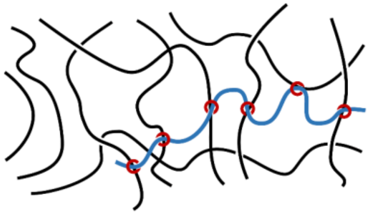
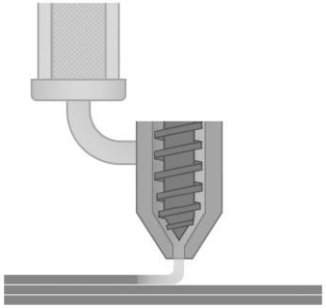
Rutledge Group Meeting
December 5, 2022

Application of the Sliplink model in polymer extrusion-based 3D printing





Visiting Student: **Daniel Silva**

Visit Supervisors: **Profesor Gregory C. Rutledge, Ph.D.**
Marat Andreev

Massachusetts Institute of Technology ChemE

POLITÉCNICO DE LEIRIA
CDRSP CENTRE FOR RAPID AND SUSTAINABLE PRODUCT DEVELOPMENT

Universitat Autònoma de Barcelona

Outline

- Personal Background
- Research Center Presentation
- 3D Printing
- Opportunity
- Previous Studies
- Motivation
- Project Idea
- Using the Sliplink Model
- Results and Discussion
- Conclusions and Future Work

Outline

- Personal Background
- Research Center presentation
- 3D Printing
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Background

- Mechanical Engineering

↓

- Manufacturing Work Experience

↓

- **Research in Design and Manufacturing**

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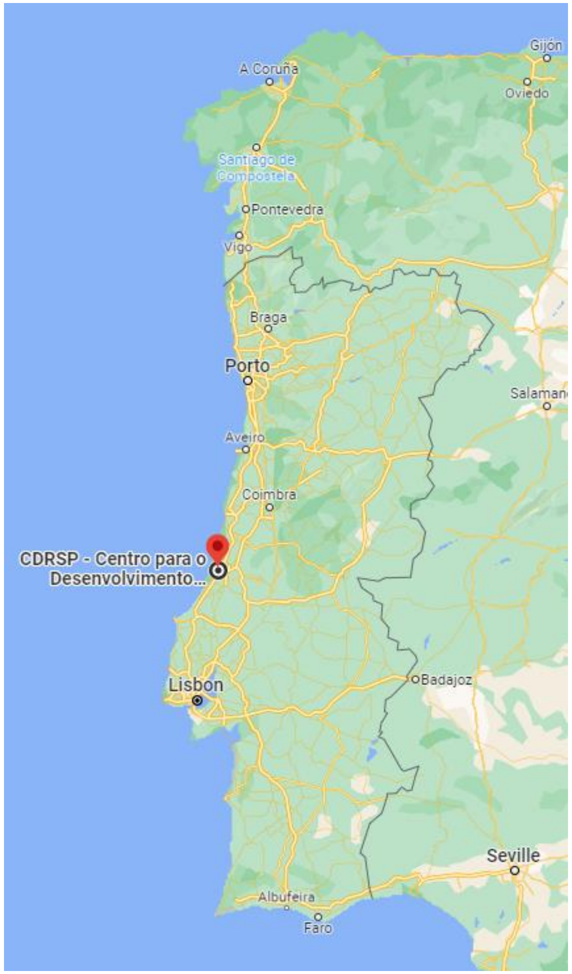

Background

- Doctoral Program in Materials Science

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UAB Universitat Autònoma de Barcelona

- Exploratory Project in 3D Printing

MIT Portugal

FCT Fundação para a Ciência e a Tecnologia + MIT Massachusetts Institute of Technology

CDRSP - What we do?

- Academic Research and Training
- Joint projects with companies

Within one of the largest **mould making** clusters

CDRSP - What we do?

- Academic Research and Training
- Joint projects with companies

→ Within one of the largest **mould making** clusters

Key Topics:

✓ Emerging Technologies in Manufacturing

  ○ Additive Manufacturing

✓ Materials → Biopolymers, Smart Materials, Metamaterials

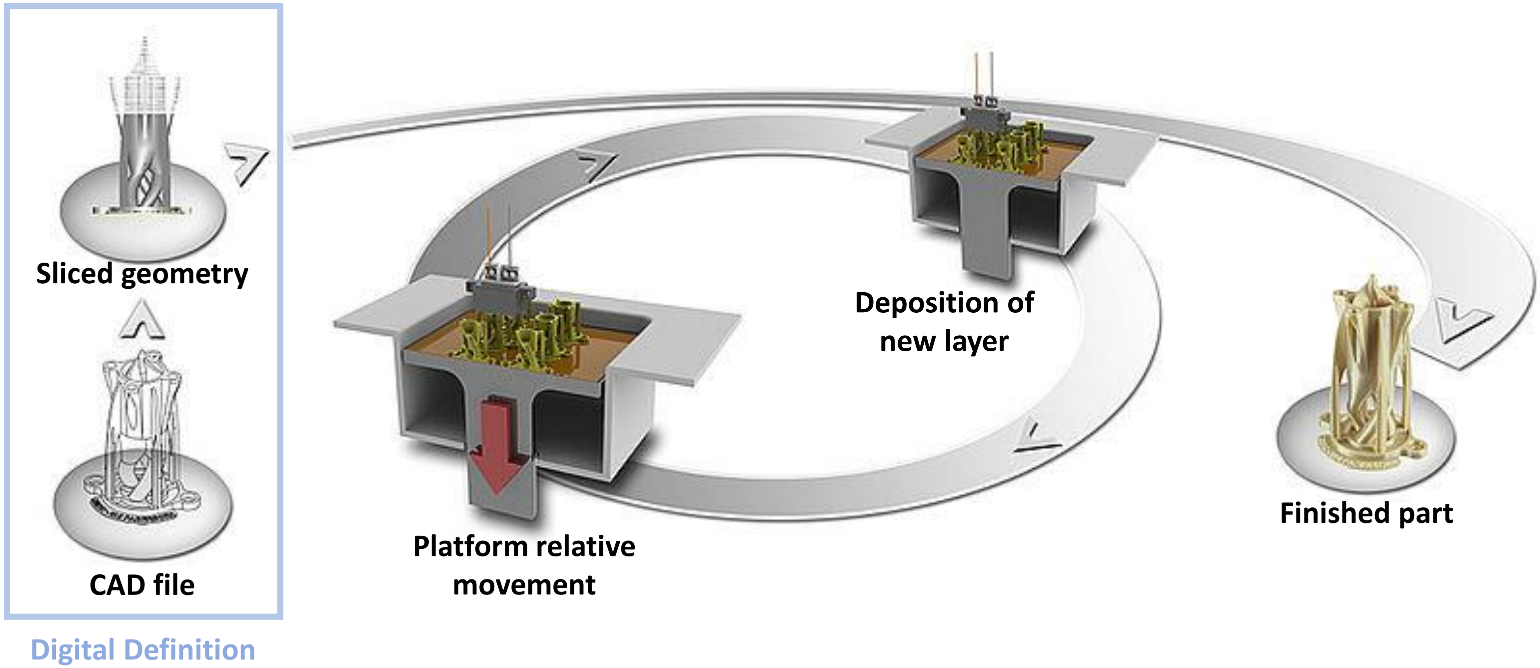
✓ Biomedical Applications

✓ Sustainability

✓ Circular Economy

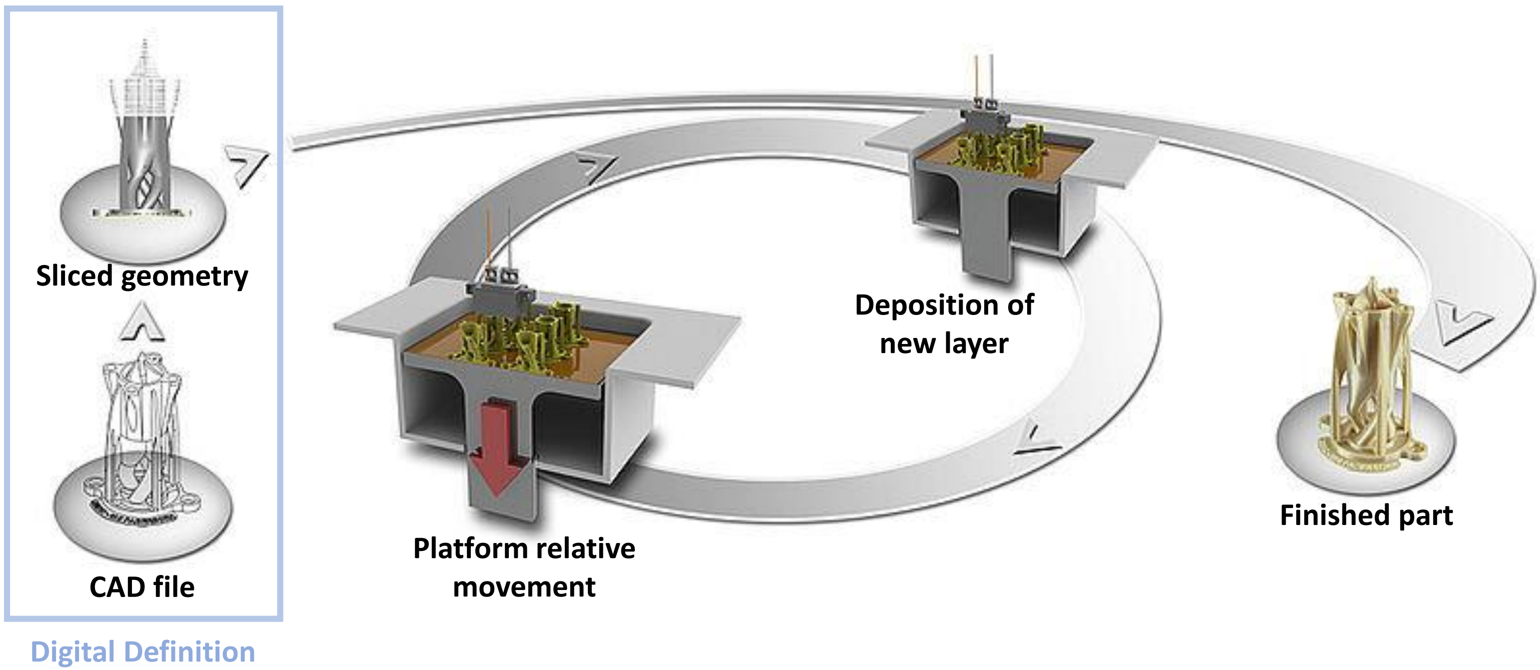
What we do?

Direct Digital Manufacturing (DDM)



What we do?

