#### University of Liège



### Departement of Aerospace and Mechanical Engineering

#pragma omp parallel for num\_threads(nbt)

# Effective development of a finiteelement solver at the University

Romain BOMAN,

Luc PAPELEUX,

Jean-Philippe PONTHOT

int inx2=0

for(int nbt=trange.getMin(); nbt<=trange.getMax(); nbt+=trange.getStep())



idx2++; double tstart = omp\_get\_wtime(); test.execute(nbt); double tstop = omp\_get\_wtime():

ICSAAM August 28-31, 2018 – Tarbes, France

# Our lab within the university





(Faculty of Applied Sciences)





# **Computational Mechanics**

- Numerical simulation
- Solid mechanics
- Finite element method
- Software development





J.-P. Ponthot

# Our main simulation code: Metafor

### Implicit Finite-Element solver for the numerical simulation of large deformations of solids

#### **Metal Forming applications**

3



- ALE Formalism, remeshing.
- Thermomechanical time-integration schemes.

# Crash / Impact

- Modelling of cracks, fracture.
- Contact algorithms.

# Fluid/structure interaction

- Fluid finite elements.
- Monolithic schemes.
- Coupling with extenal solvers.





 Mesh generation from medical images.

# Typical simulation

# Modelling of a roll forming mill

(forming of beams and tubes from steel sheets)

step 0 t=0/64.872 dt=0.12





# Current team



D. Boemer (PhD student)



R. Boman (Senior Researcher)



M.L. Cerquaglia (PhD student)



L. Papeleux (Senior Researcher)



C. Laruelle (PhD student)



P. Flores (visiting academic)

#### 3 PhD students – 2 senior researchers – 1 visiting academic

# Former developers

G. Deliége



6

C. Canales



A. Stephany



L. Noels



R. Koeune



E. Biotteau

S. Hannay

25 contributors to the present code – from 2000

G. Wautelet



Y. Crutzen



C. Laurent



M. Mengoni



S. Trichon





V.Q. Bui



C. Hennuyer





Y. Carretta





P.-P. Jeunechamps



W. Guo

L. Adam



P. Bussetta

V. d'Otreppe







# Industrial partners



💾 = owns a Metafor license

Scope



# 1. Practical Management of Simulation Codes

• Metafor... from 1992 to 2018

# 2. Numerical Applications

- Introduction to ALE formalism
- Thixoforming
- Continuous Roll forming
- Friction Stir Welding
- Additive manufacturing

# 3. Conclusions

eads(nb)

# Scope

#### void mxv

#pra

for

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• Metafor... from 1992 to 2018

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eads(nbt

# My PhD project in 1997



### Source Code?

- "Spaghetti" code (Fortran 77)
- Several versions of the code

### **Regression testing**?

 Non-automatic and incomplete procedure.



# **Portability?**

- Depends on a library only available as binaries on supercomputers.
- Post-processing with a non-free product.

# Input files?

- Home-made input files.
- Error-prone obscure syntax.

# **Documentation?**

 An outdated technical report from 1992 printed on paper.

### **Extensibility?**



During 3 years I did **almost no research at all**!

In 2000, I seriously considered stopping my PhD research...



FORTUNATELY,

my supervisor gave me the opportunity to **solve all these problems** and build a **framework** that would allow us to avoid the errors from the past.





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**Extensibility**?

Very long tradition of Fortran 77 for implementing the finite element method...



... and a lot of other computation programs. (cfr BLAS: <u>http://www.netlib.org/blas/</u> MUMPS: <u>http://mumps.enseeiht.fr/</u>, etc.)

... also in the industry:



# Main problems of Fortran 77

Yes, it is obviously **possible** to write a good finite-element solver in Fortran...

### BUT

- the language does not help you produce clean/maintainable code
- the maintenance effort increases with time!

