LBRAI2219 - 2017/2018

MODÉLISATION DES SYSTÈMES BIOLOGIQUES

X. DRAYE & G. LOBET

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1. INTRODUCTION

X. DRAYE & G. LOBET

THÈMES ABORDÉS

- Introduction à **biologie des systèmes**
- Introduction aux notions de **réseaux** dynamiques et compartimentés
  - **Formalismes mathématiques** et outils logiciels pour l'exploration des données de type omics
- Initiation à la **modélisation** (exercices pratiques)

ACQUIS D'APPRENTISSAGES

- Connaître et comprendre un socle de savoirs approfondis dans le domaine de l'analyse et de la gestion de l'information en ingénierie biologique (M1.1, M1.2, M2.2)
- Maîtriser des outils spécialisés en Sciences de l'ingénieur ' analyse des systèmes et modélisation (M2.3)
- Résumer un état des connaissances (M3.1)
- Analyser et interpréter les résultats pour une problématique scientifique complexe (M3.6)
- Faire preuve d'une capacité d'abstraction conceptuelle et de formalisation dans l'analyse et la résolution de problèmes complexes (M4.4)
- Comprendre et exploiter des articles scientifiques et documents techniques en anglais (M6.1)
- Elaborer des schémas logiques pour poser une problématique complexe de façon synthétique (M6.3)
- Communiquer de manière synthétique et critique l'état des connaissances dans un domaine specifique (M6.4)

CONTENU DU COURS

- Vue générale de la **biologie des systèmes**
  - Théorie des systèmes et biologie
  - Topologie, éléments de graphes et attributs de réseau
  - Identification des noeuds et cartographie des interactions
  - Inférence de réseaux
  - Intégration des données
  - De la structure à la dynamique
- 2. **Outils informatiques** pour l'exploration de données (omics)
- 3. Langages et **études de cas**
  - L-Systems (structure) et FSPM (structure et fonction)
  - Interactions organisme - environnement
  - Etudes de cas à diverses échelles (réseau de gène, cellule, tissu, organe, organisme)

MÉTHODES D'ÉVALUATIONS

- Présentation d'un ou plusieurs séminaires

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2. BIOLOGIE DES SYSTÈMES

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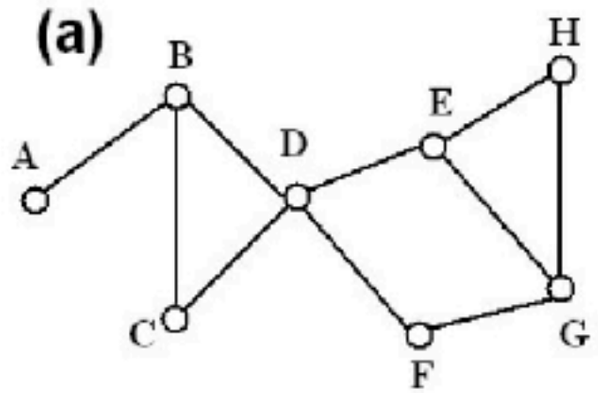
AN OVERVIEW OF SYSTEMS BIOLOGY

- Lecture d'acticle
- **Concepts clés:**
  - Systems theory
  - Graph and network theory
  - Biological networks

Albert, R. & Assmann, S. M. **An Overview of Systems Biology**. in *Annual Plant Reviews Volume 35: Plant Systems Biology* 41–66 2009

GRAPH ELEMENT AND NETWORK ATTRIBUTES

- Node
- Edge
- Node degree
- Neighbourhood
- Clique
- Clustering coefficient
- Graph distance
- Between centrality

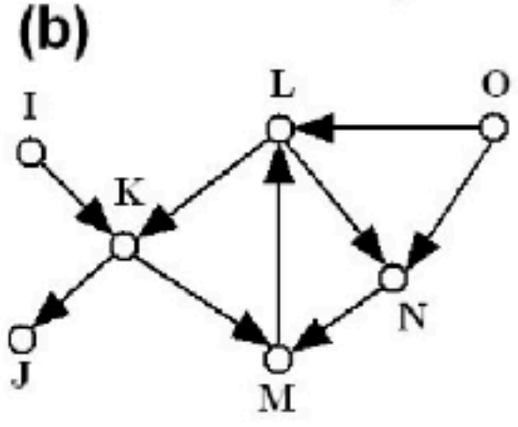


k	P(k)
1	1/8
2	3/8
3	3/8
4	1/8

C	P(C)
n.d.	1/8
0	1/8
1/6	1/8
1/3	3/8
1	1/8

d	P(d)
1	10/28
2	10/28
3	6/28
4	2/28

b	P(b)
0	3/8
1.5	1/8
2	1/8
6	2/8
12.5	1/8



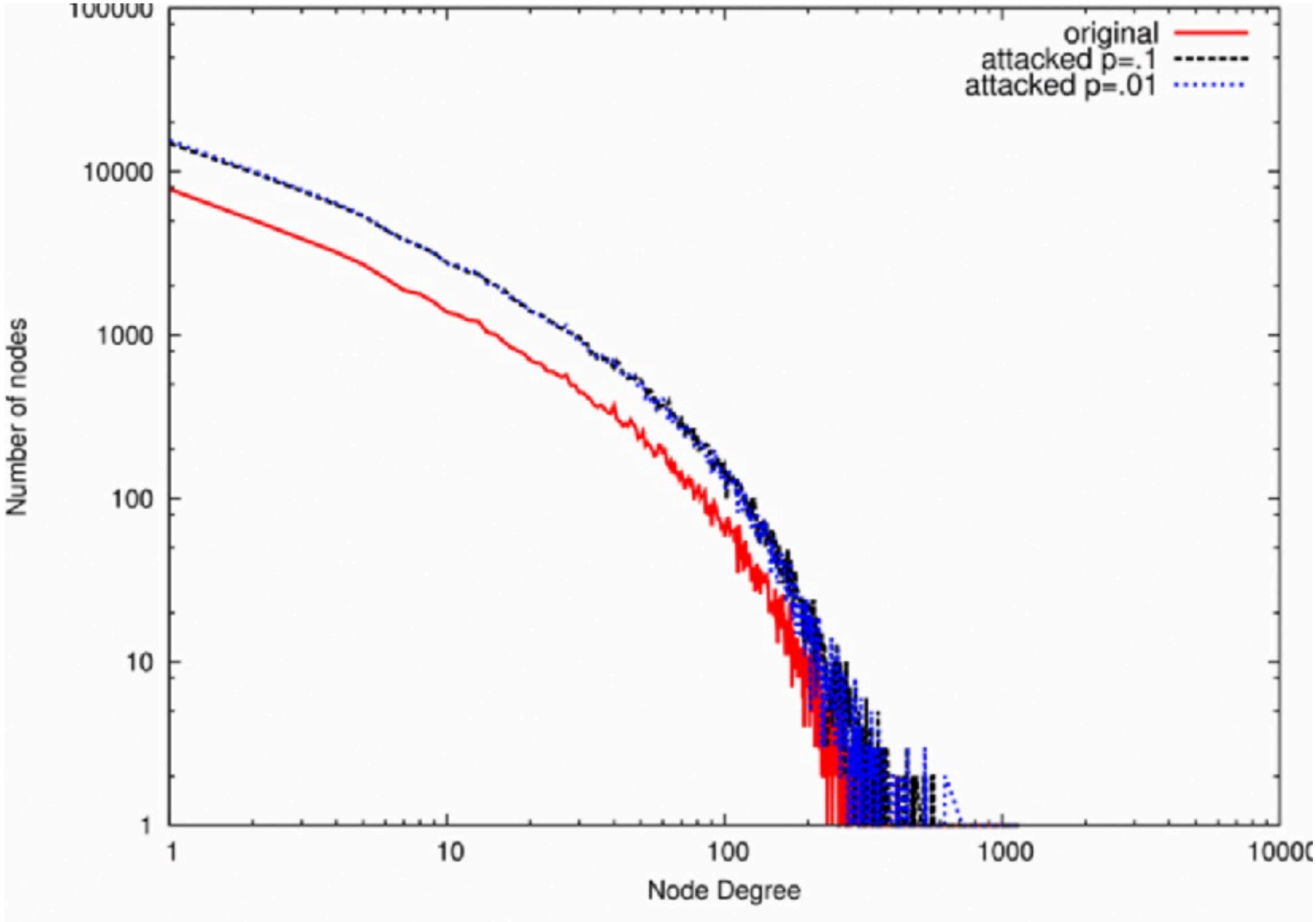
k_{in}	$P(k_{in})$
0	2/7
1	1/7
2	4/7

k_{out}	$P(k_{out})$
0	1/7
1	3/7
2	3/7

d	P(d)
∞	17/42
1	9/42
2	10/42
3	4/42
4	2/42

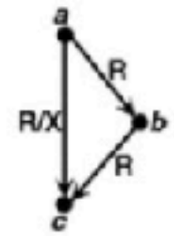
b	P(b)
0	3/7
1.5	1/7
6	1/7
7.5	1/7
9	1/7

GRAPH ELEMENT AND NETWORK ATTRIBUTES

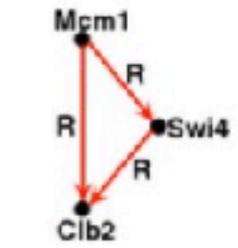


MOTIFS

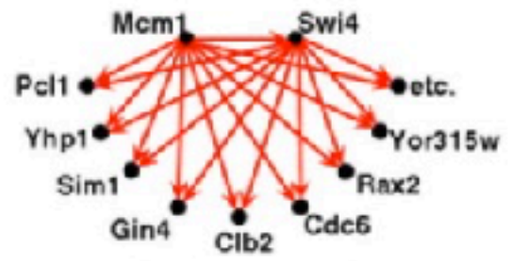
(a)



	A1	A2
N_{real}	4.7×10^{2}	3.0×10^{1}
N_{rand}	$(2.6\pm0.5)\times10^{2}$	5.4 ± 3.2

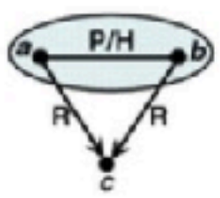


A motif example

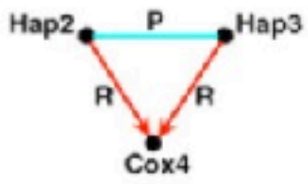


A theme example

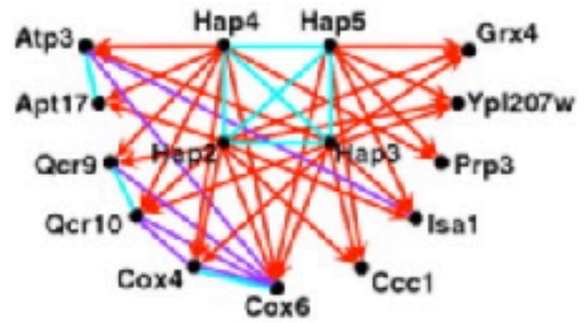
(b)