Direct Digital Manufacturing (DDM)



CDRSP is the lead institute in the **PAMI** - Portuguese Additive Manufacturing Initative project

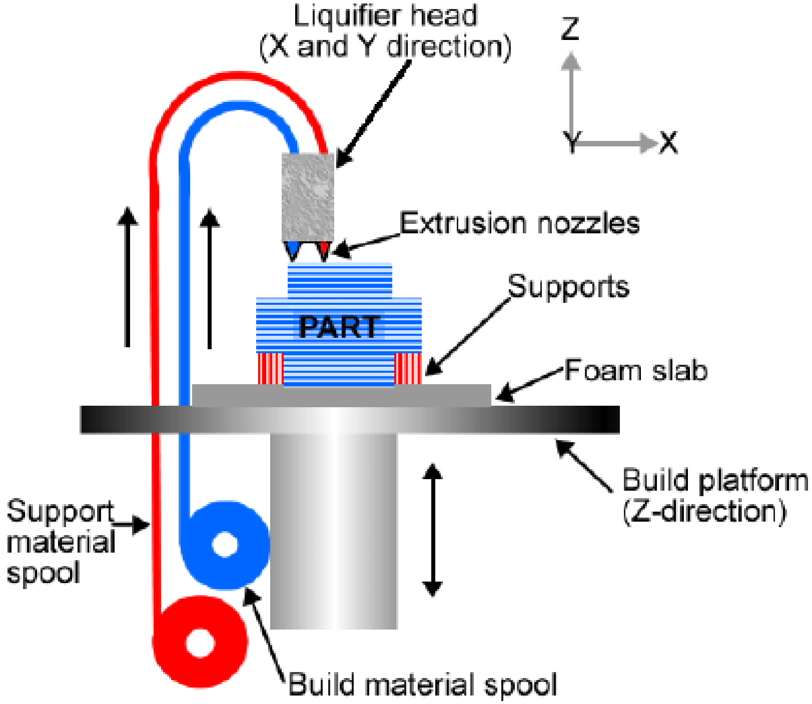
What we do?

Extrusion-based 3D Printing

Scott Crump, founder of Stratasys, invented Fused Deposition Modelling (FDM), or 3D printing in 1989.

What we do?

Extrusion-based 3D Printing



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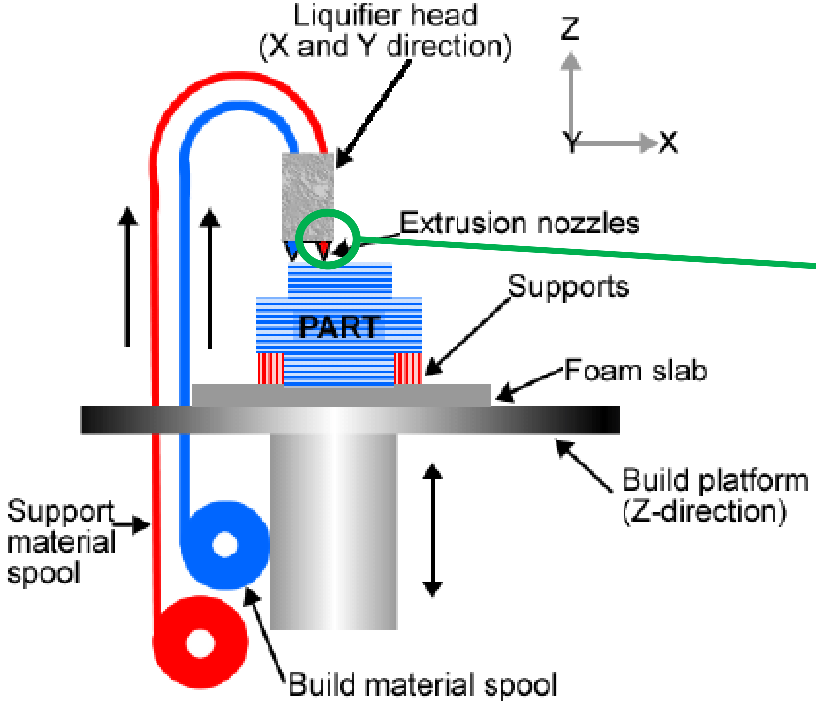
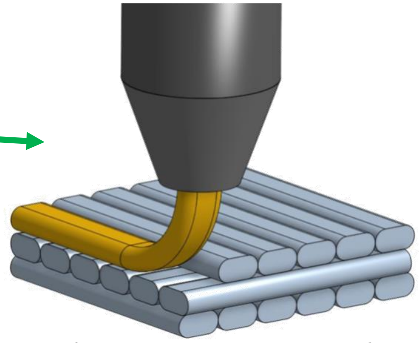
What we do?

Extrusion-based 3D Printing





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What we do?

Examples

Polymers

What we do?

Examples

Polymers

Metals

What we do?

Examples

Polymers

Metals

Ceramics

What we do?

Examples

Polymers

Metals

Ceramics

What we do?

Fields of Application

What we do?

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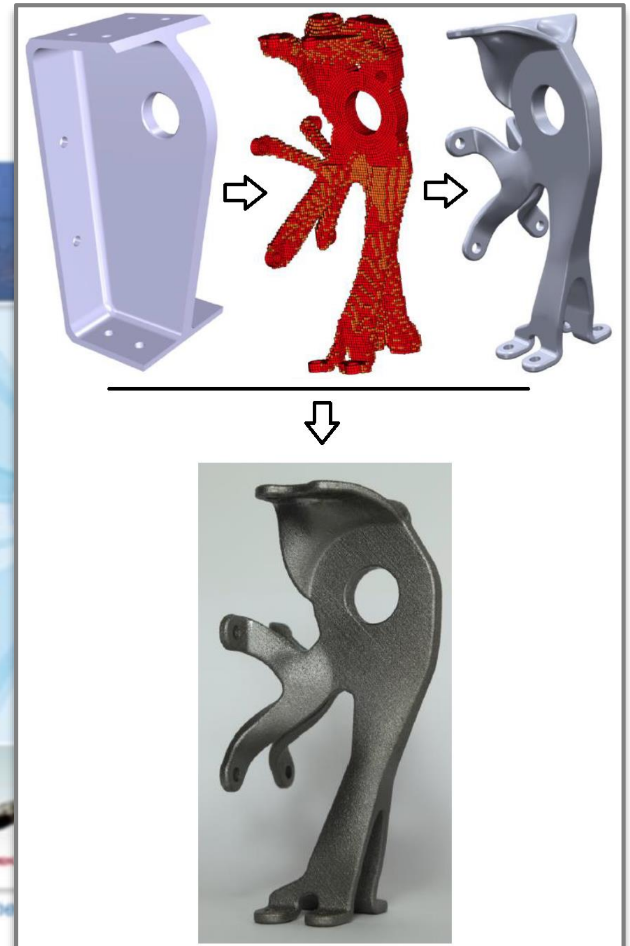
What we do?

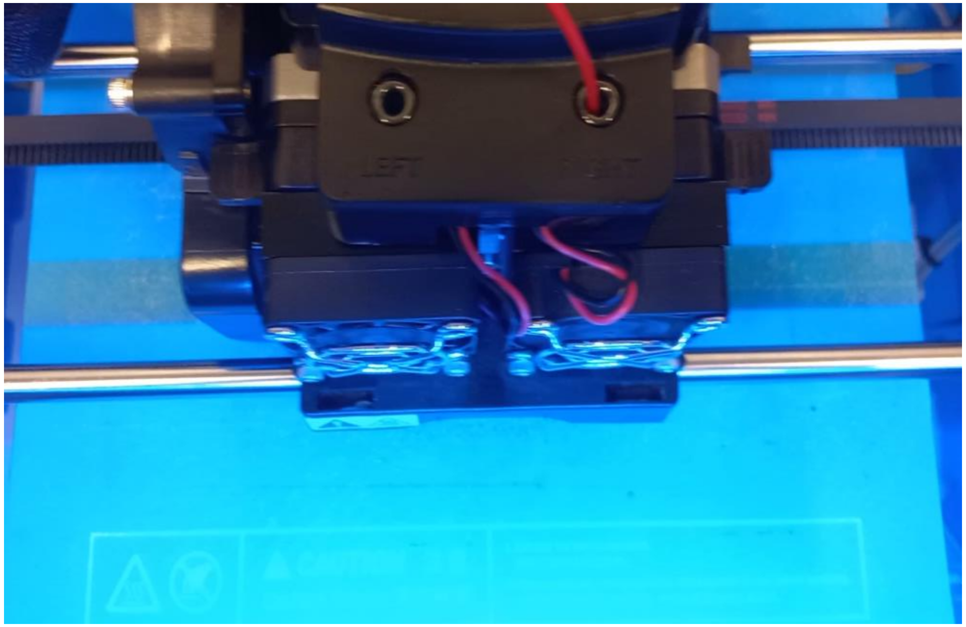
Fields of Application



What we do?

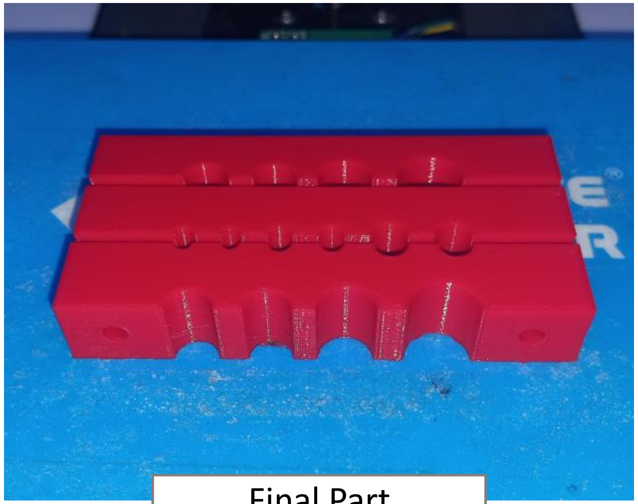
Example – Jig

FDM fabrication with PLA

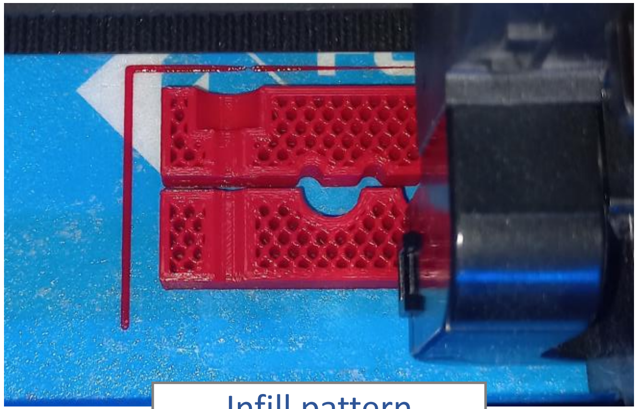


What we do?