CALL META (S,IREST,LS,INOE,NPRDOM,NTOPDO,P,Q, X00,X0,X1,X2,LOCSIG,LOCEL,LOCEL2,LOCNOD, FINT, FEXT, IDENT, ACR, NREMA, T, DEPL, NREAC, DEPKHI,NREKHI,FIMP,NFI,LOCS,LOCSIT,S(I2), S(I3), S(I4), DX2, VIT, ACC, DIAMAS, SMS, DJ, DETJØV,DETJ1V,SIGØ,SIG1,EPLØ,EPL1,BETA1, SVM1,NEPG1,S(I5),AMAT,LOCP,LOCP2,ALOCP, NGR, ANGR, LOCC, LOCC2, VLOCO, ICONT, CODIR, RCONTØ, RCONT1, LMATER, PMATER, NAEL, RAY0, RAY1, DRM, MDE, MAINOE, IMPTIME, IMPDDL, EPS0, EPS1, NOTIN, VALTIN, NFIXT, VALFIX, LOCLT, LOCLT2, ALOCLT, DETFV0, DETFV1, F0,F1, SIGV0, SIGV1, SIGH0, SIGH1, INTMET, LISNOE, LISMAI, HGQ0, HGQ1, ALP0, ALP1, ICTM, TT, STPG, HHT, HHTA, CONMAS, LIA, LIA2, END0, END1, COEHYP, DCHYP, NAELCL, DXT, RHO0, RH01, FTCAP, AMULA0, AMULA1, FPENAL, XFON, MATMOR, IDON INV(1+IPOPT),IDON INV(1+IPOPT+NXOPT), RDON INV(1+IPOPT), RES INV(2), RES INV(2+NPOIOPT), RES INV(1), TRAV1JP, X1SSB, X2SSB, SIG1SSB, DETJ1VSSB, EPL1SSB, RAY1SSB, EPS1SSB, END1SSB, HGQ1SSB, ALP1SSB, DETFV1SSB, F1SSB, RH01SSB, RCONT1SSB, UEFPLUS, UEFMOINS, SIG0SSB, DETJ0VSSB, EPL0SSB, RAY0SSB, EPS0SSB, END0SSB, HGQ0SSB, ALP0SSB, DETFV0SSB, F0SSB, RH00SSB, SIGV0SSB,SIGV1SSB,SIGH0SSB,SIGH1SSB, RCONTØSSB, XØSSB, RESPLUS, XØØSSB, PMATERSSB, VLOCOSSB, IDIFFSSB, DPSSB, VITSSB, ACCSSB, HHTSSB, HHTASSB, STPGSSB, PSSB,QSSB,X000,XM00,XM0,XM1,XM00SSB, XM0SSB,XM1SSB,S(I12),S(I8),S(I9),S(I13), S(I10),S(I11),S(I14),S(I15),S(I6), S(I7), IROBO, NNZ, DJSSB, UPWTMP, S(I16),S(I17),S(I18),S(I19), LOCGAU, LOCELM, LOCNG, MAIADJ, LOCSITG, FCL, MAIADJ2, LOCGAP, LOCSITP, S(I20), S(I21), S(I22), S(I23), NBRNOETFX, LNOETFX, NBRPTSFCT, FIXT\_TIME, VALFCT, ALNPSY, DIAMT, ALNKPSY, ACCLNM1, ACCLN, FINERLN, FINERLNM1, MQLN, DX2LN,ALPN0,ALPN1,EVPL0,EVPL1,SMALLR0,SMALLR1,V FCT)

Example of a subroutine call in Metafor written in Fortran (2000)

# Main problems of Fortran 77



- Memory management?
  - No dynamic memory allocation:
    - > any modification is very instrusive
- Modularity?
   No easy way to gather similar variables/ subroutines together
   > structures?

partially solved with later versions of Fortran



Features?

Necessity to learn another programming language: (graphics, GUI, use of libraries, network, etc.) remaining problem

We finally decided to **rewrite Metafor in C++** and take advantage of Object Oriented Programming

The resulting source code (300k lines) can be split into **33 dynamic libraries** 



# How to have one single set of source files?

# **Our goals**

- One single reference version for everybody (4-10 simultaneous researchers).
- Try to gather all the results / code / models from past projects.
- Keep track of the whole history of modifications in the source code.



# *Version control systems - How does it work?*

#### Most basic workflow



Daily usage should be very easy and intuitive because my colleages will not read the manual...

