoto, N. Charitonidis, F. Cerutti, L. Peroni.



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A painting of a Dutch landscape featuring a windmill in the background and a field of tulips in the foreground. The sky is a mix of blue and purple, suggesting a sunset or sunrise. The tulips are in various colors, including red, orange, and yellow.

Backup slides



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MECHANICAL & MATERIALS ENGINEERING
FOR PARTICLE ACCELERATORS AND DETECTORS

Modelling techniques

HYDROFORMING: 1.3 GHz single cell elliptical

Using keywords principle with LS-DYNA standalone:

Definition of the tube:

```
*PART
*MAT_PIECEWISE_LINEAR_PLASTICITY
*SECTION_SHELL
```

Definition of the die and punch:

```
*PART
*MAT_RIGID
*SECTION_SHELL
```

Elements will be assigned in a part
 Plastic material low
 Assignment of the element formulation and thickness
 Tools defined as rigid

Boundary conditions:

```
*BOUDARY_PRESCRIED_MOTION_RIGID
*LOAD_SEGMENT
*BOUNDARY_SPC
```

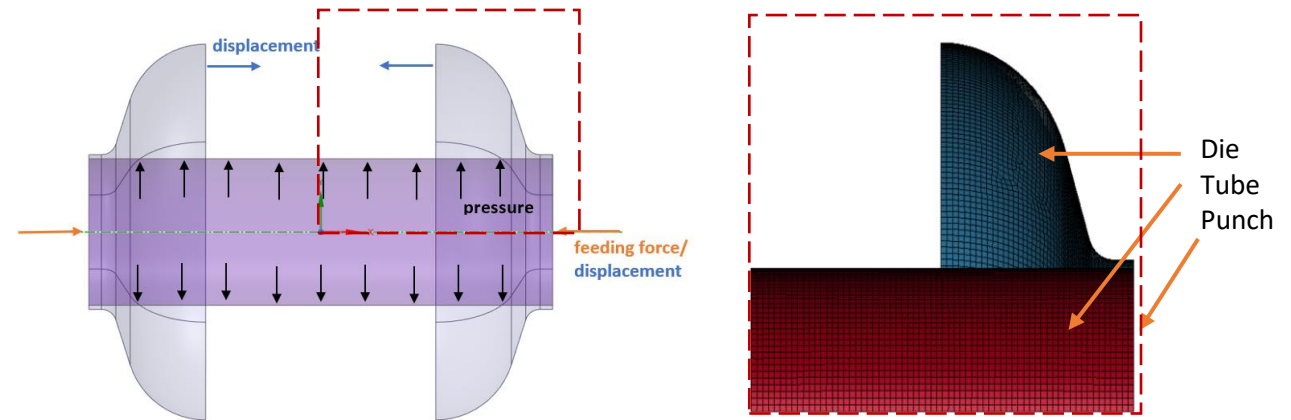
Tool displacement
 Applying pressure

Contact:

```
*CONTACT_FORMING_ONE_WAY_SURFACE_TO_SURFACE
```

Controls and activates the output files:

```
*DATABASE
```



Full symmetry used

All part as surfaces (shell elements)

- inner pressure
- axial displacement

Keywords definitions based on user manual

***PART**

***PART**

| Card 2 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|----------|------|----------|----------|----------|----------|------|--------|----------|
| Variable | PID | SECID | MID | EOSID | HGID | GRAV | ADPOPT | TMID |
| Type | I/A | I or A10 | I or A10 | I or A10 | I or A10 | I | I | I or A10 |
| Default | none | none | none | 0 | 0 | 0 | 0 | 0 |

VARIABLE

DESCRIPTION

| | |
|---------|---|
| HEADING | Heading for the part |
| PID | Part identification. A unique number or label must be specified. |
| SECID | Section identification defined in a *SECTION keyword. See Remark 7. |
| MID | Material identification defined in the *MAT section. See Remark 7. |
| EOSID | Equation of state identification defined in the *EOS section. Nonzero only for solid elements using an equation of state to compute pressure. See Remark 7. |
| HGID | Hourglass/bulk viscosity identification defined in the *HOURLASS Section. See Remark 7. EQ.0: default values are used. |

Failure model

How to assess the failure?