Example – Jig



Final Part

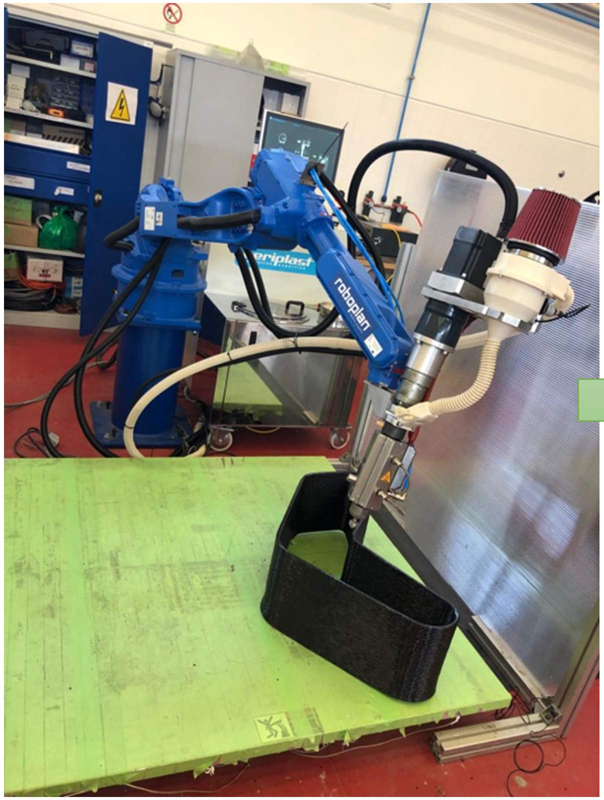


Infill pattern

Jig Fitting

What we do?

Example – Big parts



What we do?

<u>Example</u> – Big parts

More information

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Reserch Center

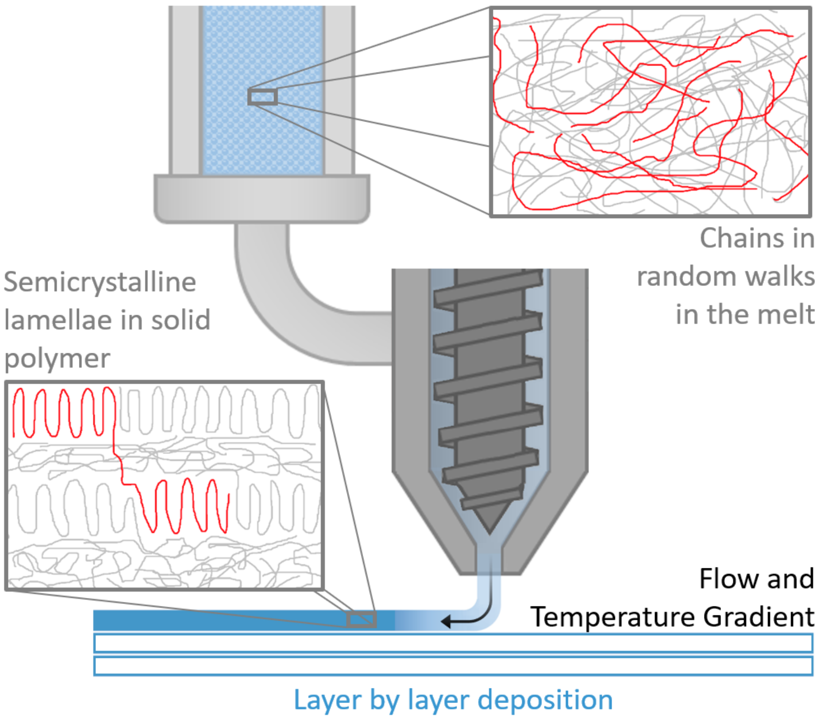
https://cdrsp.ipleiria.pt/

The 3D printing revolution - Documentary

https://www.youtube.com/watch?v=k0poVtBhIsQ

Project Idea - Origin

"Any processing operation applied to a polymer may have both chemical and physical effects on the material." – Roger T. Fenner, Principles of Polymer Processing, The Macmillan Press, 1979, pp. 15 ISBN 0-8206-0285-X



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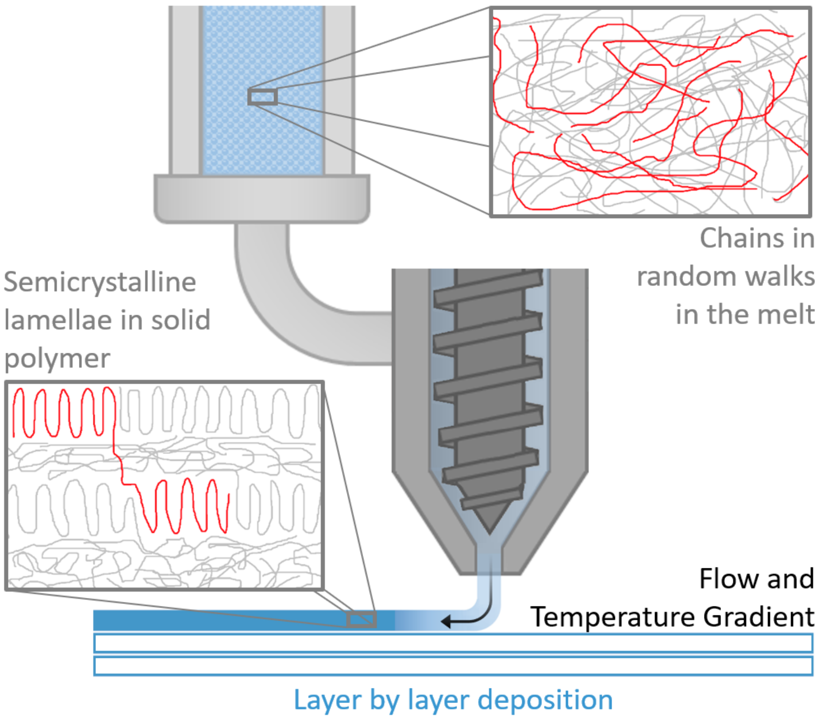

Material property mapping during manufacturing

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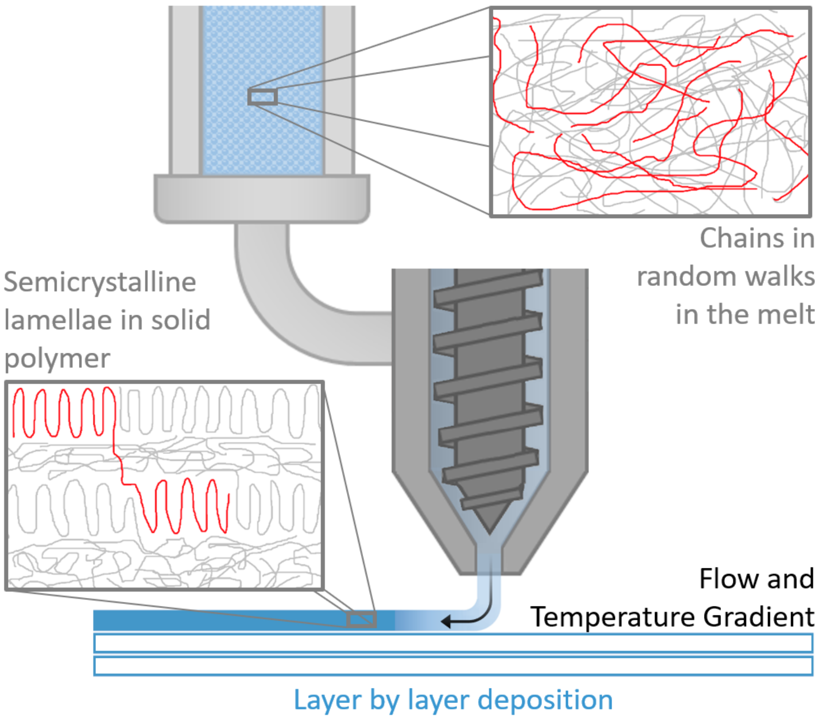


Material property mapping during manufacturing

Single Material → Different Behaviors

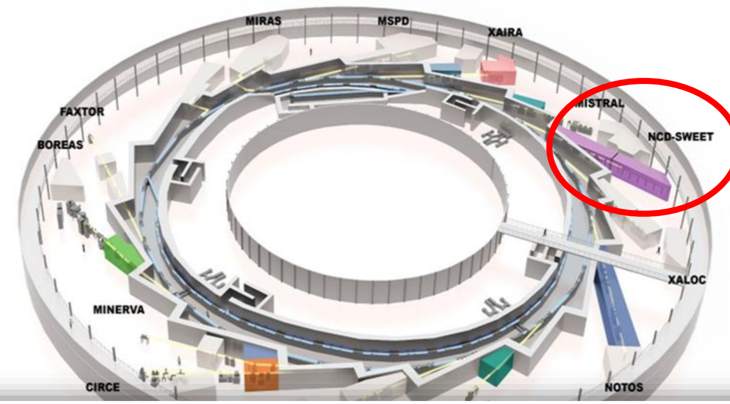
Project Idea

- How to monitor the changes in the material?
- How far can we change the material behavior under a certain load?
- Can we predict the behavior of the material after production?

Previous Studies

ALBA

ALBA Synchrotron, Barcelona - Spain



polymers MDPI

Article

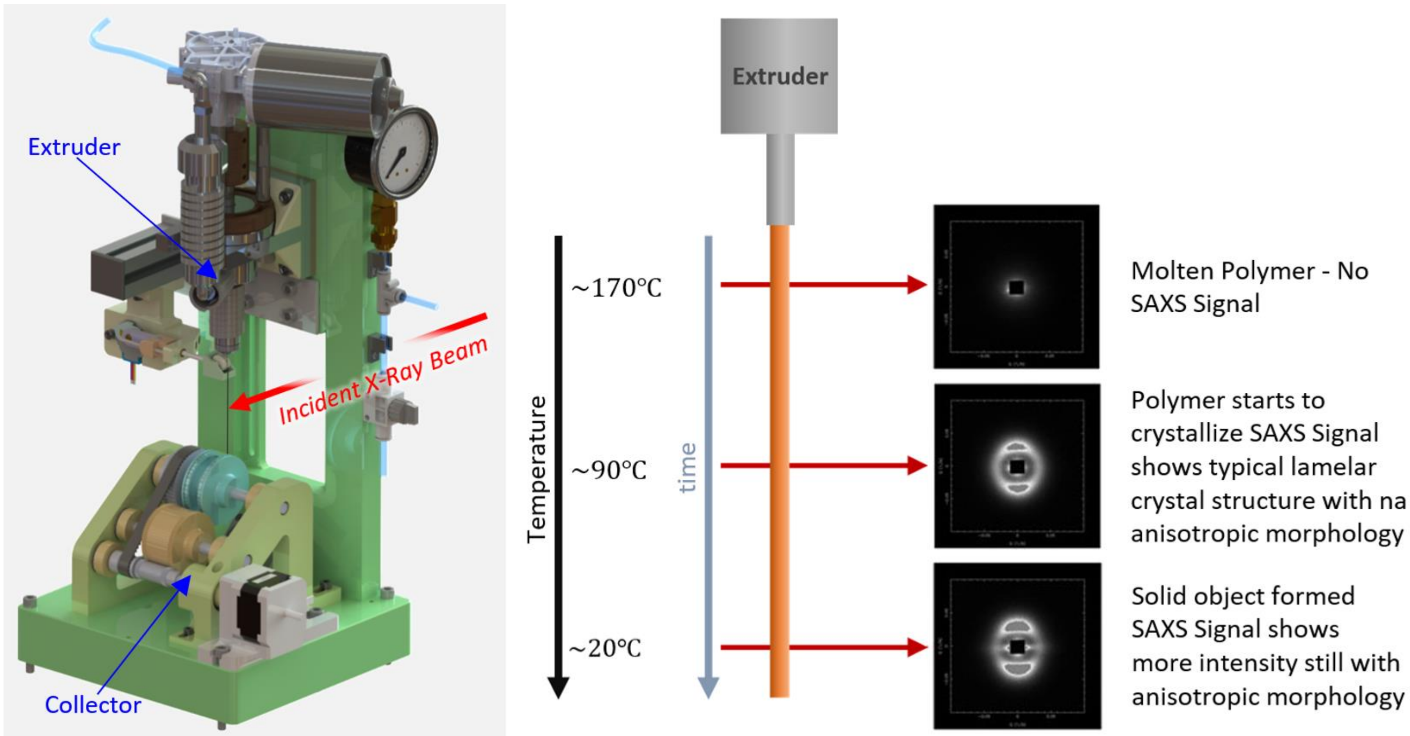
Changing the Paradigm-Controlling Polymer Morphology during 3D Printing Defines Properties