	P	H
N_{real}	1.3×10^{2}	6.1×10^{2}
N_{rand}	3.3 ± 3.7	$(8.0\pm2.3)\times10^{1}$



A motif example

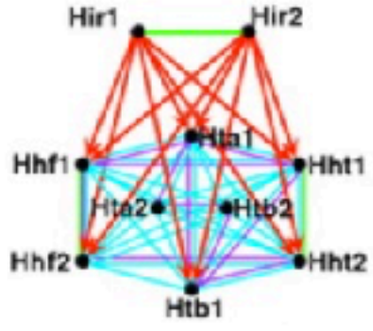


A theme example

(c)

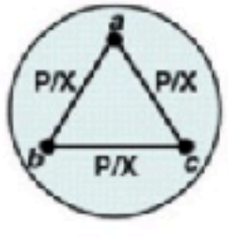
	C1	C2	C3
N_{real}	5.9×10^{3}	3.5×10^{3}	1.9×10^{3}
N_{rand}	$(5.4\pm0.5)\times10^{2}$	$(2.7\pm0.3)\times10^{2}$	$(5.3\pm0.5)\times10^{2}$

A motif example



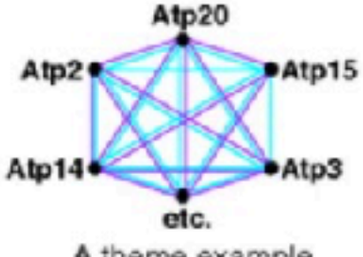
A theme example

(d)



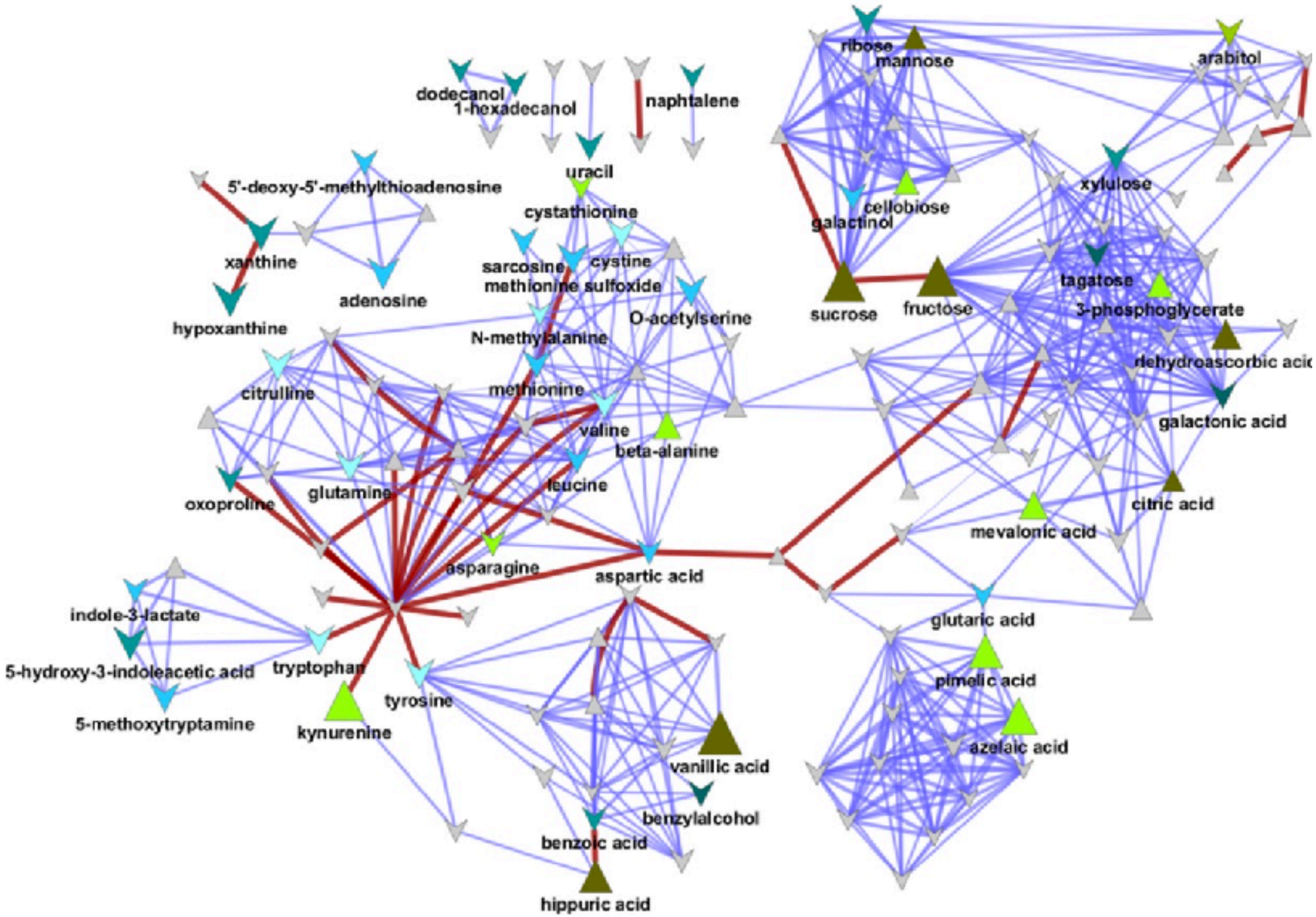
	D1	D2	D3	D4
N_{real}	5.7×10^{5}	9.9×10^{4}	6.7×10^{4}	1.2×10^{6}
N_{rand}	$(1.1\pm0.0)\times10^{5}$	$(8.2\pm0.3)\times10^{3}$	$(5.2\pm0.2)\times10^{3}$	$(2.7\pm0.1)\times10^{4}$

A motif example



A theme example

MODULES


dodecanol
1-hexadecanol
naphtalene
uracil
5'-deoxy-5'-methylthioadenosine
cystathionine
xanthine
sarcosine
cystine
methionine sulfoxide
adenosine
hypoxanthine
O-acetylserine
N-methylalanine
citrulline
methionine
valine
beta-alanine
oxoproline
glutamine
leucine
asparagine
aspartic acid
indole-3-lactate
5-hydroxy-3-indoleacetic acid
tryptophan
tyrosine
5-methoxytryptamine
kynurenine
vanillic acid
benzylalcohol
benzoic acid
hippuric acid
ribose
mannose
arabitol
xylulose
cellobiose
galactinol
tagatose
sucrose
fructose
3-phosphoglycerate
dehydroascorbic acid
galactonic acid
citric acid
mevalonic acid
glutaric acid
pimelic acid
azelaic acid

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3. MODEL EXAMPLES

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ALL MODELS ARE WRONG, BUT SOME ARE USEFULL...

GEORGE BOX

WHY DO WE NEED MODELS?

- Theory testing
- Experimental design
- Sensitivity analysis
- ...