A commonly used failure criterion:

- Maximal principal strain:

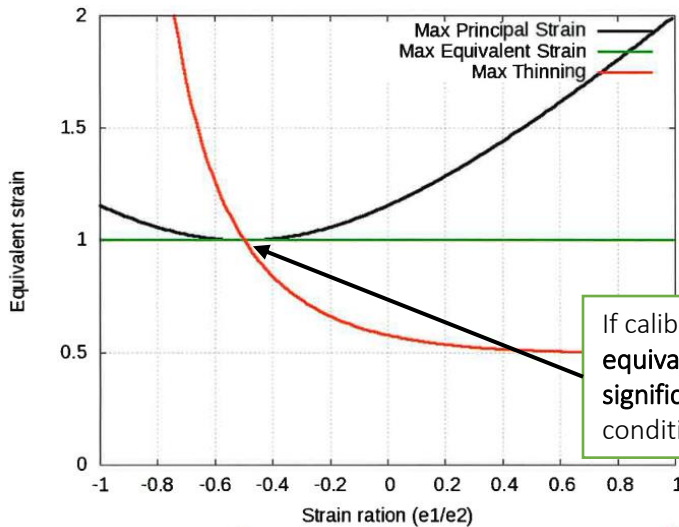
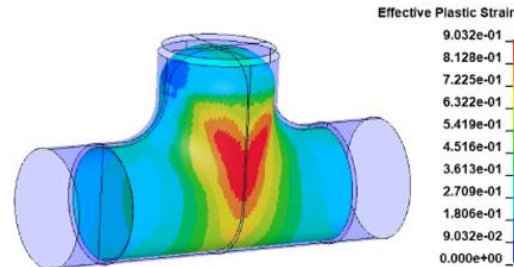
$$\epsilon_1 \leq \epsilon_{max}$$

- Maximal equivalent strain:

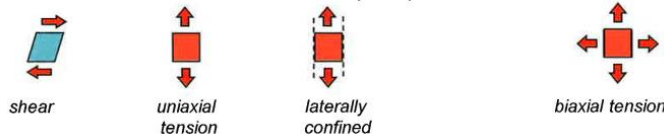
$$\epsilon_{eq} = \sqrt{\frac{4}{3}\epsilon_1^2(1+b+b^2)} \leq \epsilon_{max}$$

- Maximal thinning:

$$\epsilon_3 \leq -\frac{\epsilon_{max}}{2}$$



If calibrated based on uniaxial tensile (UA),
equivalent only for UA deformation,
significantly different for three-directional forming
conditions