Daniel P. da Silva [1], João Pinheiro [1], Saba Abdulghani [1], Christina Kamma Lorger [2], Juan Carlos Martinez [2], Eduardo Solano [2], Artur Mateus [1], Paula Pascoal-Faria [1] and Geoffrey R. Mitchell [1,*]

1 Centre for Rapid and Sustainable Product Development, Polytechnic of Leiria, 2430-080 Marinha Grande, Portugal; daniel.p.silva@ipleiria.pt (D.P.d.S.); joao.d.pinheiro@ipleiria.pt (J.P.); saba.abdulghani@nms.unl.pt (S.A.); artur.mateus@ipleiria.pt (A.M.); paula.faria@ipleiria.pt (P.P.-F.)

2 NCD-SWEET Beamline, Alba Synchrotron Light Source, Cerdanyola del Vallès, 08290 Barcelona, Spain; ckamma@ansto.gov.au (C.K.L.); guilmar@cells.es (J.C.M.); esolano@cells.es (E.S.)

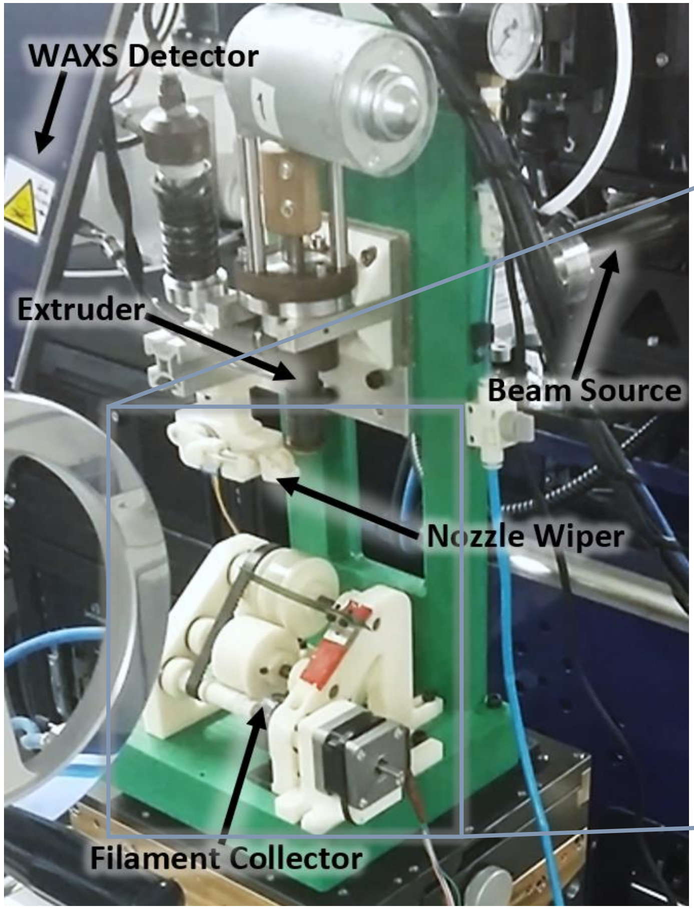
Previous Studies

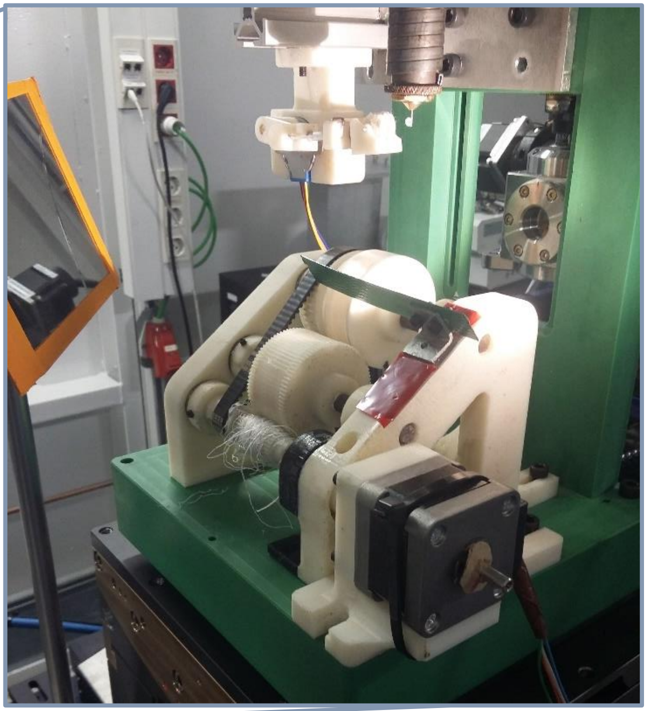


- Point measurements on the Z direction, observing the polymer scattering **as it crystallizes**;

- Static extrusion means that measurements along the Z axis relate to the **evolution in time**.

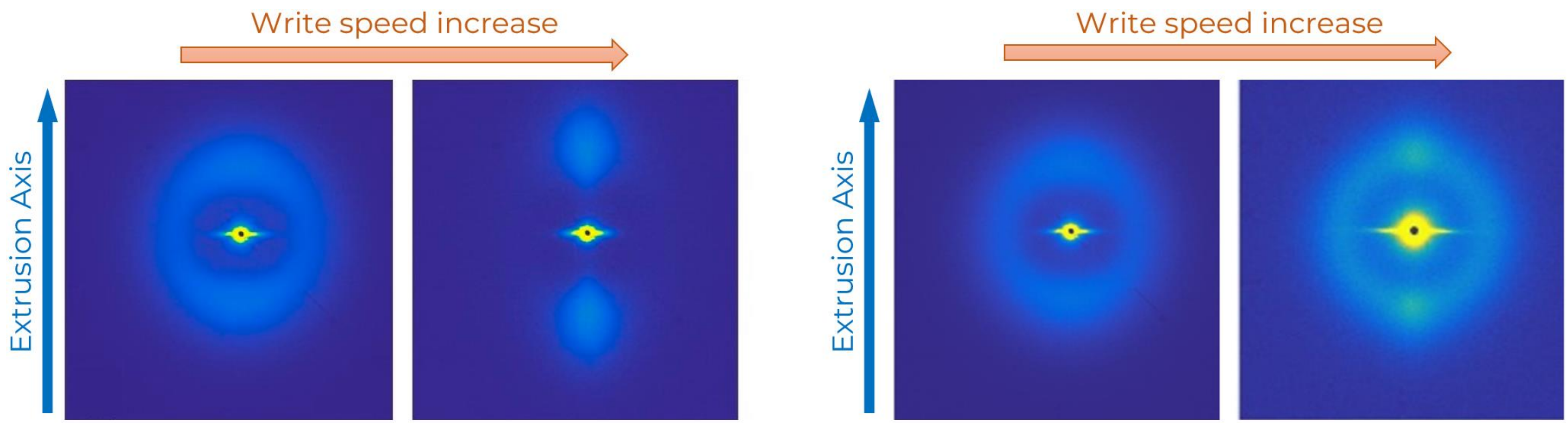
Previous Studies





Previous Studies

SAXS patterns obtained at different write speeds



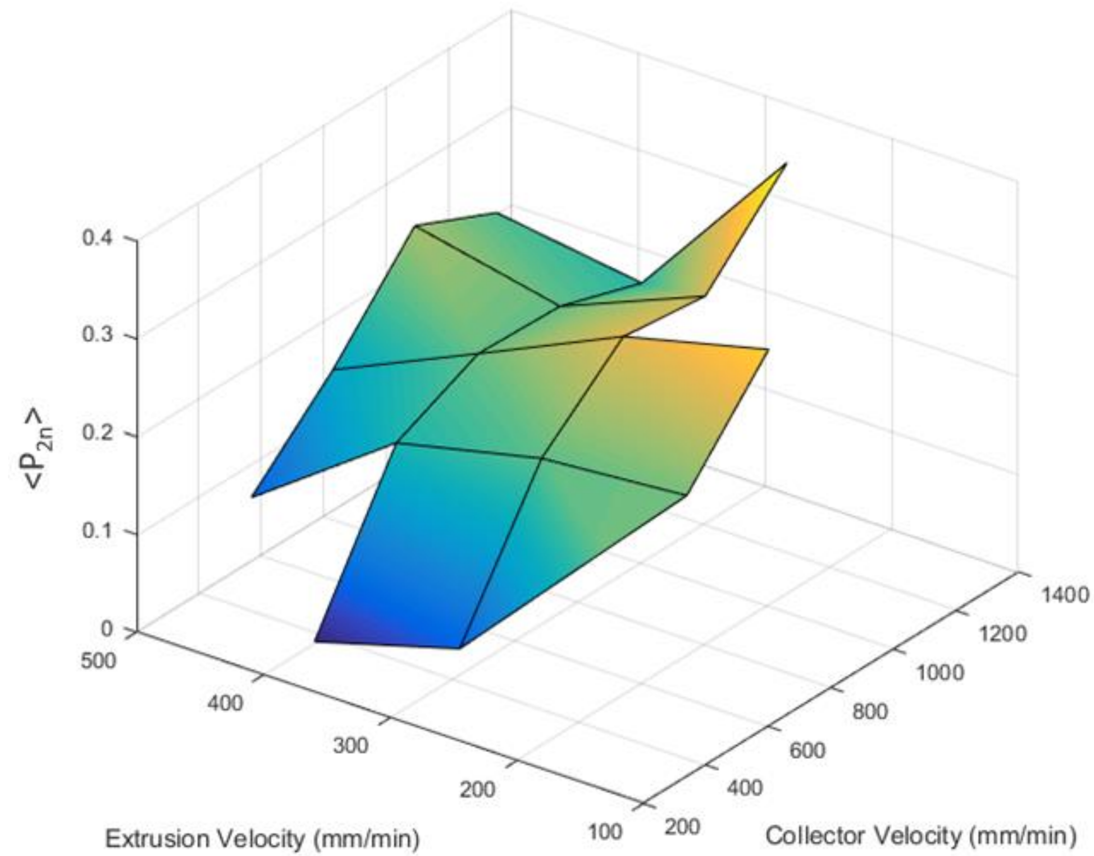
Low-density Polyehtylene

Poly(ε-caprolactone)