ORGAN SCALE

PLANT SCALE

FIELD SCALE

STRUCTURE

FUNCTION

SOIL

B

Root cross section imaging

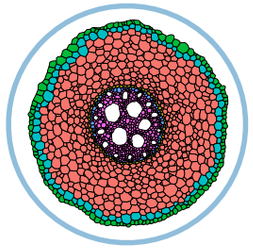
Root cross-section image analysis tool

Root anatomical parameters

Full tracing

Root anatomy

Root anatomy model



D

Root system imaging

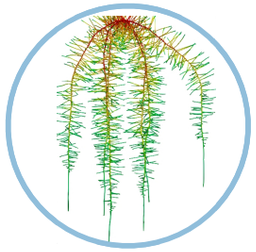
Root image analysis tool

Root architecture parameters

Full tracing

Root architecture

Root architecture model



F

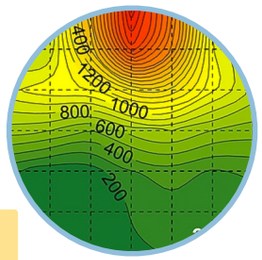
Field root phenotyping

Root image analysis tool

Root density parameters

Root length density profile

Root density model



A

Root axial water flow model

Root-type axial conductivity

Root pressure probe

Root radial water flow model

Root-type radial properties

Cell-type hydraulic properties

Cell pressure probe

Water pathway contributions

C

Pressure chamber

Timelapse mass balance

Plant water status dynamics

Plant transpiration dynamics

Root system water flow model

High Pressure Flow Meter

E

Lysemeter experiment

Standard uptake fractions

Root system conductivity

Macroscopic root water uptake model

Canopy transpiration dynamics

Canopy water status dynamics

Remote sensing

G

Experimental procedure

Image analysis tool

Data

Modelling tool

Hypothetical tool or connection

Water content measurment

Soil water status dynamics

Water uptake distribution

Water uptake measurement

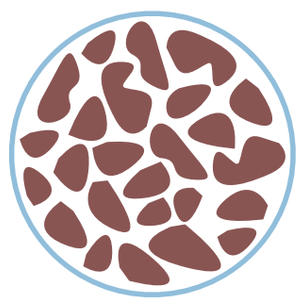
Soil retention curve measurement

Soil retention curve

Soil water flow model

Soil conductivity curve

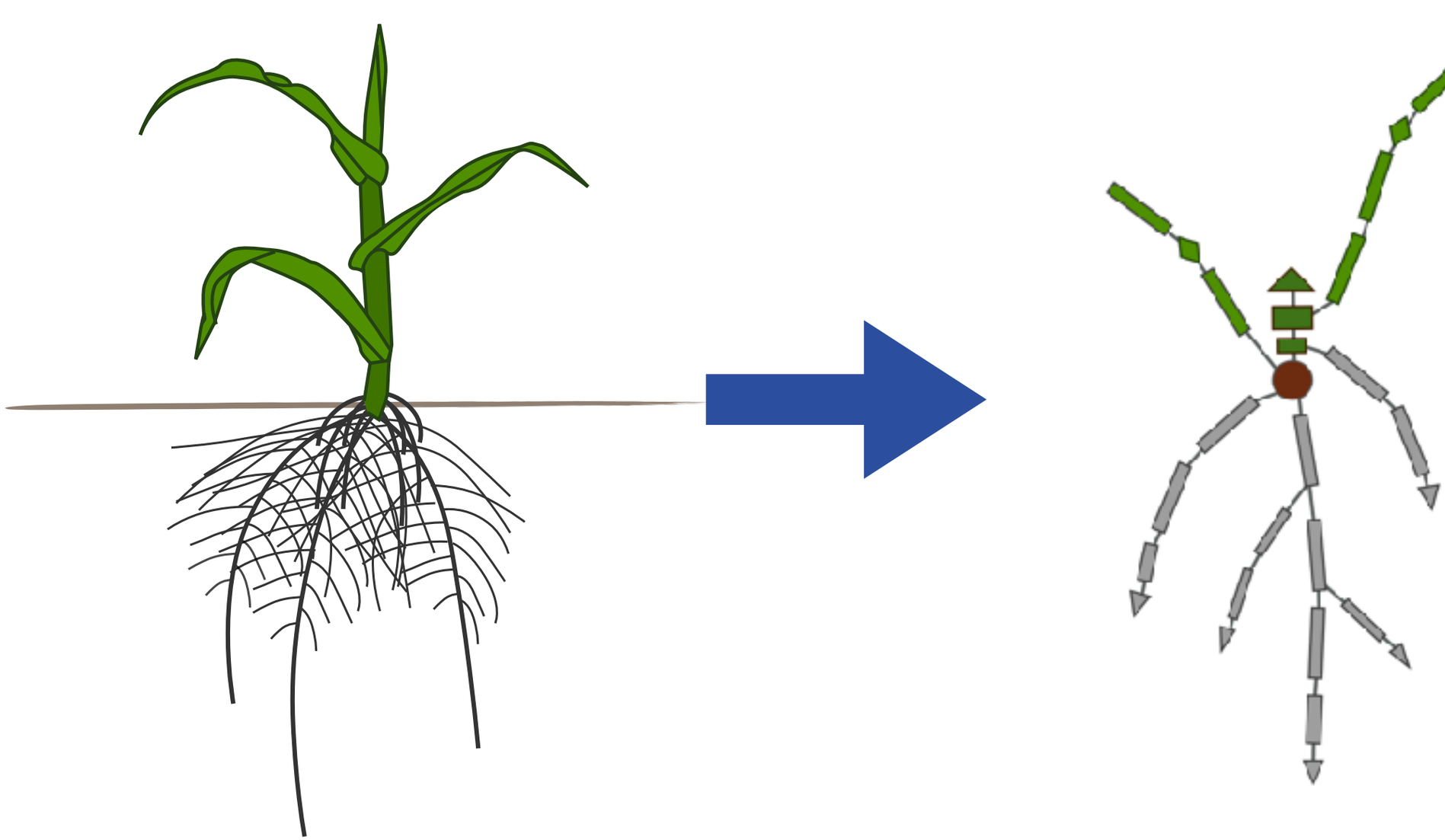
Soil conductivity measurement



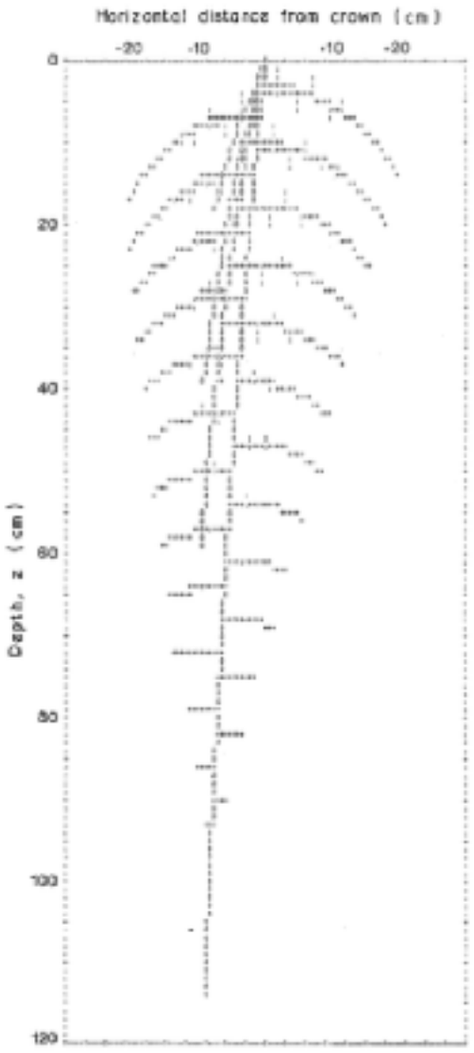
STRUCTURAL MODELLING

Represent the structure (and growth) of the root system

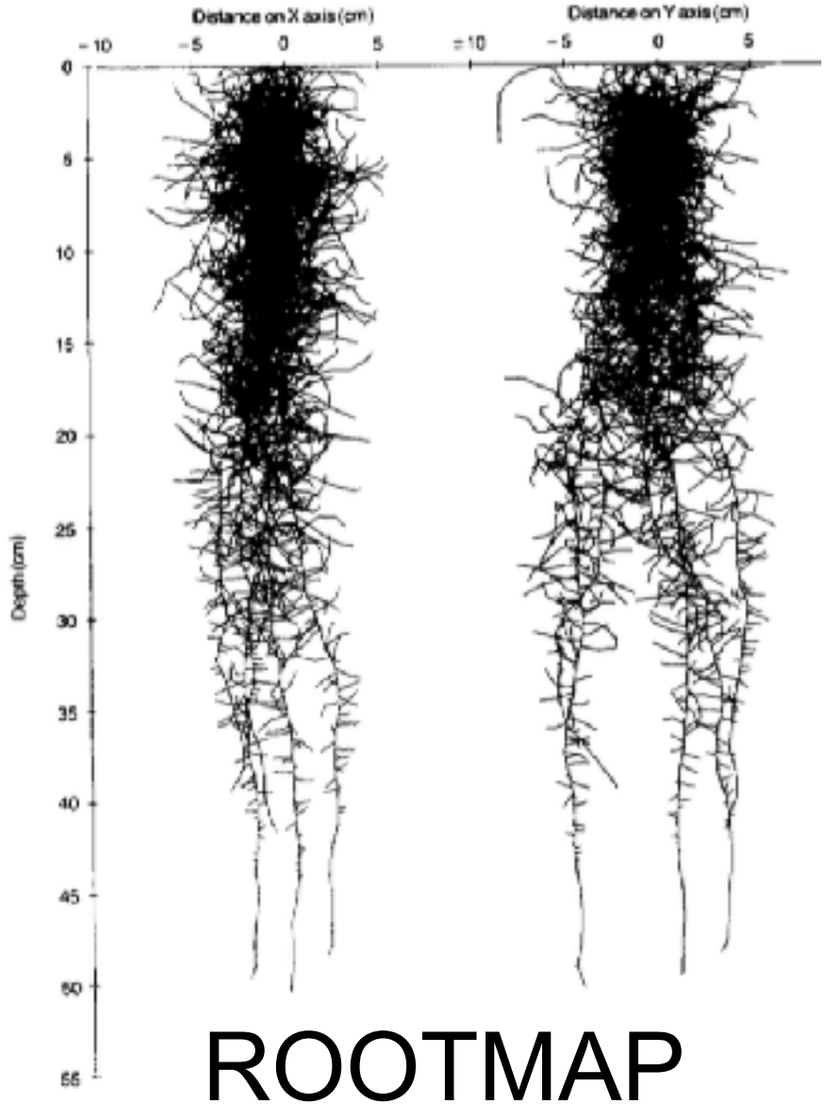
Helps you understand the dynamics (underlying processes) of the root system formation



STRUCTURAL MODELLING



1973

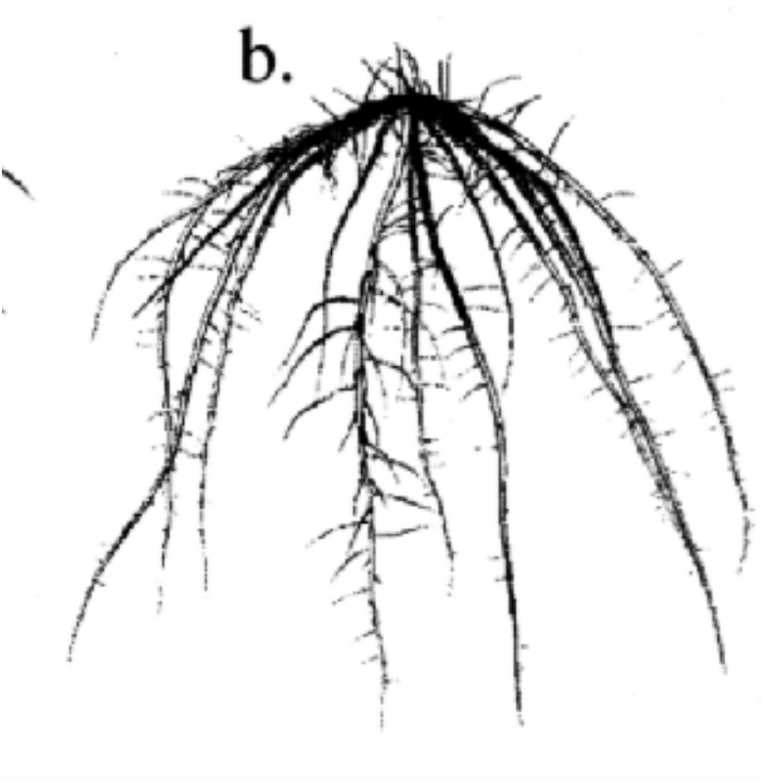


ROOTMAP

1988

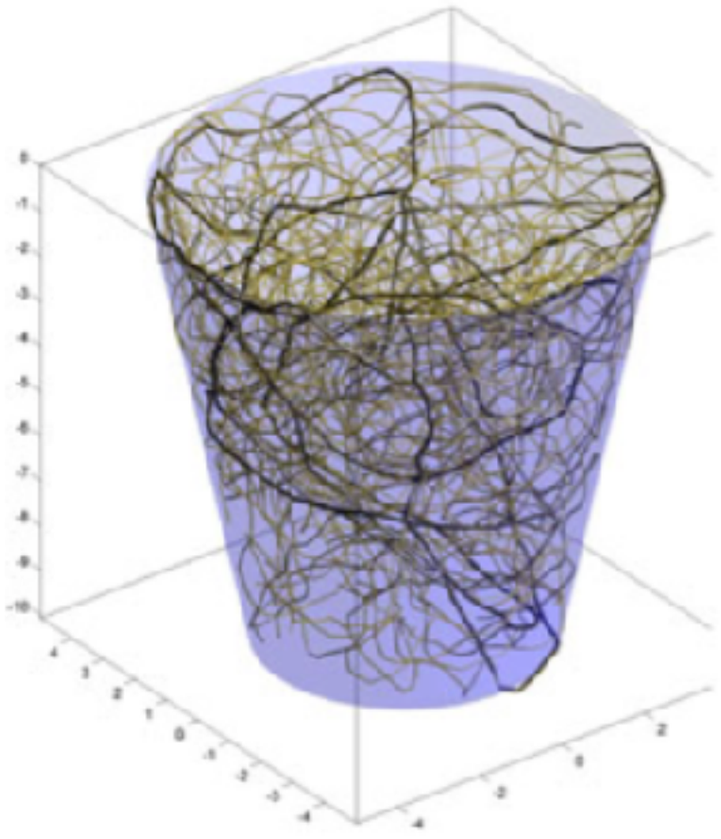
1989

STRUCTURAL MODELLING



1997

2004



2010

STRUCTURAL MODELLING

http://bit.ly/crootbox

This app displays the capabilities of the CRootBox model. Choose a dataset, unleash CRootBox, then try changing the parameters.