➔ No "branches"

# *Version control systems - How does it work?*

#### Most basic workflow



### Additional safeguard:

➔ A series of tests ("test suite") should succeed before any commit.

→ The latest version is <u>always</u> stable.

### Source Code?

- "Spaghetti" code (Fortran 77)
- Several versions of the code

### **Regression testing?**

• Non-automatic and incomplete procedure.



# **Portability?**

- Depends on a library only available as binaries on supercomputers.
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**Extensibility**?

# **Regression testing**

# Aims

- Non regression of the algorithms and the numerical models.
- Avoid conflicts between people.





# **Regression testing**

# Principles of our "test suite"

- In-house python script.
- Easy procedure "just run the script!"
- Runs a series of about 3100 FE models, in parallel if the machine allows it.
- Lasts less than 1 night on a classical desktop PC (~75000s CPU = ~5h30 on a 4core PC).
- 4 configurations (various OS/compilers):
- Each test extracts "well chosen" results that are compared to the results of the previous version of the code (these results are committed with the source code.)



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- Mandatory.
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• None.

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**Extensibility**?





### **Strong points**

- Created 14 years ago.
- Very easy installation (text-based DB).
- Numerous plugins.
- Regular / automatic updates.
- ... and no need to read a long manual to edit a page.

# Wiki system: Dokuwiki



#### As any wiki:

- Online editing.
- Keep track of all changes.
- Importation of images, videos, etc.

#### **Online editor**

Edit the page and hit Save. See Formatting Syntax for Wiki syntax. Please edit the page of test some things, learn to make your first steps on the playground

#### B I U TT S H H H H @ @ E E = S @ O 7 5 5 () 1

=== Description === The damage tensor is denoted \$D\$

\$\$ \dot D = \left(\dfrac{\tilde\sigma {eq}^2 R \nu}{2ES}\right)^s |D^{pl}| \ \varepsilon^{pl}\_D \$\$

where  $D^{pl}$ , and eigenvalues equal to the absolute value of \$D^{pl}\$ eigenvalues. The triaxiality function is defined as :

\$\$ R\_\nu = \dfrac{2}{3}\left(1+\nu\right) + 3\left(1-2\nu\right) \left(\dfrac{p}{\sigma\_{eq}}\right)^2 \$\$

where \$ n \$ is the pressure and \$ \sigma Seal \$ Von Mises stress

Preview Cancel Edit summary Save Minor Changes

doc/user/elements/volumes/continuousanisodamage.txt · Last modified: 2016/03/30 15:

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### javascript rendering engine for equations: MathJax

#### Online view



# Documentation of source code changes ("commits")

$\begin{array}{cccccccccccccccccccccccccccccccccccc$				
	Date	Version	Auteur	Résumé
	7 Août 2018	3224	DB	Traction at trans ContactTraction
	1 Août 2018	3220	RoBo	Surroundednes
	27 Juillet 2018	3216	Luc	Bug Fix Thermi
	23 Juillet 2018	3211	Marco	Center of gravit
	19 Juillet 2018	3206	Luc	refactoring The
	17 Juillet 2018	3202	DB	Out-of-plane thi area computatio
	13 Juillet 2018	3198	DB	New ContactTr
	09 Juillet 2018	3194	Luc	bug fix YieldGp
	05 Juillet 2018	3190	Luc	YieldGpState
	03 Juillet 2018	3186	DB	New coupling p
	25 Juin 2018	2102	Luc	ValaaHuparDk2



# Table of Contents **Commit August**

commit:2018:08 17

Previously, in commit 3198, the ContactTractionElement, which sets the resultant traction forces equal to zero at the nodes that are in contact, was introduced. Setting the traction forces equal to zero might, however, be incoherent at a node belonging to an element at the transition from "no contact" to "contact", since the majority of the element is still stressed by the traction as can be seen in the following figure (red triangle). For this reason, an additional property was added to the ContactTractionElement, i.e. TRACTION\_AT\_TRANSITION\_ON. In the past, the ContactTractionElement computed the forces as in the case TRACTION\_AT\_TRANSITION\_ON = False. In the other case, the traction force is not set equal to zero, if the ContactTractionElement is located at the transition from "no contact" to "contact" (see red arrow below). The new default case is TRACTION\_AT\_TRANSITION\_ON = True.