Extended chains during crystallization…

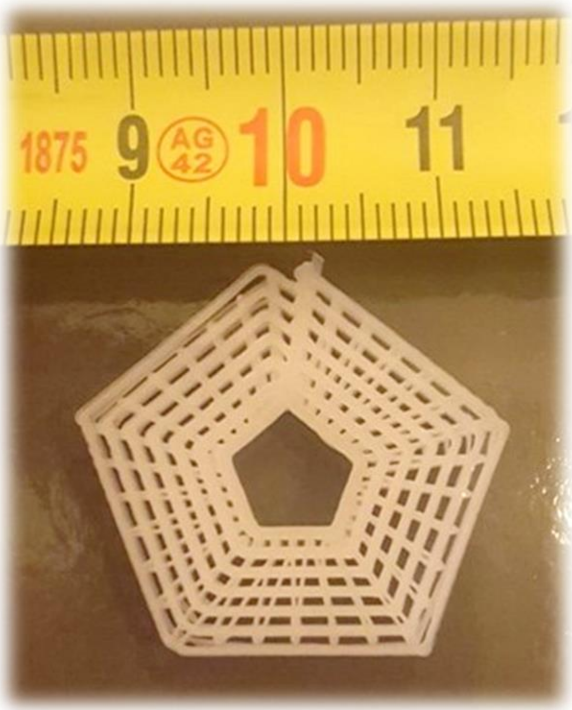
Previous Studies

Orientation Parameter < P_{2n}>



P_{2n} = 1 → uniform orientation of crystals

Proof of Concept

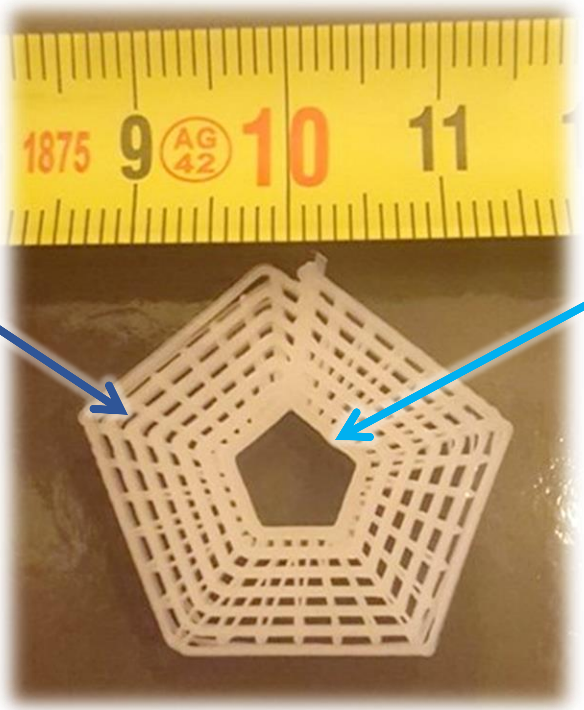


Deposition velocity proportional to radial distance

Proof of Concept

Higher print speed

Lower print speed



Deposition velocity proportional to radial distance

Motivation

- Doctoral Program in Materials Science

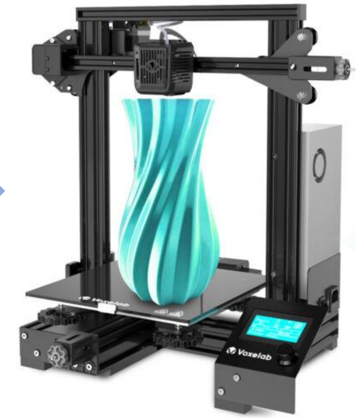
Degradation
during Recycling

Polyethylene as
the world's most
used polymer.

Source: Ruben Demets, et al.; Addressing the complex challenge of understanding and quantifying substitutability for recycled plastics.

Property Mapping

Monomaterial
Design and Printing

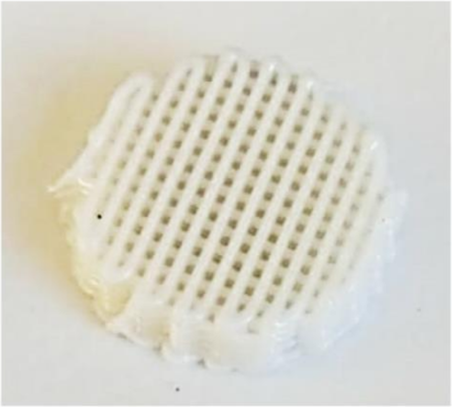


Same material,
Different responses!
Increasing reliability.

High Recyclability

Motivation

- Exploratory Project in 3D Printing - Case Study



Biodegradability:
Requirement and
Constraint

Project Idea

- How to monitor the changes in the material?
- How far can we change the material behavior under a certain load?
- Can we predict the behavior of the material after production?

Multiscale Simulation

Project Idea

- How to monitor the changes in the material?
- How far can we change the material behavior under a certain load?
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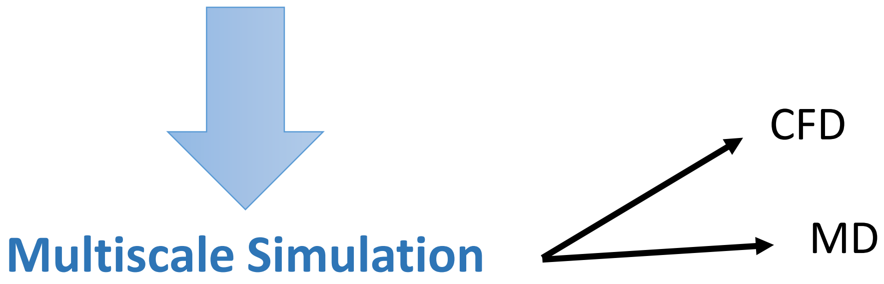

Project Idea

- How to monitor the changes in the material?
- How far can we change the material behavior under a certain load?
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Multiscale Simulation → CFD, MD

- Material Characteristics
  - Process Parameters

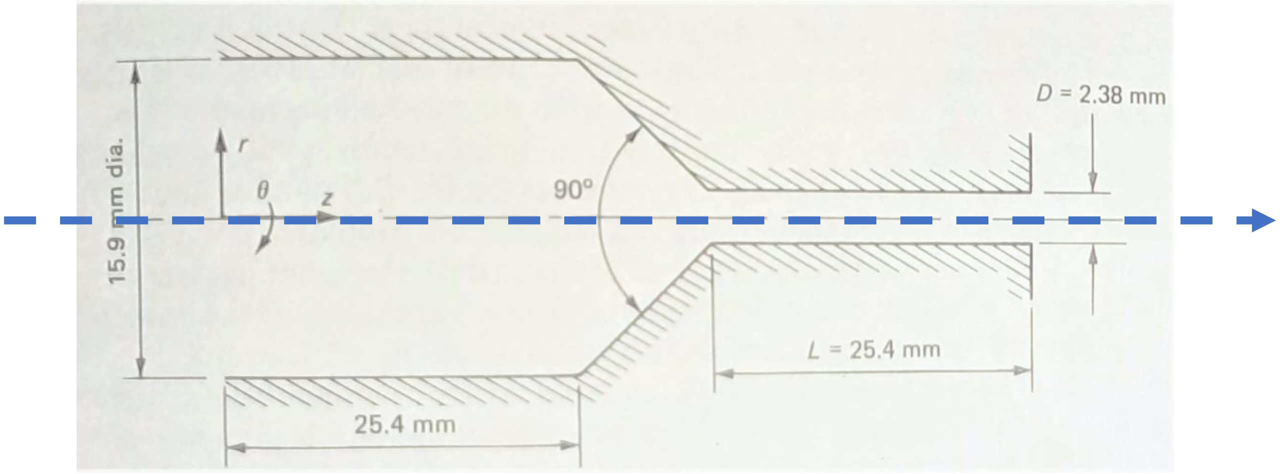
Deformation → **Sliplink Model** → Stresses

- Conformation Tensor – C

Project Idea

Originally:

- Modelling polymer flow and crystallization.
- Analysis of the elastic modulus of a partially cristalized poylmer melt.



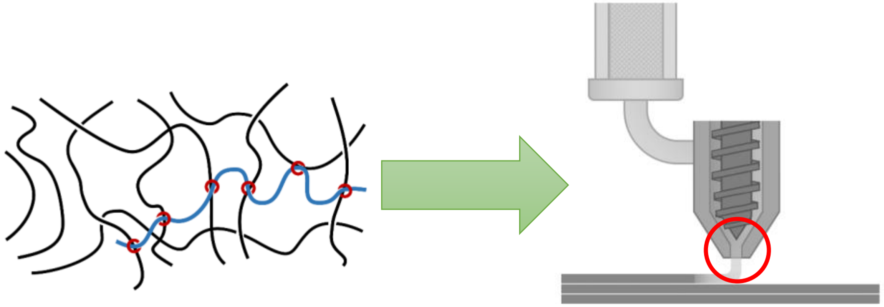
Adapted from: Roger T. Fenner, Principles of Polymer Processing, The Macmillan Press, 1979, ISBN 0-8206-0285-X

Project Idea

3 Months Visit

Learning how to use the Sliplink Model

Application in 3D Printing!