Forschungszentrum Juelich GmbH

1. Load parameter set

1. Select root system dataset

Triticum aestivum a

Simulation of wheat growth using the 3D root architecture model SPACSYS: Validation and sensitivity analysis
Bingham I J, Wu L
European Journal of Agronomy, 34, 181-189, 2011
View paper

Black and white root system

Unleash CRootBox

JÜLICH
FORSCHUNGSZENTRUM

2. Update parameters

2. Select root type

Select parameter to change

Length of basal zone [cm]

Parameter mean:

0 1

Parameter deviation [%]:

0 50

Length of basal zone [cm]
Length of the unbranched basal zone of the root

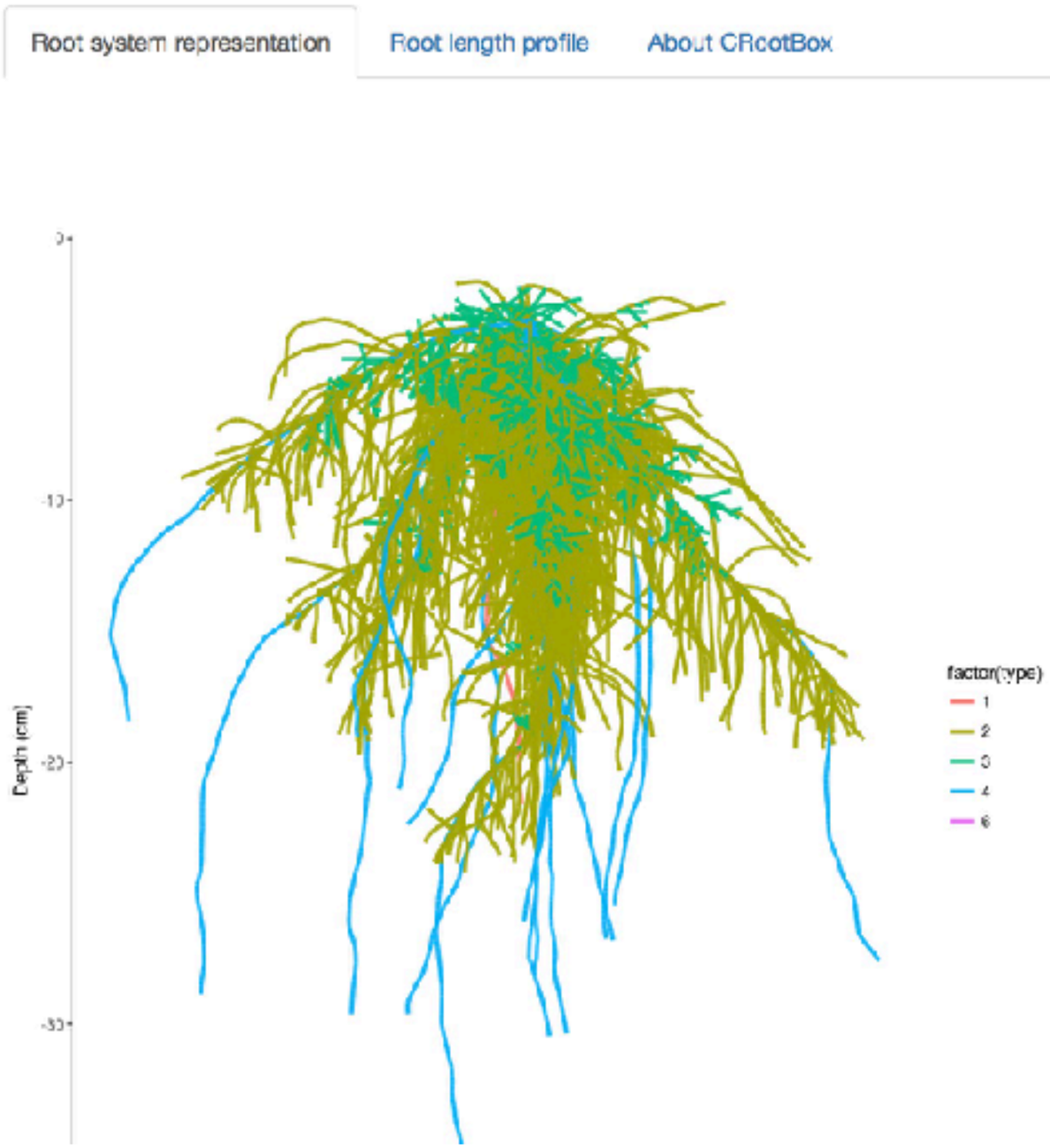
3. Select plant parameter to change

Planting depth [cm]

Parameter value:

0 3 6

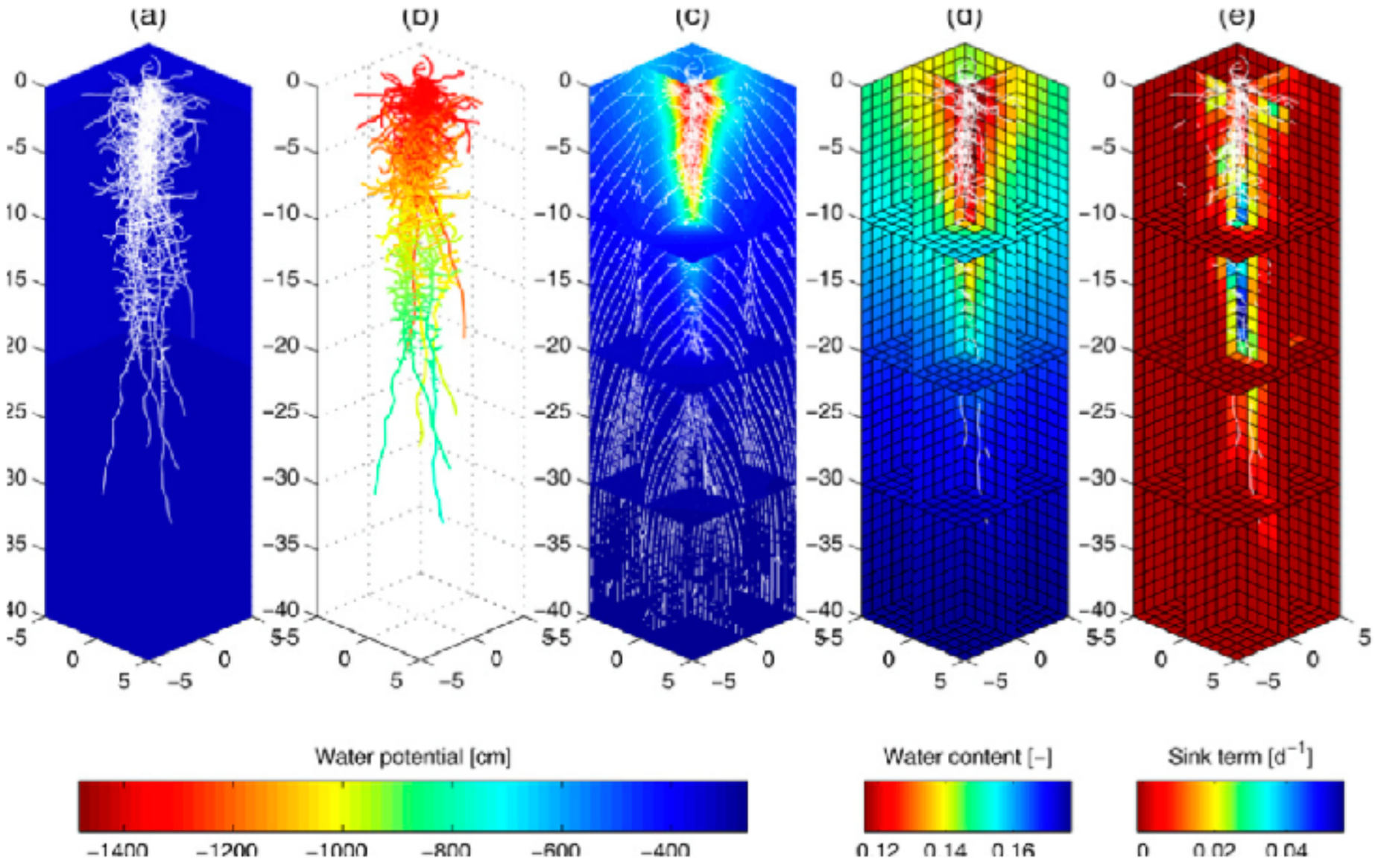
Root system representation | Root length profile | About CRootBox