#### Test cases

17th, 2018
### Source Code?

- Modular (C++).
- Source Code Management with Subversion.

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• A wiki system on the web.

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**Extensibility**?

# Rule: The code should be easily built/tested on any (recent) platform



#### Main problems

- the build system should be multi-platform (CMake).
- the dependencies should be limited and multi-platform.

# Visualisation

# **Example: Real-time visualisation during the simulations**

### Initially, 2 aims

- To see what we are doing, anytime.
- To make the software usage easier for students and the industry.

### **Features**

- 1 thread exclusively dedicated to graphics running in parallel.
- The state of the memory is continuously displayed in 3D.
- Nothing is written to disk.

### **Multi-platform libraries:**





3D display of the problem



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- Modular (C++).
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#### Portability?

- Runs on any recent desktop computer and supercomputers.
- Own GUI / post-processor,

#### **Regression testing**?

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**Extensibility**?

# Input files

# Python scripts as input files





- Parsing requires a lot of code.
- Error handling?
- New syntax to learn.

- Almost no source code at all!
- Error handling by python.
- Same syntax as internal C++.

# Input files

# Python scripts as input files





• all these features come at no cost!

# Input files

# No cost? Really?



Yes! a Python class is **automatically** created by SWIG (free tool) for each C++ class.



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## Input files?

• Python.

#### **Documentation?**

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**Extensibility?** 

# **1.** Extensibility with "Inheritance" in C++

- In any object-oriented language, you can extend a class using "inheritance".
- Example: extension of an elastic material to handle elasto-plasticity:

```
ELASTIC MATERIAL
```

```
class ElasticMat
{
   double E, nu;
public:
   virtual
   T computeStress(T &strain);
};
```

ELASTO PLASTIC MATERIAL

```
class ElPlastMat : public ElasticMat
{
    double sig_yield, hardening;
public:
    virtual
    T computeStress(T &strain);
};
```

#### Purpose?

• The code using the material can be written without any conditional statements and should never be modified.

➔ " if the material is elastic, do this.... else, do that" is avoided.

• But, of course, the new code should be recompiled.

# **2.** Inheritance of C++ classes in Python : "user subroutines"

Thanks to SWIG, the derived class can be written in Python!



✓ Very useful for students (FYP)

# 3. Extensibility via "python as a glue language": coupling with another solver

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*Summary – Advantages of the Python interface* 

- Less source code: no need to code a home-made parser,
- **Safety**: errors are never ignored and can be correctly handled.
- **Complete Language**: possibility to use loops, conditional statements, objects, functions, ... in the input file.
- **Extensibility**: inheritance of C++ classes.
- Glue language: call to external programs, solvers.

### Source Code?

- Modular (C++).
- Source Code Management with Subversion.

#### Portability?

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- Own GUI / post-processor,

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## Input files?

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### **Documentation?**

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### Input files?

• Python.

### **Documentation?**

• A wiki system on the web.

### Extensibility?

- Python user-subroutines.
- Coupling with external solvers.

# Scope

#### void mxv

#pra

for

# 1. Practical Management of Simulation Codes Metafor... from 1992 to 2018

# 2. Numerical Applications

- Introduction to ALE formalism
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- Continuous Roll forming
- Friction Stir Welding
- Additive manufacturing

# 3. Conclusions

eads(nbt)

# Introduction to ALE formalism

x

x

# Kinematic description of the motion



# Eulerian formalism

- Undistorted mesh
- Free boundaries are difficult to track
- History-dependent materials are difficult to handle

# Lagrangian formalism

- The mesh can be rapidly distorted
- Free boundaries are automatically computed
- History-dependent materials are easier to handle

# Introduction to ALE formalism

# Kinematic description of the motion



# Arbitrary Lagrangian Eulerian (ALE) formalism

- Extension of both previous formalisms
- The mesh motion is uncoupled from material motion
- ALE can be crudely seen as a continuous remeshing procedure
- Mesh topology does not change
- Remapping of variables is faster than classical remeshing

# 2 Families of ALE Problems

# **1.** Problems involving excessive mesh distortion

### Benefits of ALE vs. Lagrangian models

- Helps us keep well-shaped elements despite large deformations
- Most often remeshing is completely avoided

# ALE model Lagrangian model

**Example:** axisymmetric forging

# 2 Families of ALE Problems



### Benefits of ALE vs. Lagrangian models

- The size of the model is decreased in the flow direction.
- Loading is easier.
- The element size may be optimised in the flow direction.
- The contact regions do not change.