Project Idea

New plan:

- Simulation for printability assessment

Flowability	Buckling	Shape Stability	Die Swell	Interlayer Adhesion

polymers MDPI

Article

FDM Printability of PLA Based-Materials: The Key Role of the Rheological Behavior

Rossella Arrigo * and Alberto Frache

Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, Viale Teresa Michel 5, 15121 Alessandria, Italy; alberto.frache@polito.it
* Correspondence: rossella.arrigo@polito.it; Tel.: +39-0131229363

Abstract: Fused deposition modeling (FDM) is one of the most commonly used commercial technologies of materials extrusion-based additive manufacturing (AM), used for obtaining 3D-printed parts using thermoplastic polymers. Notwithstanding the great variety of applications for FDM-printed

Project Idea

New plan:

- Simulation for printability assessment

Flowability	Buckling	Shape Stability	Die Swell	Interlayer Adhesion

Flowability → Shear Thining

polymers MDPI

Article

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Abstract: Fused deposition modeling (FDM) is one of the most commonly used commercial technologies of materials extrusion-based additive manufacturing (AM), used for obtaining 3D-printed parts using thermoplastic polymers. Notwithstanding the great variety of applications for FDM-printed

Project Idea

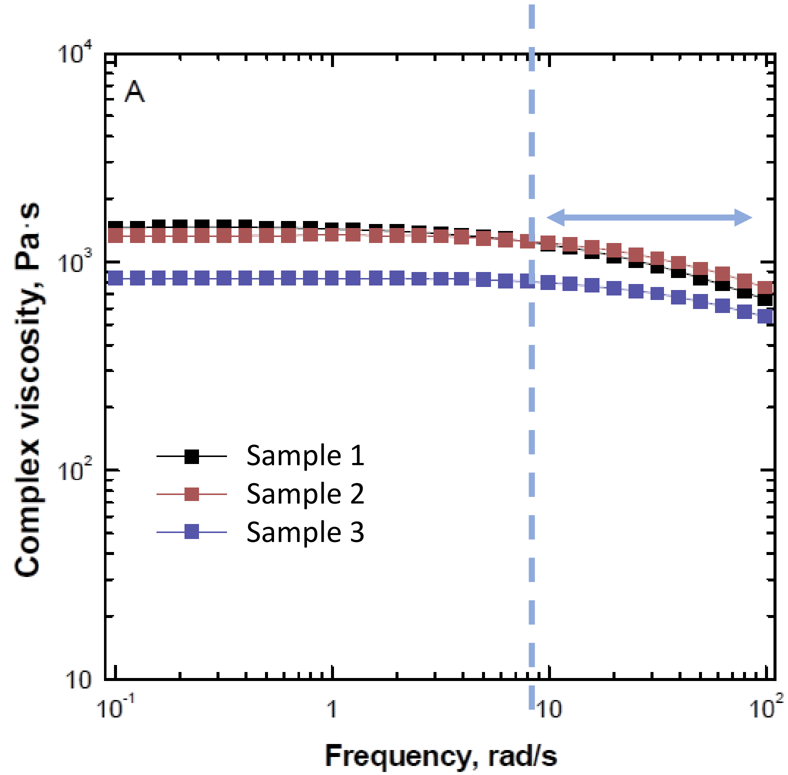
Shear thining given by ***n*** in the Carreau Model:

$$\eta(\omega) = \eta_0[1 + (\lambda\omega)^2]^{\frac{\boldsymbol{n}-1}{2}}$$

$\boldsymbol{n} \in [0; 1]$ in pseudo-plasticity domain

$\boldsymbol{n} \downarrow \rightarrow$ shear thining $\uparrow$

Experimental Data →



Project Idea

Shear thining given by ***n*** in the Carreau Model:

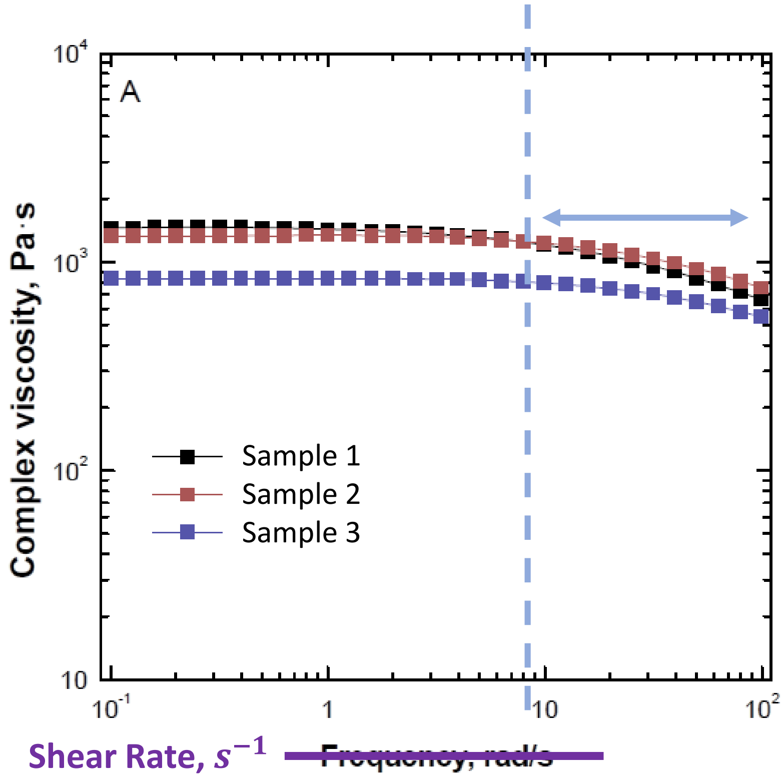
$$\eta(\omega) = \eta_0[1 + (\lambda\omega)^2]^{\frac{n-1}{2}}$$

$$\eta(\dot{\gamma}) = \eta_0[1 + (\lambda\dot{\gamma})^2]^{\frac{n-1}{2}}$$

$n \in [0; 1]$ in pseudo-plasticity domain

$n \downarrow \rightarrow$ shear thining $\uparrow$

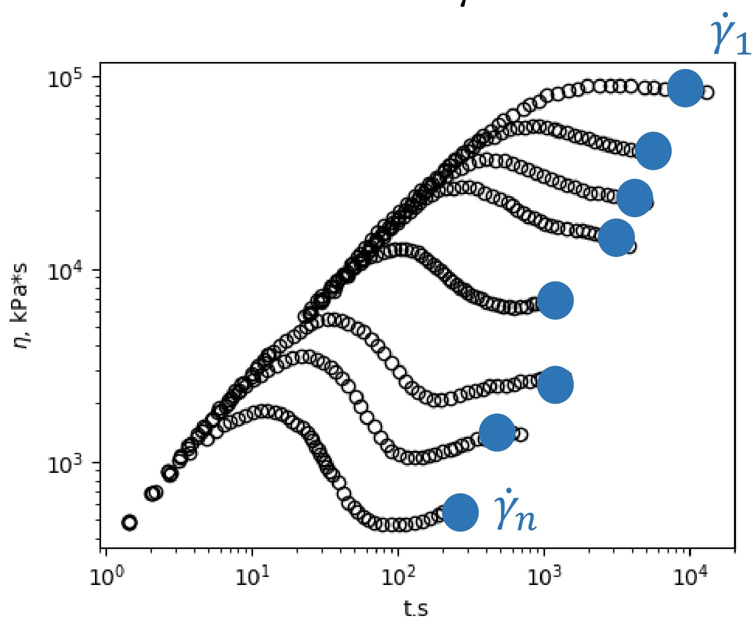
~~Experimental~~ Data
Simulation



Project Idea

- Obtainment of the <u>Flow Curves</u>

$$\eta(t) = \frac{\sigma_{xy}(t)}{\dot{\gamma}}$$



$\eta_S \equiv Steady\ State\ Viscosity$

Plot $\boldsymbol{\eta_S}$ as a function of $\dot{\boldsymbol{\gamma}}$

↓

Mean value
of Viscosity

Project Idea

Input variables

- Material: Polyisoprene (PI)

$$M_w = 94.9\ kg/mol$$

$$N_s = 46$$

$$\tau_S @ 25°C = 0.1 s$$

- $T = 200°C$

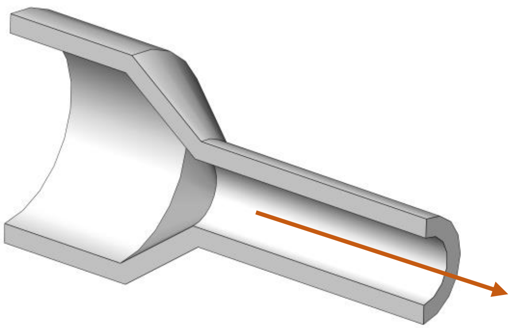
- $\dot{\gamma}$ = ?

Using the model

Input variables

Shear rate for a circular capillary die:

$$\dot{\gamma}_w = \frac{4Q}{\pi r^3}\left(\frac{3f+1}{4f}\right)$$

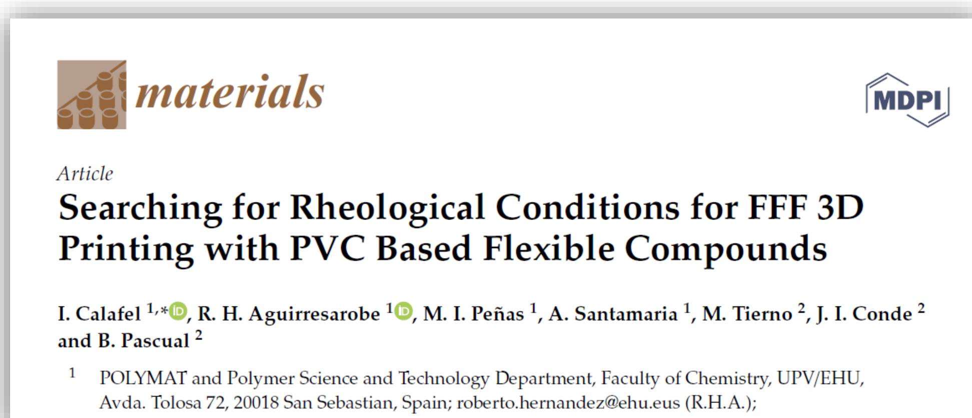


$\dot{\gamma}_w \equiv shear\ rate\ at\ the\ wall\ [s^{-1}]$

$f \equiv profile\ shape\ index \quad (f < 1)$

$Q \equiv volumetric\ flow\ rate\ \left[{m^3}/{s}\right]$

$$Q = \pi R^2 v_p$$



materials

MDPI

Article

Searching for Rheological Conditions for FFF 3D Printing with PVC Based Flexible Compounds

I. Calafel [1,*], R. H. Aguirresarobe [1], M. I. Peñas [1], A. Santamaria [1], M. Tierno [2], J. I. Conde [2] and B. Pascual [2]

1 POLYMAT and Polymer Science and Technology Department, Faculty of Chemistry, UPV/EHU, Avda. Tolosa 72, 20018 San Sebastian, Spain; roberto.hernandez@ehu.eus (R.H.A.);

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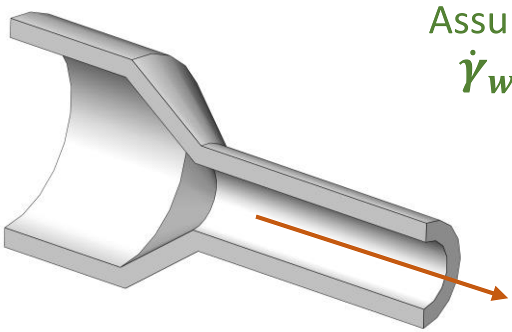