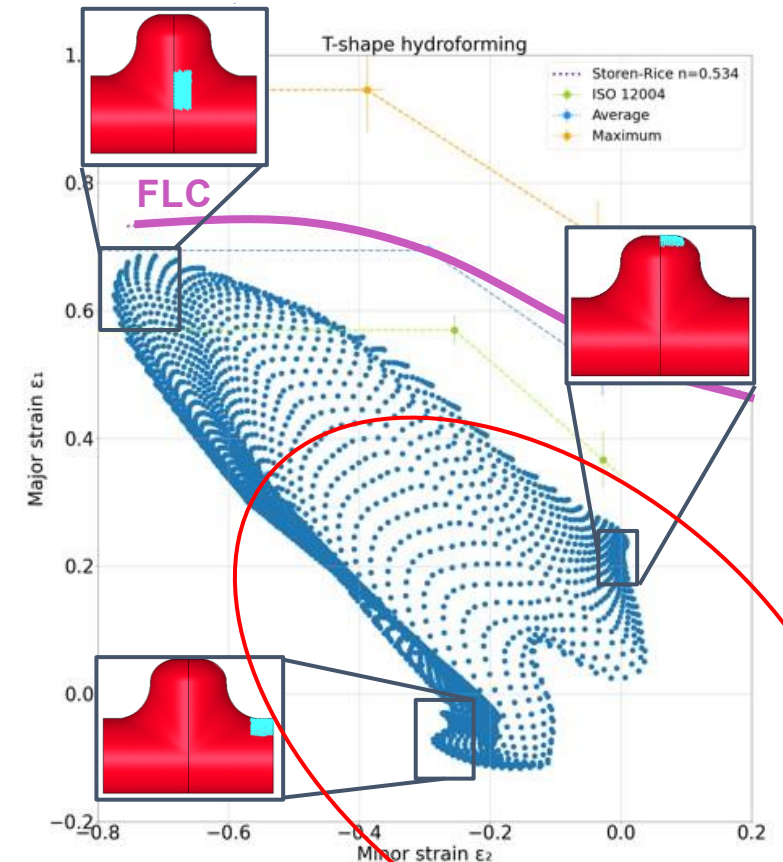


Forming Limit Diagram

for failure prediction

- 1) Simulate
- 2) Correlate ϵ_1 and ϵ_2
- 3) Observe part deformation paths
- 4) Assess feasibility

Standard approach for sheet metal forming:
Failure Model : maximum strain criteria
(Distortion Energy, **FLD** Forming Limit Diagram)



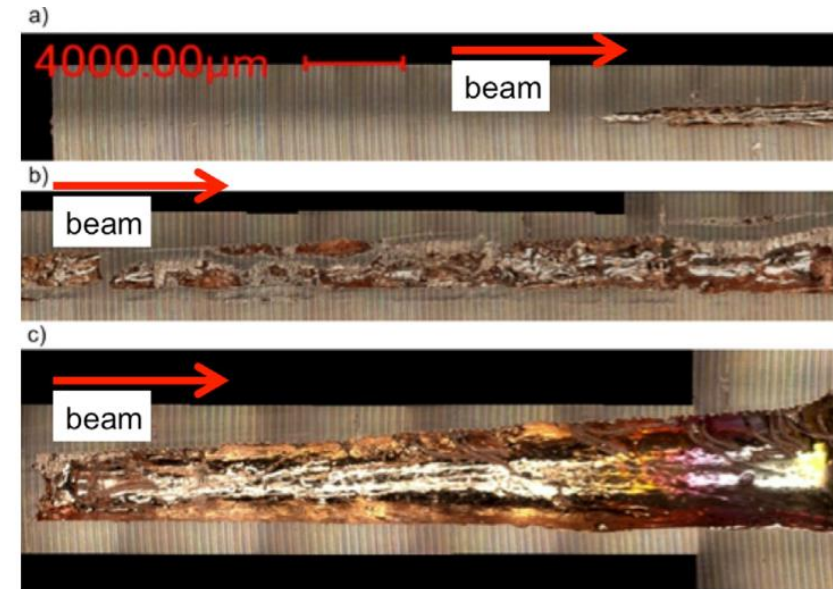
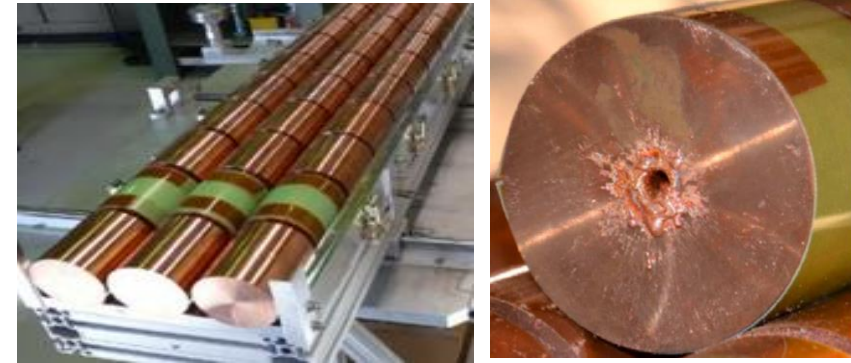
Maximal equivalent strain criterion
Too conservative and inaccurate for large deformation