# Scope

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eads(nbt)

# What is thixotropy?

- A thixotropic material behaves...
  - ... like a solid, at rest (a billet can sustain its own weight).
  - ... like a liquid, during shearing (can be cut easily).
- Common examples: clays, muds, paints, tomato ketchup.
- Some alloys (Magnesium, Aluminium, Steels) exhibit a semi-solid behaviour in a narrow range of T.

# What is thixoforming?

- Taking advantage of this semi-solid state.
- The process combines advantages of casting and forging.



## **Constitutive behaviour**

"Extended yield criterion" for thixotropy

$$\bar{f} = \bar{\sigma}^{VM} - \sigma_y - \eta \, \bar{\varepsilon}^{vp}$$



R. Koeune

modified yield stress

$$\sigma_{y} = \sigma_{y}(\,\bar{\varepsilon}^{vp}, \bar{\varepsilon}^{vp}, \lambda, f_{l})$$

apparent viscosity

$$\eta = \eta \left( \, \bar{\varepsilon}^{vp}, \bar{\varepsilon}^{vp}, \lambda, f_l \right)$$

2 NEW INTERNAL VARIABLES

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liquid fraction (phase change)  $f_l = f_l(T)$  cohesion degree (microstructural state)  $\lambda = \lambda(\, \dot{\overline{\varepsilon}}^{vp}, f_l)$ 

Both liquid and solid formalisms are contained in the proposed models!



## **Double cup extrusion – process description**

- Production of an axisymmetric H-shape part, starting from a cylinder.
- Temperature controlled by induction heating.
- Experiments made in PIMW, Liège in collaboration with ENSAM, Metz.
- Material: 100Cr6 steel alloy.





Example of (half) part

### Double cup extrusion – mesh management

ALE mesh management (numerical trick): → An initial thin squeezed mesh is added to the top of the billet



### **Double cup extrusion - results**







- Good agreement between experimental and numerical results.
- The model is able to predict the residual stresses after unloading and cooling to room temperature.

## A PhD project built from the results of other projects



# Scope

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eads(nbt)

# **Continuous Roll forming**

### **Process description**

A metal strip is incrementally bent by sets of rolls (called "forming stands") until the desired cross section is obtained

→ Key advantage: OK for Advanced High Strength Steels



FE Modelling of roll forming is essential (roll design, prediction of defects, residual stresses, springback, etc.) ... but very time-consuming!

# **Continuous Roll forming**

# Forming of a rocker panel (closed section)



# **Continuous Roll forming**

# 

Drawbacks of Lagrangian modelling

In a Lagrangian model, the continuous strip is modelled by a sheet of limited length.

ArcelorMitto

- Non-realistic boundary conditions or friction coefficents to make the sheet move.
- The sheet hits the stands and gets sometimes blocked.

→ Incremental modifications of the geometry of the tools by trial and error.

How to model the welding and post-cut operation?

The setup of the Lagrangian model is **very tricky** and time-consuming!
### Initial ALE mesh: interpolation of the flower diagram



### Modelling of inline welding in ALE

- Actual physics in the welding process is **heavily simplified**.
- The initial mesh is built as a closed mesh.





### Modelling of the post-cut operation in ALE

• Aims:

75

- release the final product from the forming rolls
- Accurate computation of the springback
- **Perfect cut-off** is **assumed**: deactivate the finite elements located inside the roll-forming machine.
- Switch from ALE to **purely Lagrangian** formalism.
- Implicit dynamic integration scheme with viscous damping to kill out the oscillations.





### View of ALE results from a downstream point of view



		Equivalent plastic strain		
0	0.0611604	0.122321	0.183481	0.244642

### **Comparison to Lagrangian results**



#### Longitudinal strain along the 2 edges

- ALE and Lagrangian curves are very **similar**, except in the inlet region.
- Maxima values are close to each other.