Assumption 1

$$\dot{\gamma}_w = \dot{\gamma}$$

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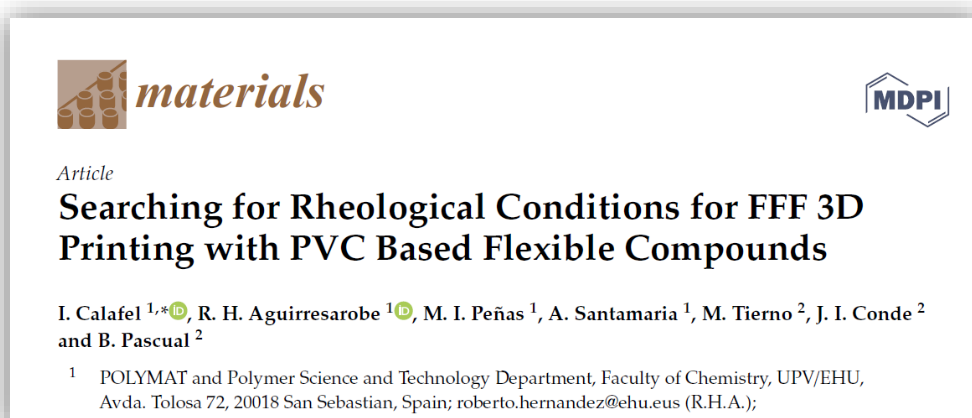
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Using the model

Input variables

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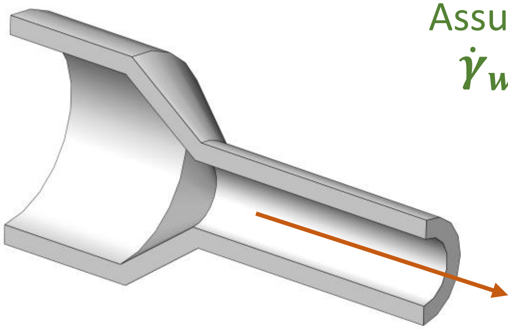


Assumption 1
$\dot{\gamma}_w = \dot{\gamma}$

$\dot{\gamma}_w \equiv$ *shear rate at the wall* $[s^{-1}]$

$f \equiv$ *profile shape index* $(f < 1)$

$Q \equiv$ *volumetric flow rate* $[m^3/s]$

$$Q = \pi R^2 v_p$$

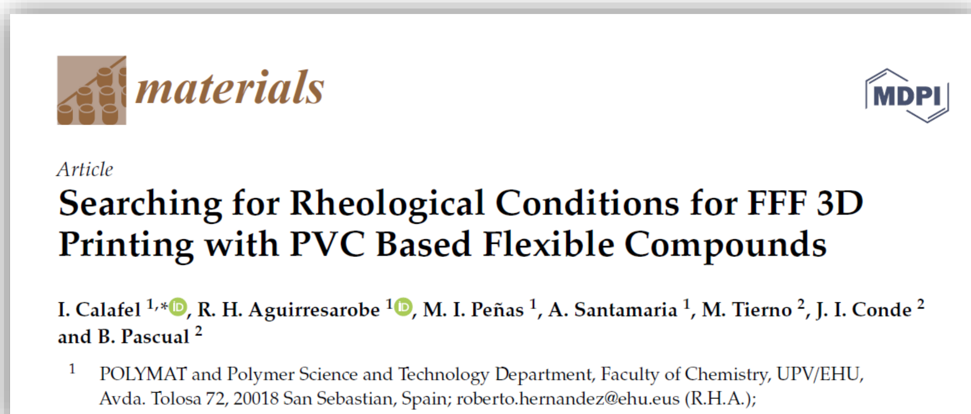
$\dot{\gamma} = 150\ s^{-1}$

For $\text{Ø} = 0{,}4mm$,

$v_p = 1{,}5mm/s$

and $f = 1$

Assumption 2



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Using the model

Procedure

1. Run the "shear_flow_exp"
   - **Time-temperature Superposition**

$$\tau_S @ 200°C$$
$$\dot{\gamma}_{sl} = \tau_S . \dot{\gamma}$$

2. "Shear_flow_dummy" edition for each shear rate

3. Job preparation and run – Cluster

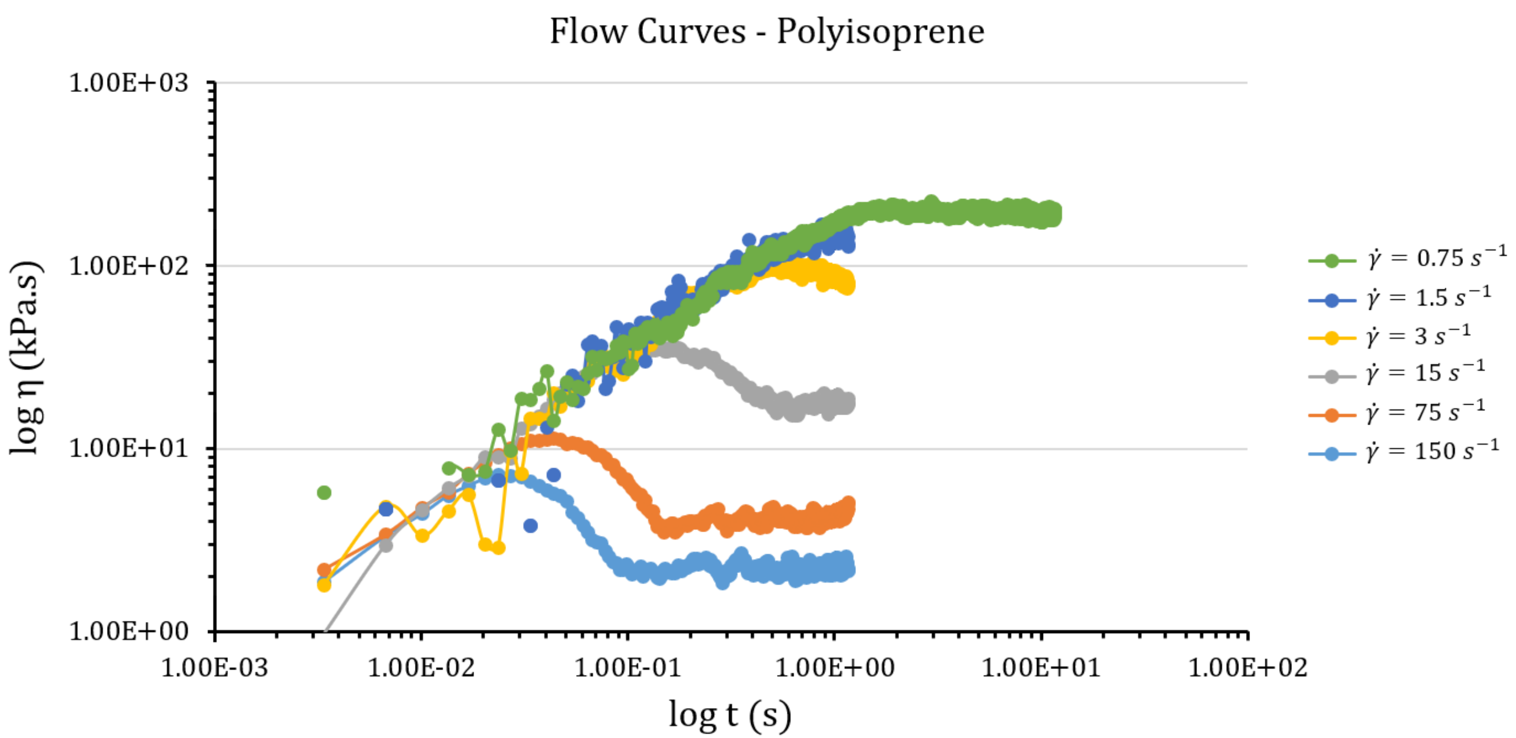
4. "Stress_aver" script run – Compilation of stress data of different output files

5. Data plotted in Excel

Using the model

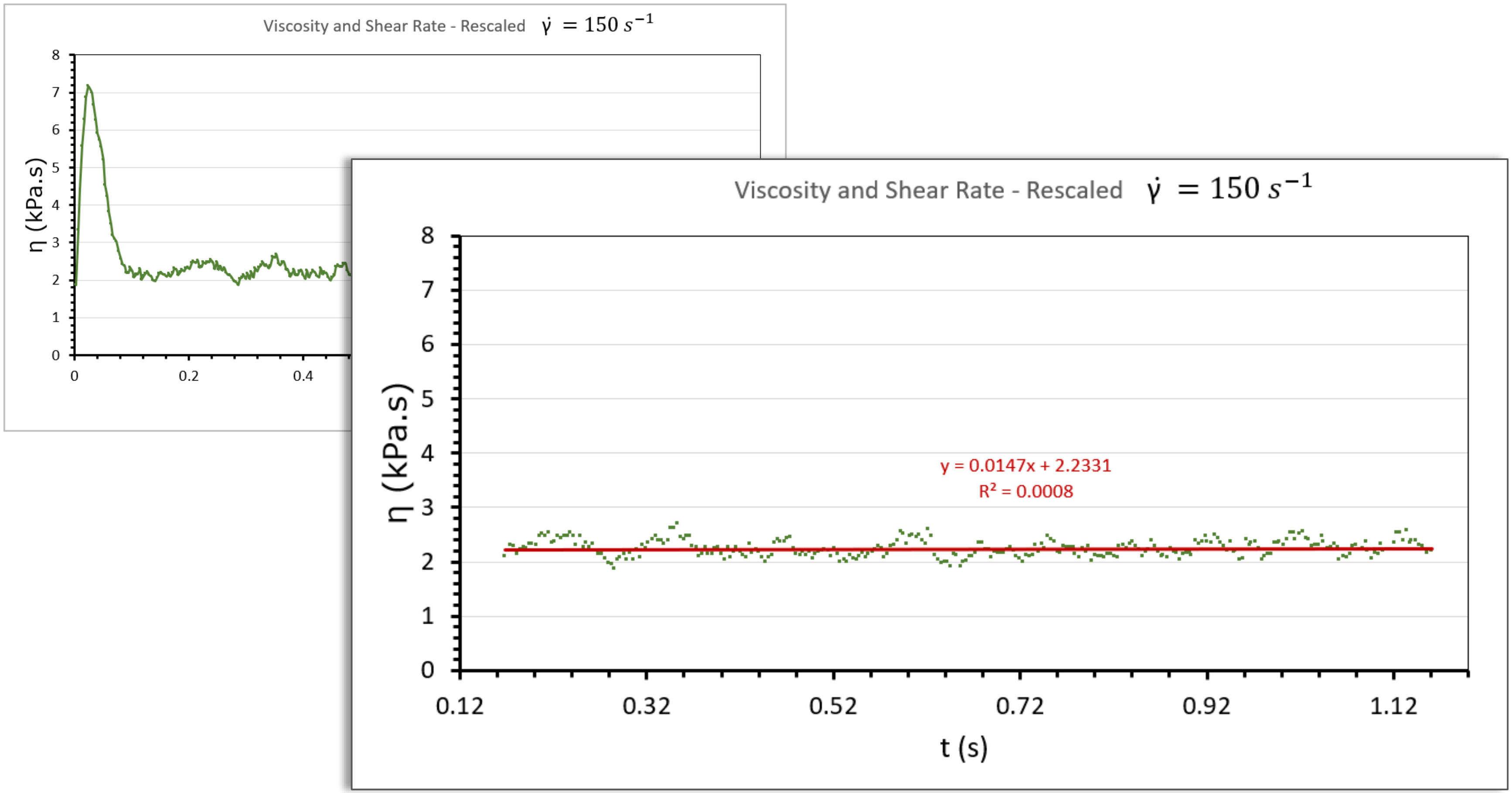
Flow curves

- 6 Simulations ran on cluster.
- Lowest shear rate → Running time ~10 min ←1000 chains | 50 chains per job