FUNCTIONAL-STRUCTURAL MODELLING

Adding function to the structure

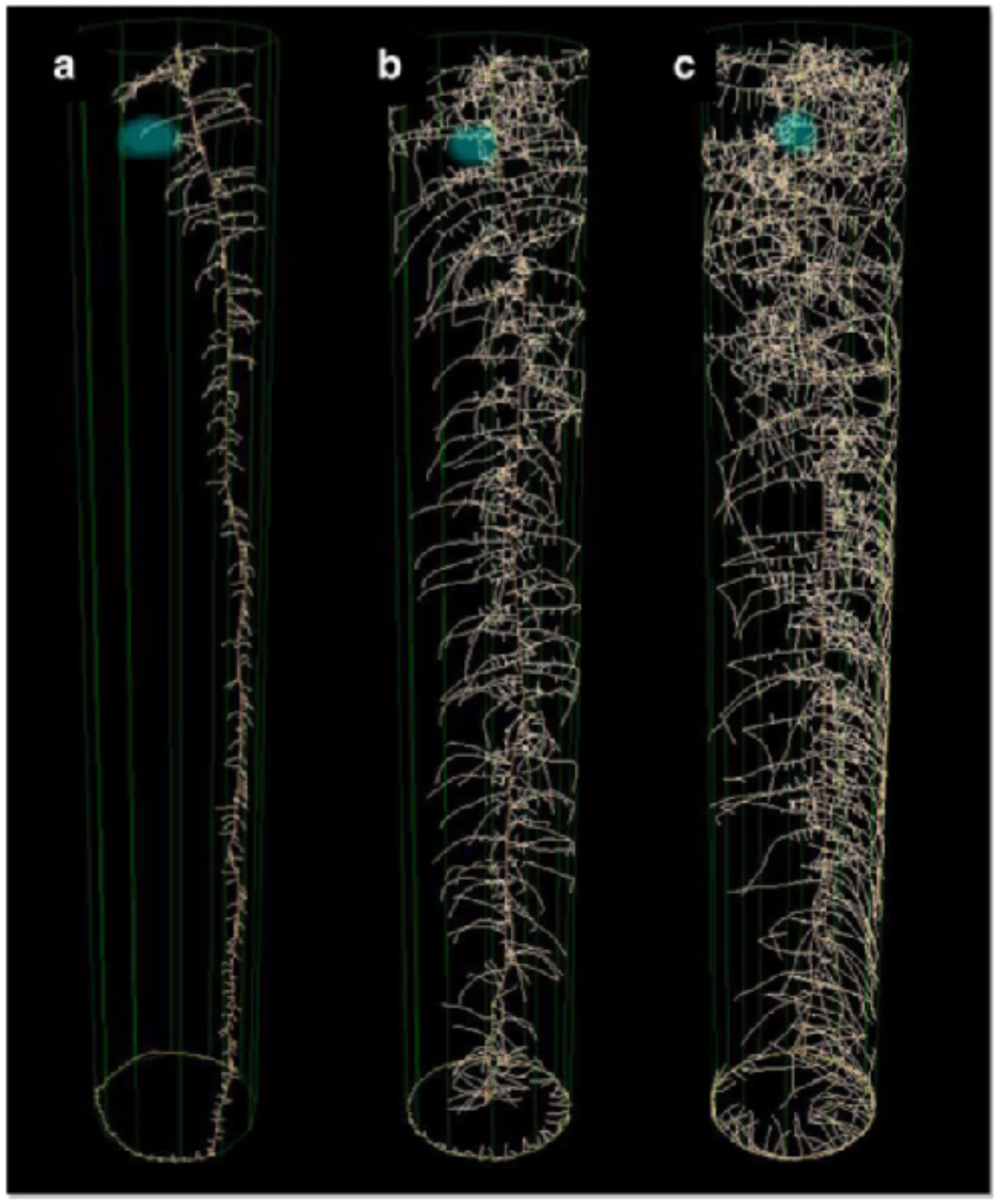
Water uptake



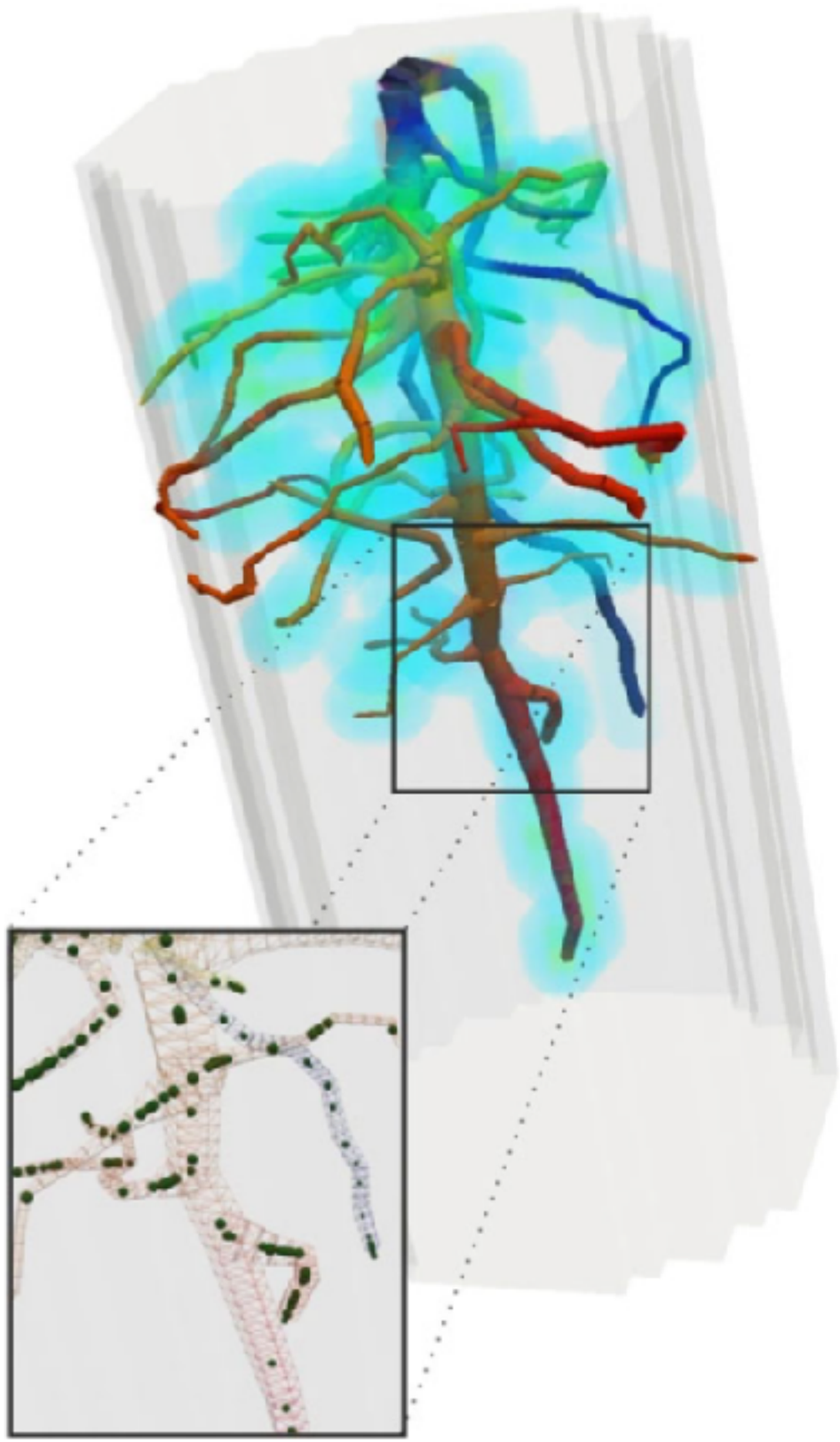
FUNCTIONAL-STRUCTURAL MODELLING

Adding function to the structure

Nutrient uptake



FUNCTIONAL-STRUCTURAL MODELLING

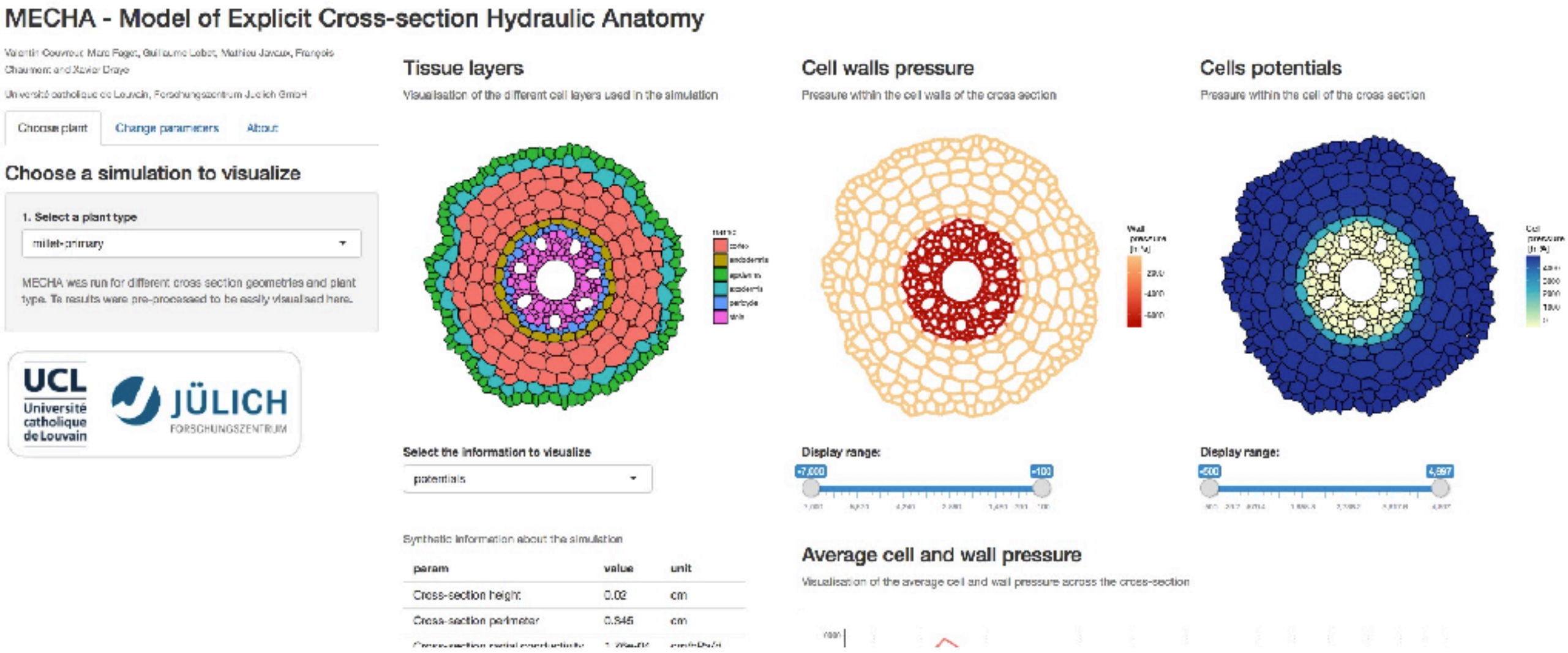


Adding function to the structure

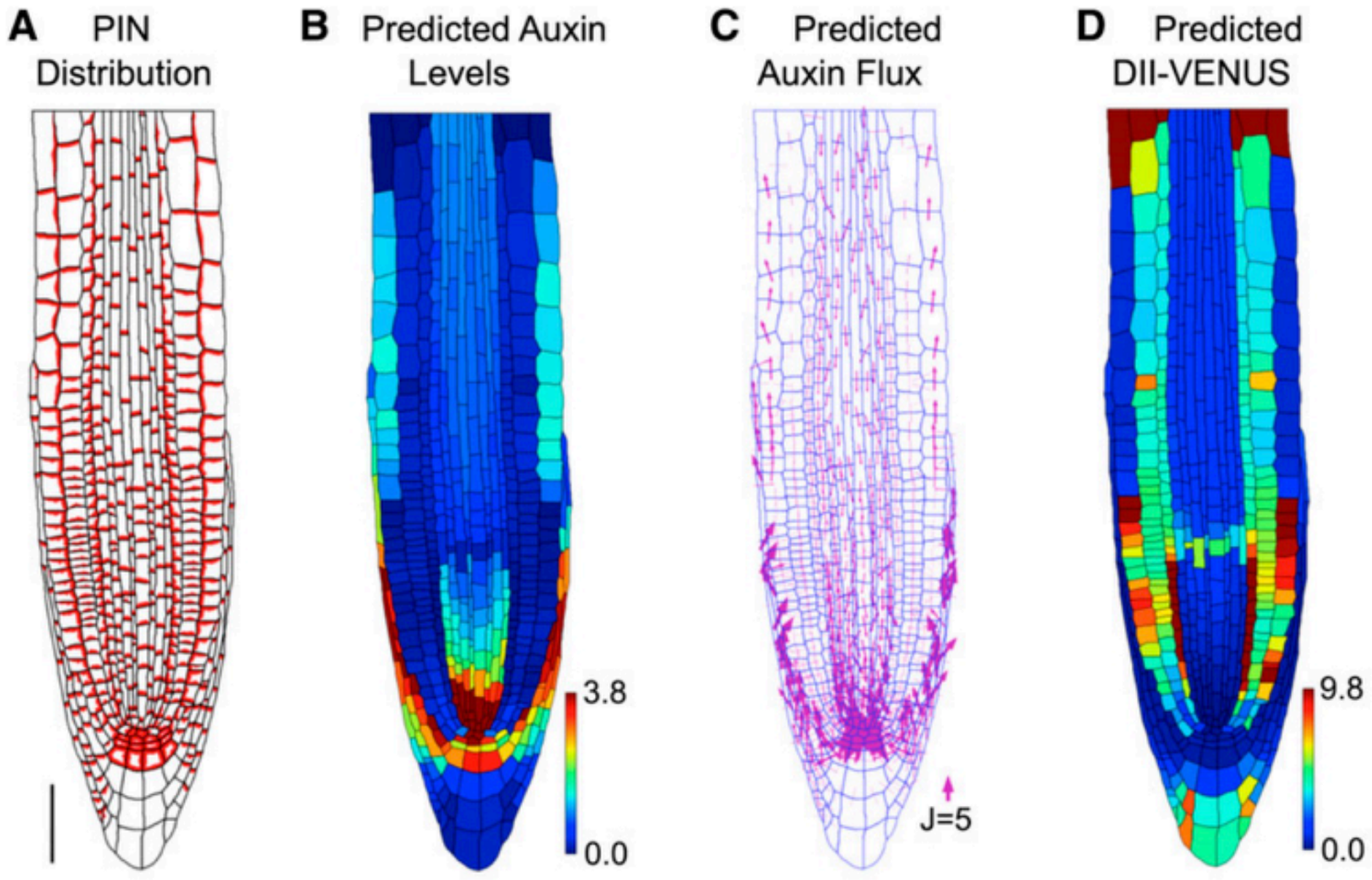
Transport

FUNCTIONAL-STRUCTURAL MODELLING

https://plantmodelling.shinyapps.io/mecha/



FUNCTIONAL-STRUCTURAL MODELLING



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4. PROJECTS

X. DRAYE & G. LOBET

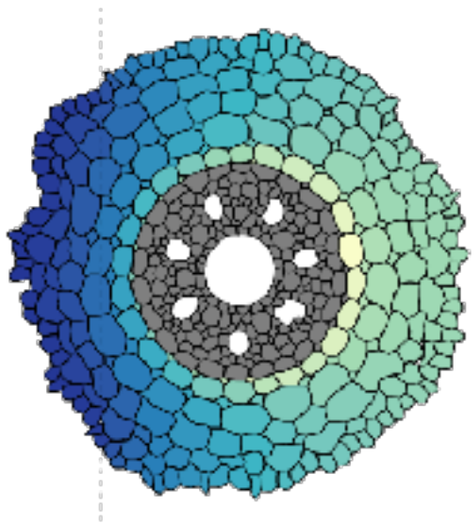
OBJECTIVES

- getting **familiar with models** in life sciences in general (why do we need models, what can they do, what are the limitations)
- knowing **examples** of successfull models in life sciences

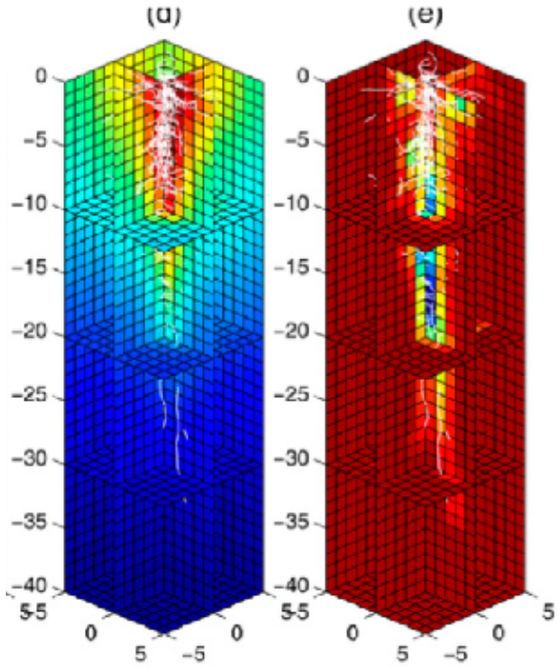
OBJECTIVES

- For a specific model:
  - understanding the underlying **theory** behind the model
  - understanding the **limitations** of the model
  - being able to **run** de model
  - being able to perform a **set of simulations** and interpret those
  - being able to **critisize** the model

MODELS NEARBY

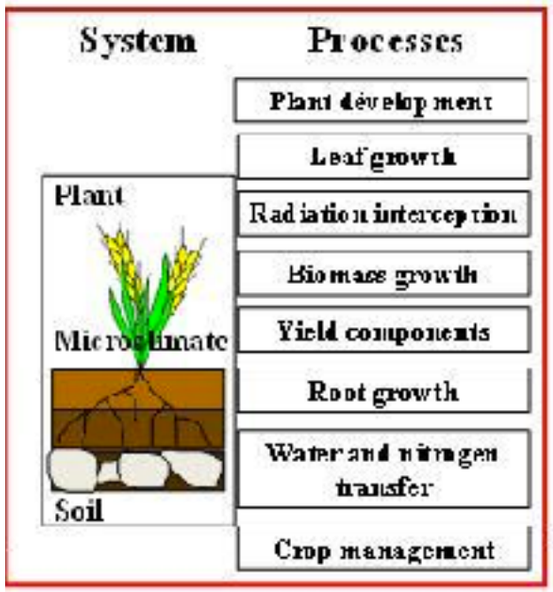


MECHA
Valentin Couvreur
Xavier Draye
UCL



R-SWMS
Valentin Couvreur