Hydrodynamic tunnelling

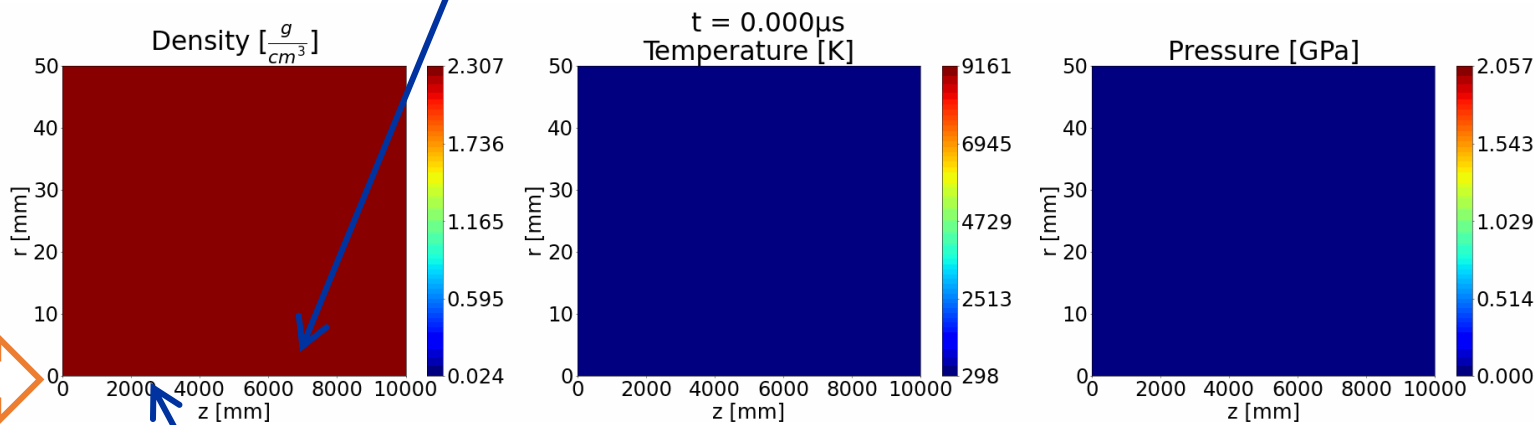
- Successive proton bunches impacting on a target **depletes the material density along the beam path** causing particle showers of subsequent bunches to penetrate deeper into the target.
- Due to the drastic change in density, **the energy distribution calculated under nominal density will cannot be used for the full beam analysis**
- **The energy distribution must be simulated again when the density change due to the beam impact is significant.**
- Done by coupling ANSYS Autodyn with the energy deposition code FLUKA iteratively. This coupling has been proven accurate by experiments conducted at HiRadMat.

Experiment at HiRadMat, CERN

440 GeV, 144b, $\sigma = 0.2$ mm, 1.5e11 p⁺, 1.5 MJ beam energy



The density depletion front reaches a constant speed into the material.



Copper targets after impact of SPS beams. **First experimental proof of hydrodynamic tunnelling.** Taken from N. A. Tahir *et al.*, "Review of hydrodynamic tunneling issues in high power particle accelerators", NIM B, 427 (2018), 70–86