Using the model

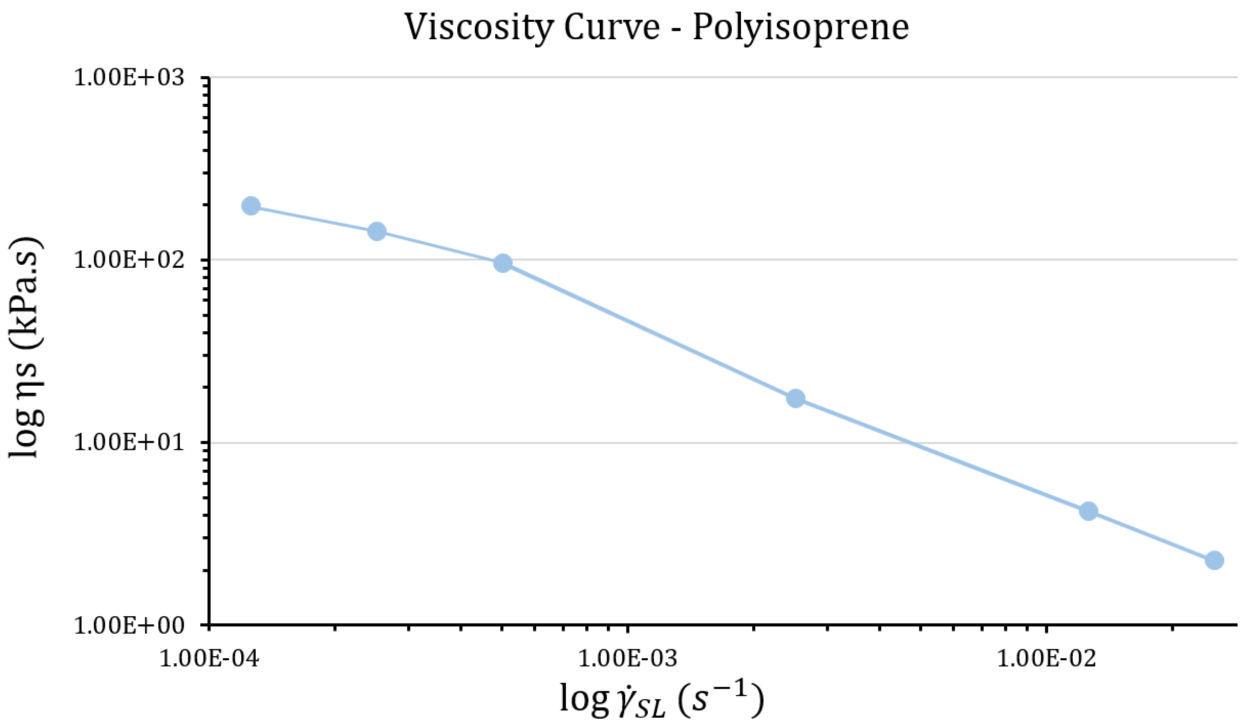
Mean value of steady state viscosity



Using the model

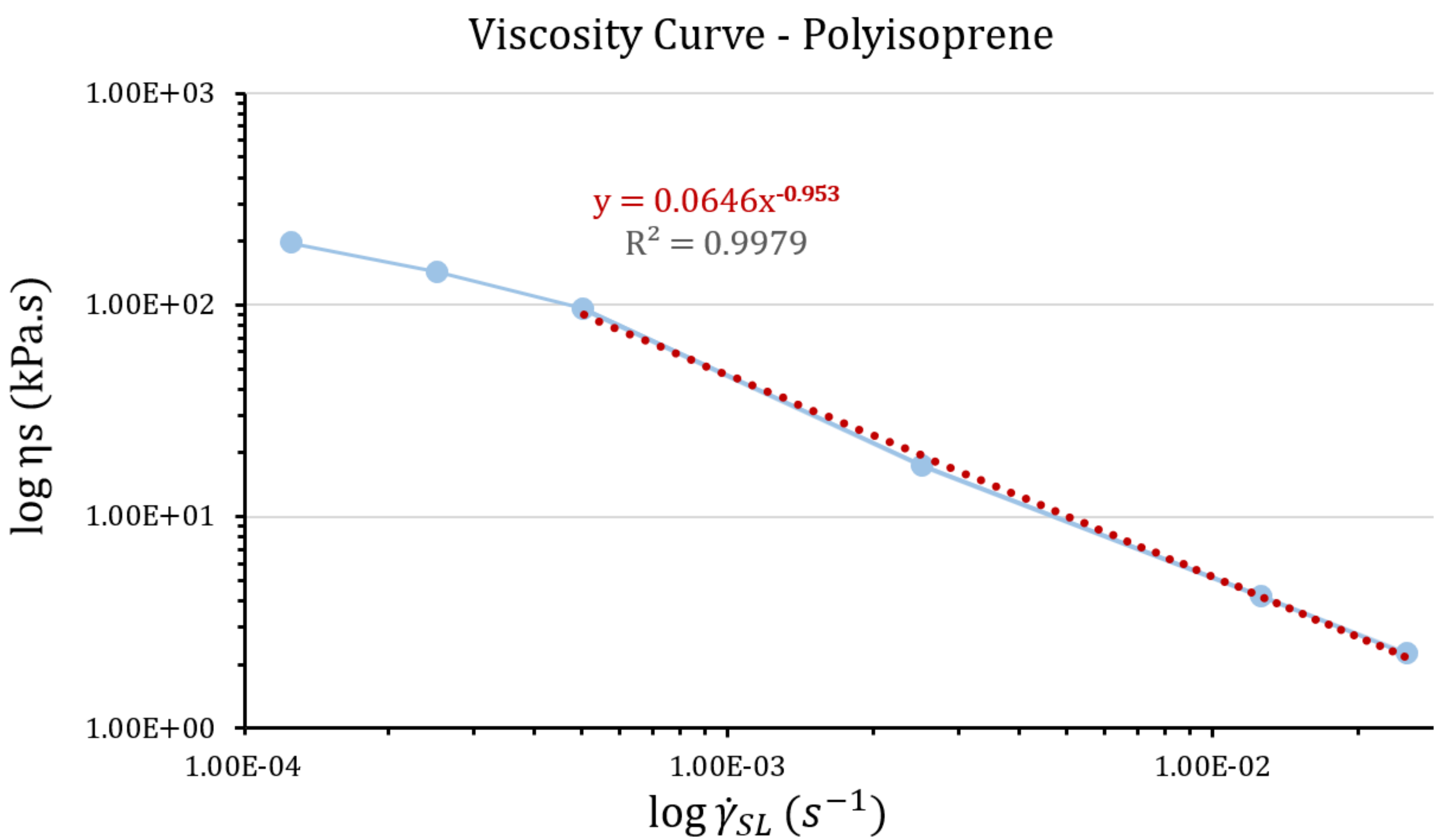
Viscosity Curve

γ'	γ'SL	ηs
0.75	0.000126	196.2317
1.5	0.000252	142.9468
3	0.000505	95.64104
15	0.002524	17.3557
75	0.012621	4.19945
150	0.025241	2.242802
$s^{(-1)}$	$s^{(-1)}$	kPa.s



Using the model

Power regression



Using the model

- Following the power-law:

$$\eta_S = K.\dot{\gamma}_{sl}^{\boldsymbol{n-1}}$$

The trendline slope is equal to the power ***n-1.***

- From the regression:

$$n - 1 = -0.953 \Leftrightarrow \boldsymbol{n = 0.047}$$

Using the model

- Following the power-law:

$$\eta_S = K.\dot{\gamma}_{sl}{}^{\boldsymbol{n-1}}$$

The trendline slope is equal to the power ***n-1.***

- From the regression:

$$n - 1 = -0.953 \Leftrightarrow \boldsymbol{n = 0.047}$$

Very high shear thining!

Observations

- Higher periods for lower shear rates should be tested;

- Value of ***n*** does not have a practical meaning – Non-application in 3D Printing.

Other materials could be tested in near future developments.

Future Work

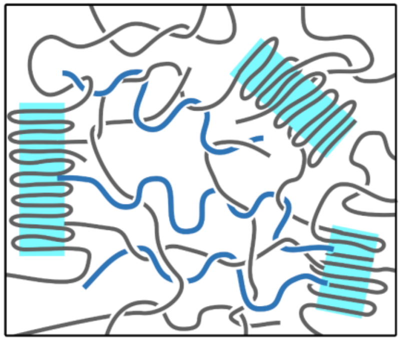
- **Conformation tensor calculation** – Near future.

<u>Consideration of:</u>

- Nozzle section variation and calculus of pressure difference as input parameter;

  Assumption of immediate freezing of the conformation tensor and the modulus.

- Conformation tensor calculation with a partially crystallized melt.



Conclusions

- I had the opportunity to be introduced to Molecular Dynamics and to successfully apply the Sliplink Model in 3D printing;

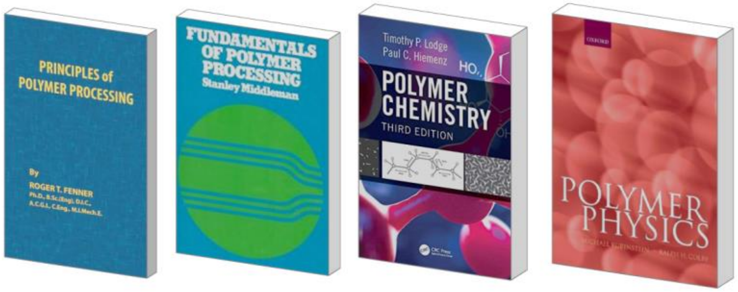
- There are several opportunities to execute new studies;

Conclusions

- I had the opportunity to be introduced to Molecular Dynamics and to successfully apply the Sliplink Model in 3D printing;

- There are several opportunities to execute new studies;

- It was very challenging and... I have a lot more to study…



Thank you, Rutledge Group!