Félicien Meunier
Mathieu Javaux
UCL

CROOTBOX
Guillaume Lobet
Andrea Schnepf
Daniel Leitner
UCL - Juelich



STICS
Benjamin Dumont
Gembloux
AgroBioTech

https://paperpile.com/shared/6MaUSf

OBJECTIVES

- "**Soft-skill**" objectives
  - being able to **communicate** about models in life sciences to an external audience (**Twitter**)
  - being able to **collaborate** on a project (**GitHub**)

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Université catholique de Louvain

AGRO LOUVAIN

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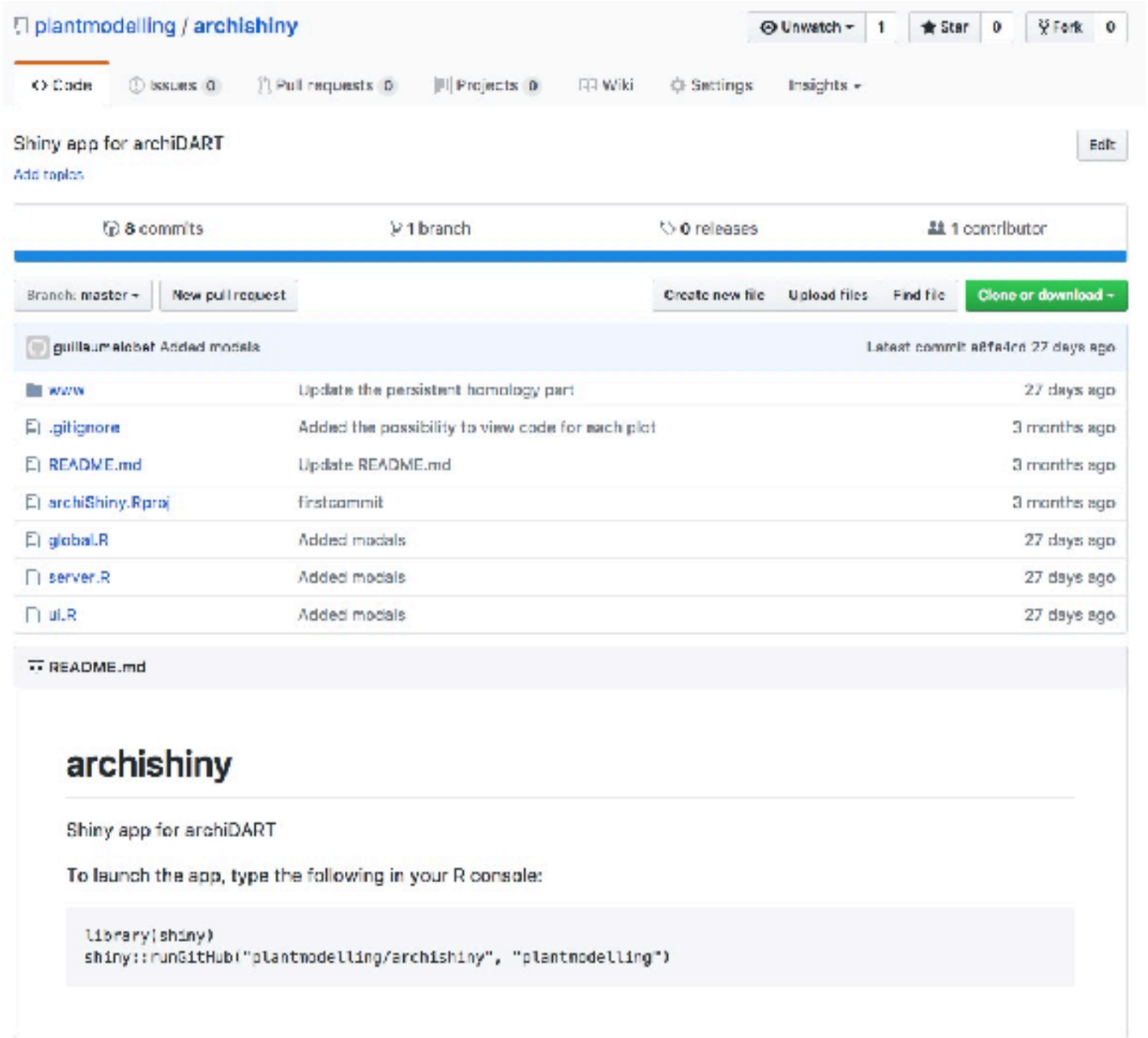
5. GITHUB

X. DRAYE & G. LOBET

WHAT IS GITHUB

- Collaboration
- Version control
- Dissemination



WHAT TO DO

- Create a GitHub account on www.github.com
- Download the GitHub Desktop
- Register to the course
- Clone the repo locally
- Modify the repo
- Submit the changes

https://try.github.io

https://classroom.github.com/g/_z0dxyTS

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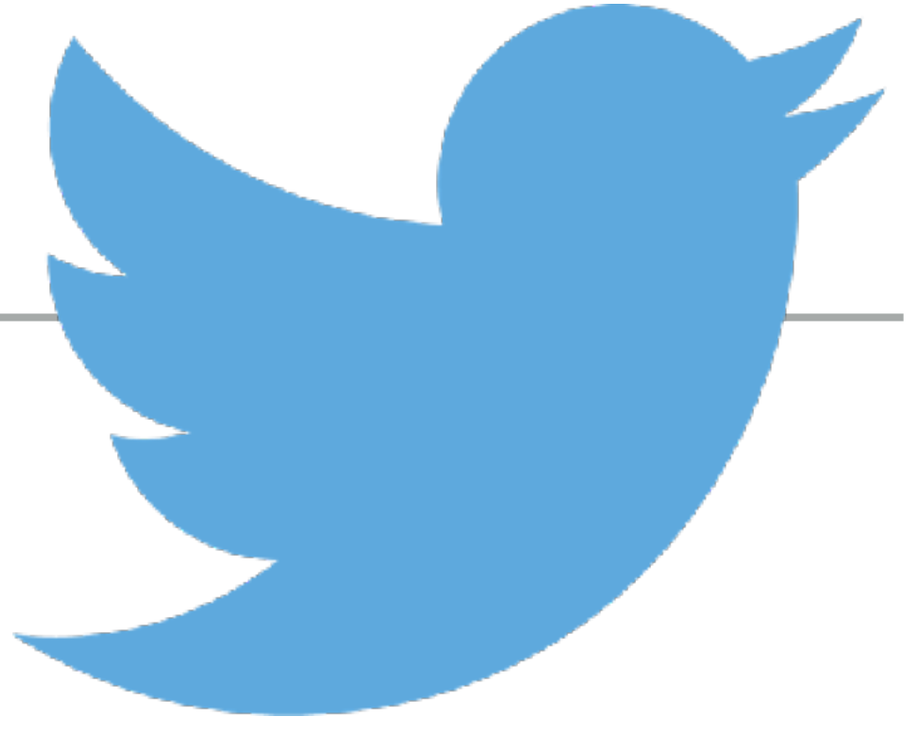
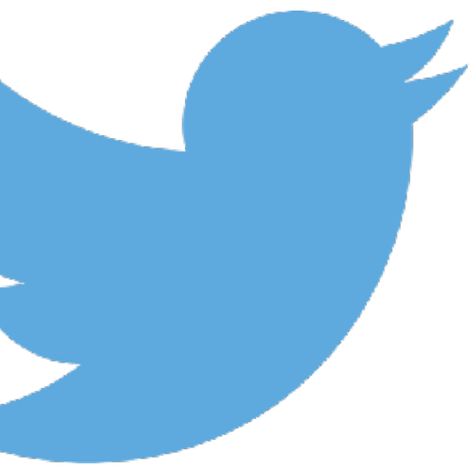
6. TWITTER



X. DRAYE & G. LOBET



8th largest website worldwide

310M
Monthly active users

1B
Unique visits monthly to sites with embedded Tweets

83%
Active users on mobile

3,800
Employees around the world

35+
Offices around the world

79%
Accounts outside the U.S.