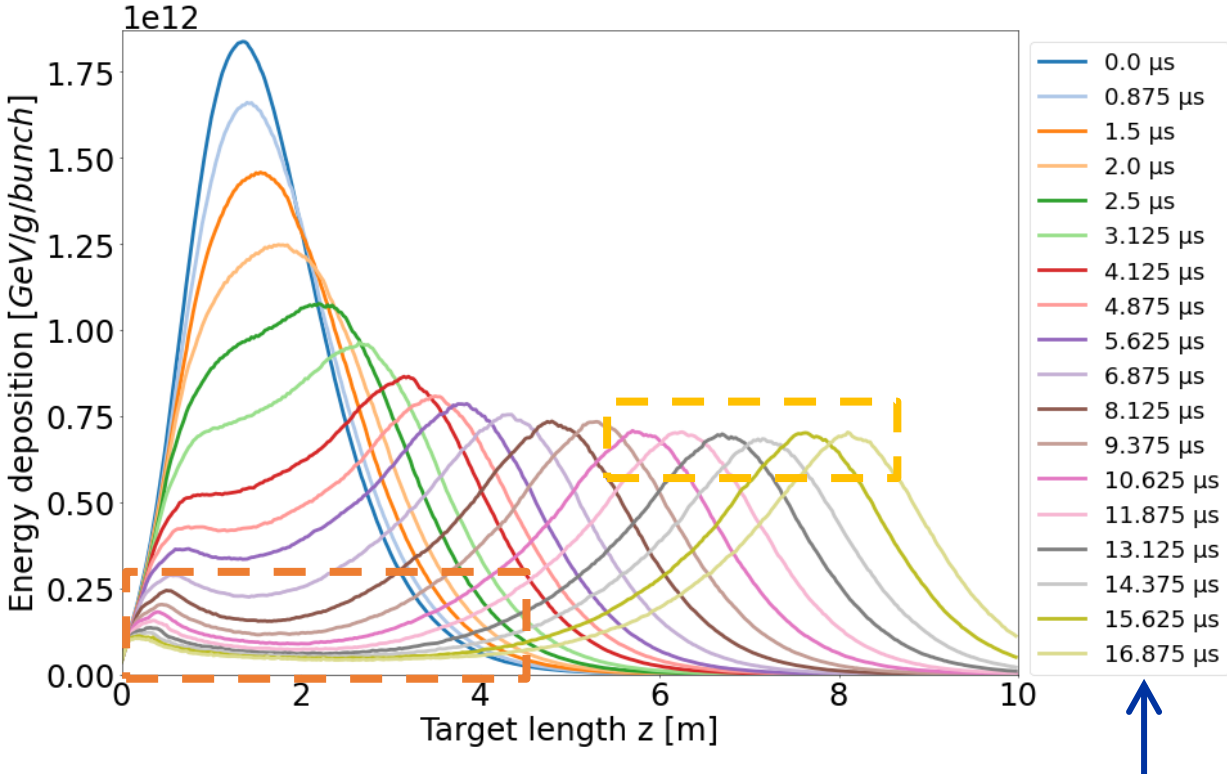
Hydrodynamic tunnelling – Results from some experiments and simulations

TABLE I. Summary of hydrodynamic tunneling studies for the SPS, the LHC, and the FCC.