### Influence of the welding operation and analysis of the final section





Shape defects predicted by the model:

- Bending radii in the lower part are much larger than the desired ones.
- Upper part is not perfectly planar.

### Analysis of the final shape of the cut-to-length strip



Shape defects predicted by the model:

- A slight longitudinal **bow defect** appears after post-cut.
- No significant twist defect (torsion)

### A project built from the results of other projects



## Scope

#### void mxv

#pra

for

# Practical Management of Simulation Codes Metafor... from 1992 to 2018

### 2. Numerical Applications

- Introduction to ALE formalism
- Thixoforming
- Continuous Roll forming
- Friction Stir Welding
- Additive manufacturing

### 3. Conclusions

eads(nbt)

### **Process description**

- Solid-state joining process → better than classical welding.
- Tprocess < Tmelting.
- Non-consumable tool.
- Mechanical intermixing + friction heating.
- Well suited for alloys with low fusion temp.





### FSW modelling with the ALE formalism

#### Mesh management – 3 zones

- 1. The mesh moves with the tool ALE formulation (red)
- 2. Remeshing (transition zone white)
- 3. Fixed mesh Eulerian formulation (grey)







P Bussetta

### FSW (ALE) – Example of mesh motion



Constitutive law:

Norton-Hoff 
$$S = 2\mu D \left(\sqrt{3}\sqrt{\frac{2}{3}D}: D\right)^{m-1}$$



### Comparison between a solid and a fluid approach



collaboration with UPC, Barcelona

#### Fluid approach – COMET (UPC)



#### **Solid approach** – Metafor (ULiège)

unknowns: displacements, temperature

### Comparison between a solid and a fluid approach



• Temperature evolution is similar with both approaches.



### Residual stresses with the solid approach

#### Plates (AA2024): thermo-elasto-viscoplastic

 $\sigma_{y} = \sigma_{0}(T) + A(T)\left(1 - e^{\xi \overline{\varepsilon}}\right) + K e^{\frac{mQ}{RT}} \dot{\varepsilon}^{m}$ 

Sonne et al (2013) JMPT 213

- ξ = 25
- K = 1.5 MPa s<sup>m</sup> (viscosity parameter)
- m = 0,12 (strain rate sensitivity parameter)
- Q = 155 kJ/mol (activation energy)
- Young modulus = E(T)
- Poisson ratio = 0.33



#### Stresses & temp. during the process



### Residual stresses with the solid approach

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#### Stresses & temp. after the process and cooling



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### **Context and challenges**

- New PhD thesis started a few months ago: Very first model of an laser solid forming with Metafor.
- The thesis focuses on mesh and geometry management.
- Material law?
  - for now: thermal calculations only.
  - future: reuse of the constitutive law developed in the frame of thixoforming.
    Reference results from Chiumenti et al.
  - Can we extend the "element deletion" algorithm (developed to compute cracks) to an **"element addition" algorithm**?





Thermal study of an AM process using Laser Solid Forming of Ti-6Al-4V metal powder



C. Laruelle

### Mesh management technique

#### Computation of new active mesh and boundary conditions



- Finite elements and boundary conditions are all created and deactivated at the start of the simulation.
- Activation/Deactivation of finite elements and boundary conditions based on the current laser position.

### Numerical results – Time evolution of the temperature field

step 0 1=0/1586.58 ctt=0



### *Results – comparison with literature*





Good agreement of the temperature evolution between COMET, Metafor and experimental measurements.



### A project built from the results of other projects



## Scope

#### void mxv

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for

## 1. Practical Management of Simulation Codes

• Metafor... from 1992 to 2018

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eads(nbt)

## Conclusions

- The development of complex models/algorithms is always the **sum of the work of many researchers**.
- Keeping their source code clean, effective, reliable, robust and easily extensible is a difficult task which is **usually underestimated** in the academic world.
- A lot of simulation codes are **continuously lost** and projects based on previous work do not reach their goals.
- The presented tools and the resulting methodology have the advantage to be rather simple and allow the researchers to spend more time on "science" and less time on "coding".