40+
Languages supported

40%
Employees in technical roles

All numbers approximate as of March 31, 2016.

DO SCIENTISTS REALLY USE TWITTER?

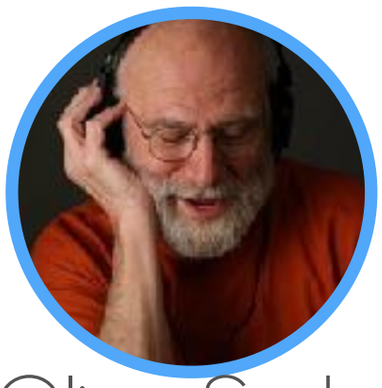
Astrophysics

Neil deGrasse Tyson
@neiltyson
4.55M

Developmental biology

David Shiffman
@WhySharksMatter
24.8K

Neurology



Oliver Sacks
@OliverSacks
113K

Evolution

Charles Darwin
@cdarwin
21.7K

http://bit.ly/twitter-stars

DO SCIENTISTS REALLY USE TWITTER?

Philippe Baret

@PhilippeBaret

728 followers

Mathieu Javaux

@MaJavx

128 followers

Guillaume Lobet

@guillaumelobet

1019 followers

Damien Debecker

@deuxbeck

3162 followers

Earth and Life Institute

@ELI_UCLouvain

167 followers

Faculté des bioingénieurs

@AGROLouvain

1013 followers

UCL

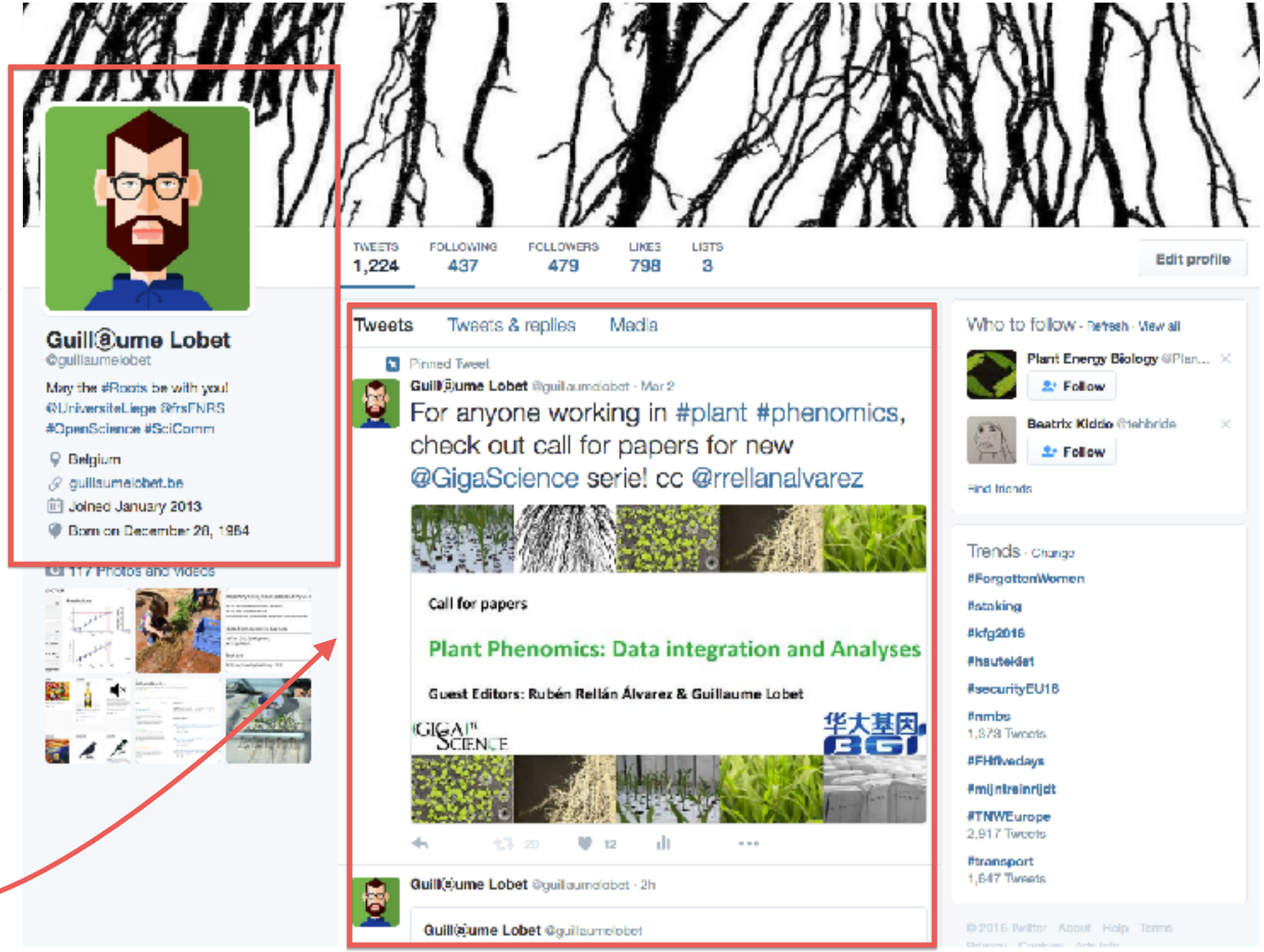
@UCLouvain_be

3966 followers

PROFILE

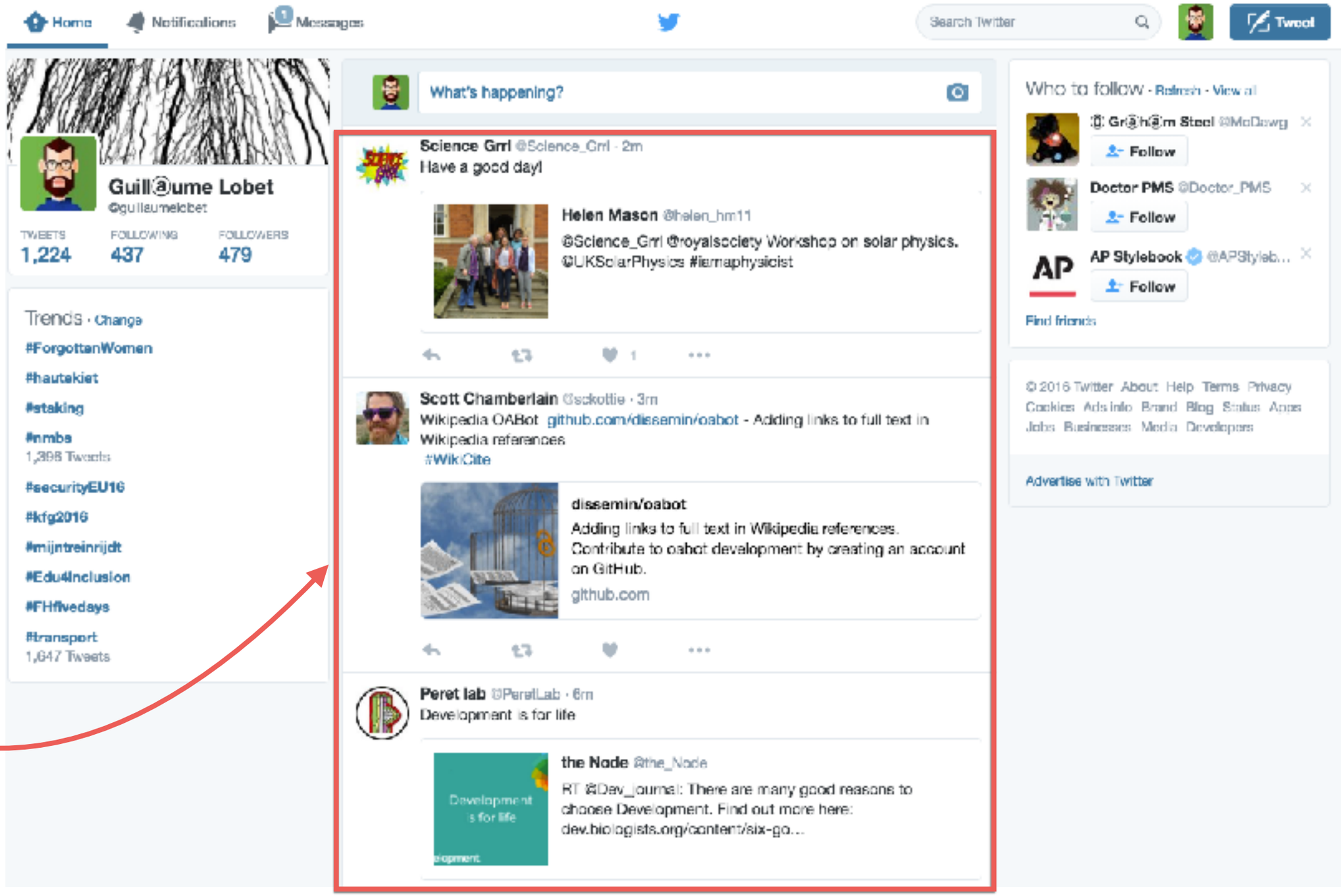
You bio.

You tweets.