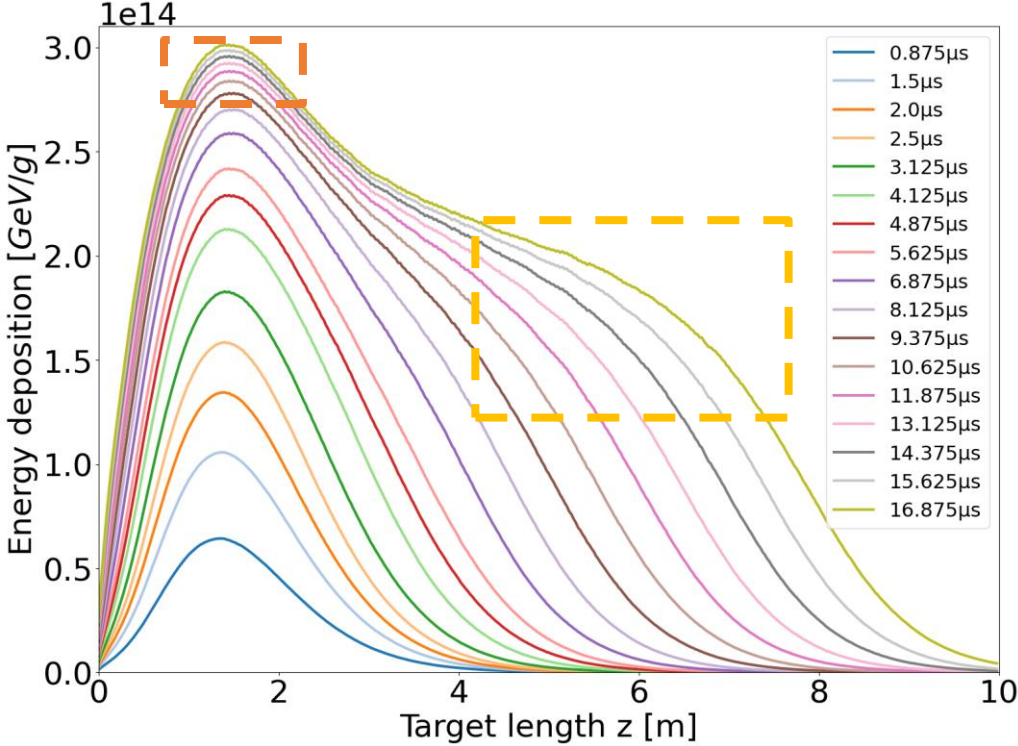
| Accelerator | Proton energy | Bunch number | Bunch intensity | Bunch separation | rms beam size | Target material | Tunneling range | Source |
|-------------|---------------|--------------|-----------------------|------------------|---------------|-----------------|-----------------|--------------------|
| SPS | 440 GeV | 108 | 1.5×10^{11} | 50 ns | 0.2 mm | Copper | 0.8 m | Simulation [23] |
| SPS | 440 GeV | 108 | 1.5×10^{11} | 50 ns | 0.2 mm | Copper | 0.795 m | Experiment [24,25] |
| SPS | 440 GeV | 144 | 1.5×10^{11} | 50 ns | 0.2 mm | Copper | 0.9 m | Simulation [23] |
| SPS | 440 GeV | 144 | 1.5×10^{11} | 50 ns | 0.2 mm | Copper | 0.85 m | Experiment [24,25] |
| SPS | 450 GeV | 288 | 1.1×10^{11} | 25 ns | 0.088 mm | Copper | 1.3 m | Simulation [11] |
| SPS | 440 GeV | 288 | 1.15×10^{11} | 25 ns | 0.2 mm | Copper | 1.1 m | Simulation [22] |
| SPS | 440 GeV | 288 | 1.15×10^{11} | 25 ns | 0.5 mm | Copper | 0.85 m | Simulation [18,22] |
| LHC | 7 TeV | 2808 | 1.15×10^{11} | 25 ns | 0.2 mm | Copper | 35 m | Simulation [13,17] |
| LHC | 7 TeV | 2808 | 1.15×10^{11} | 25 ns | 0.5 mm | Graphite | 25 m | Simulation [18] |
| FCC | 40 TeV | 10600 | 1.0×10^{11} | 25 ns | 0.2 mm | Copper | 290 m | Simulation [27] |
| FCC | 50 TeV | 10600 | 1.0×10^{11} | 25 ns | 0.2 mm | Copper | 350 m | Simulation [27] |

Hydrodynamic tunnelling – Distribution of energy in the material for the HL-LHC beam

Energy distribution over time. Each line is how energy is distributed at one specific timestep. First, we see an initial maximum peak, then as density is depleted the energy is deposited further into the material with a constant amplitude.



Accumulated energy over time. Each line is how the total energy is distributed in the material at the given time and how this increases over time as more bunches impact. Can see how, over time, there is close to no new energy distributed where the density is depleted to zero.



Each timestep represents a coupling step at which the energy distribution in the material was updated due to a significant change in density.

7 TeV, $\sigma = 0.5$ mm, 2.2×10^{11} ppb