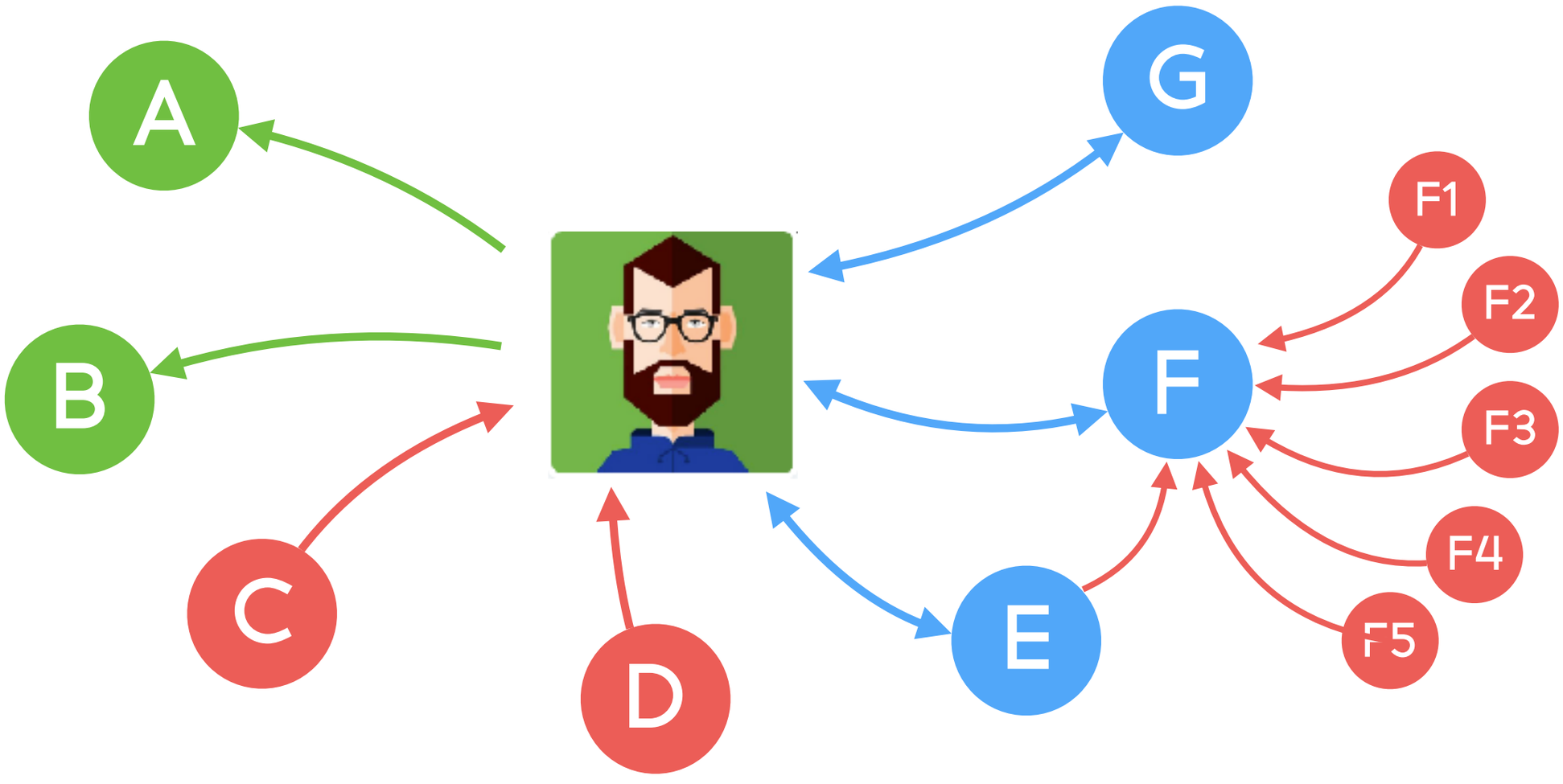


HOME

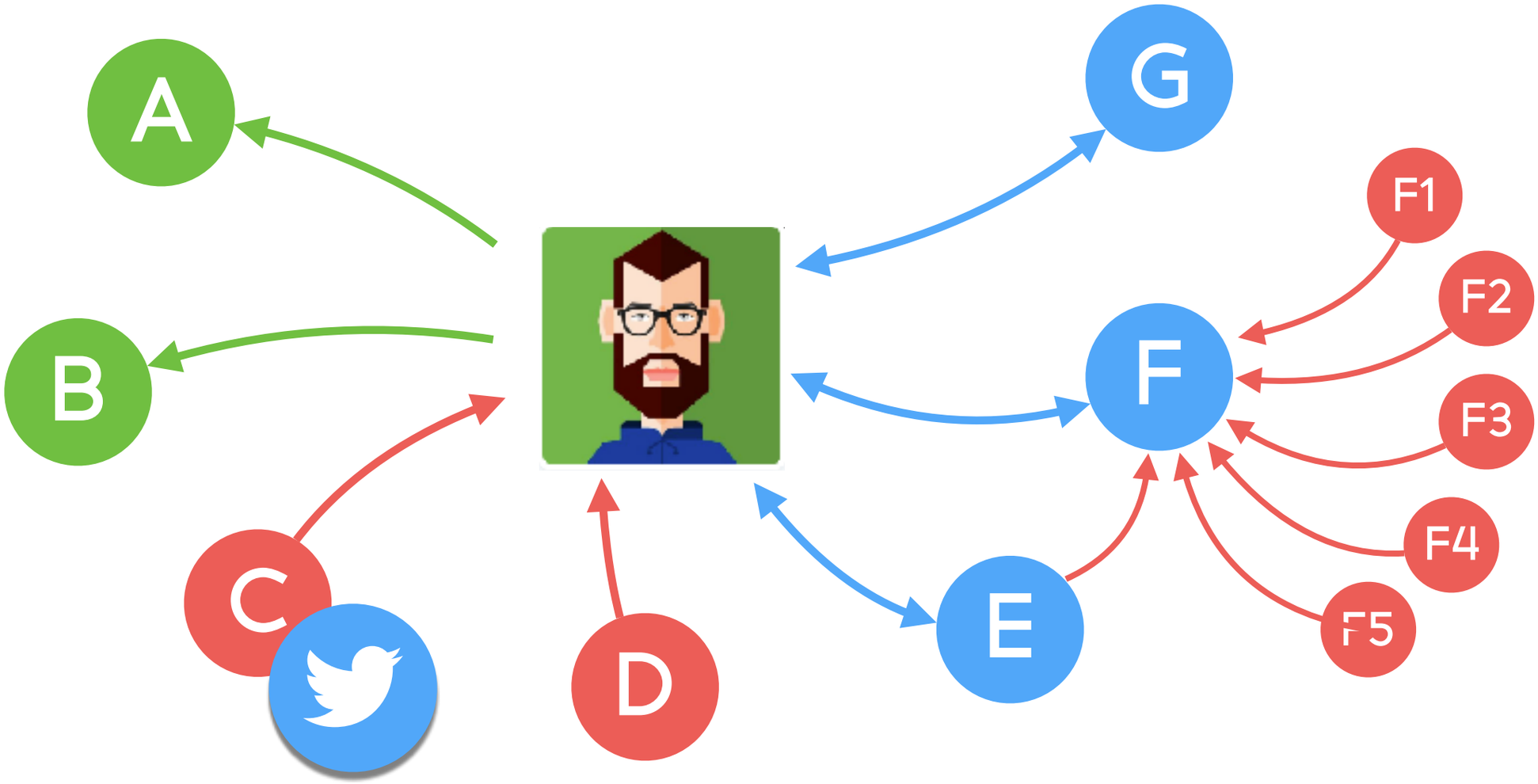
Tweets of people you follow



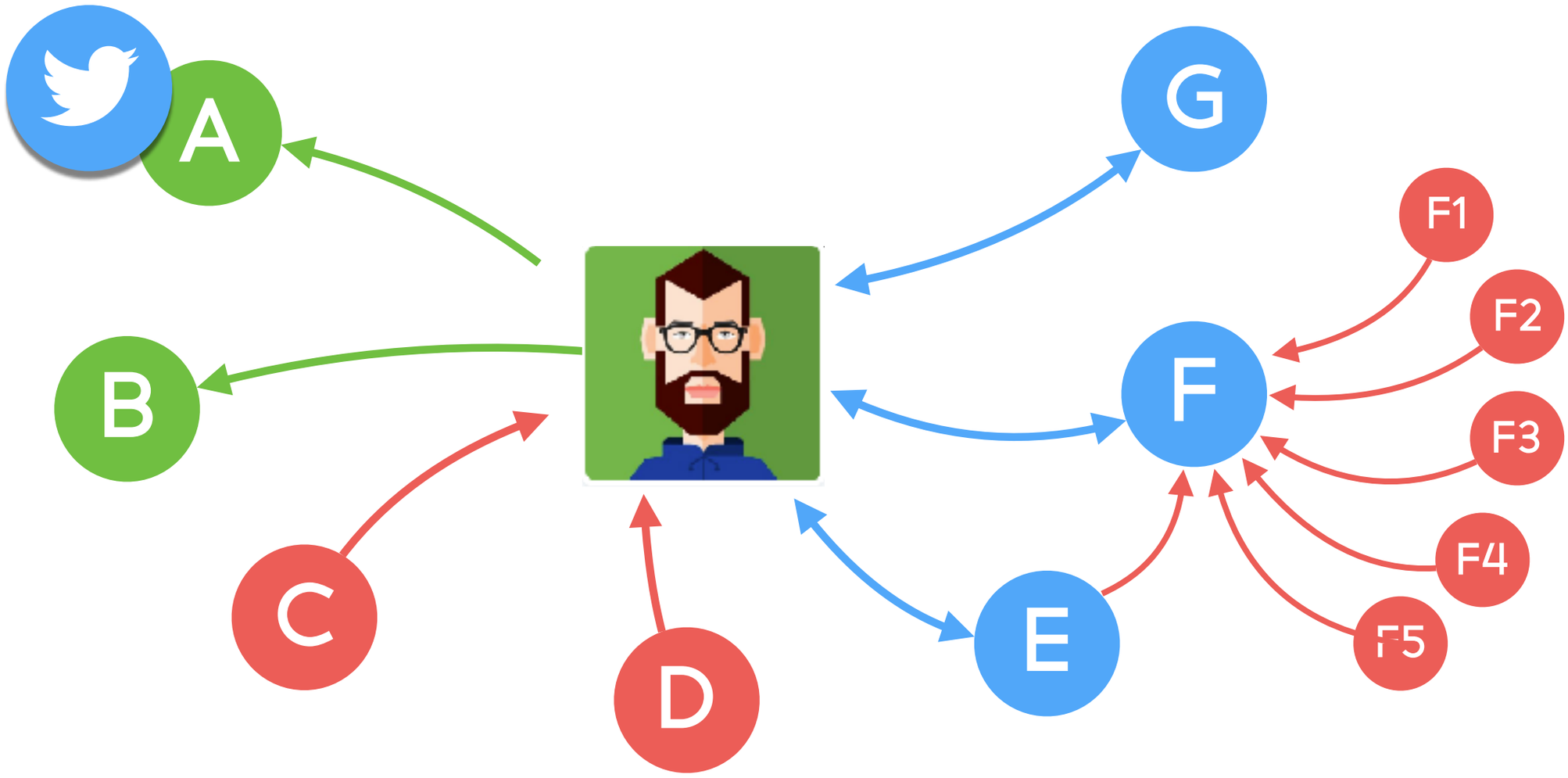
FOLLOWERS – FOLLOWING



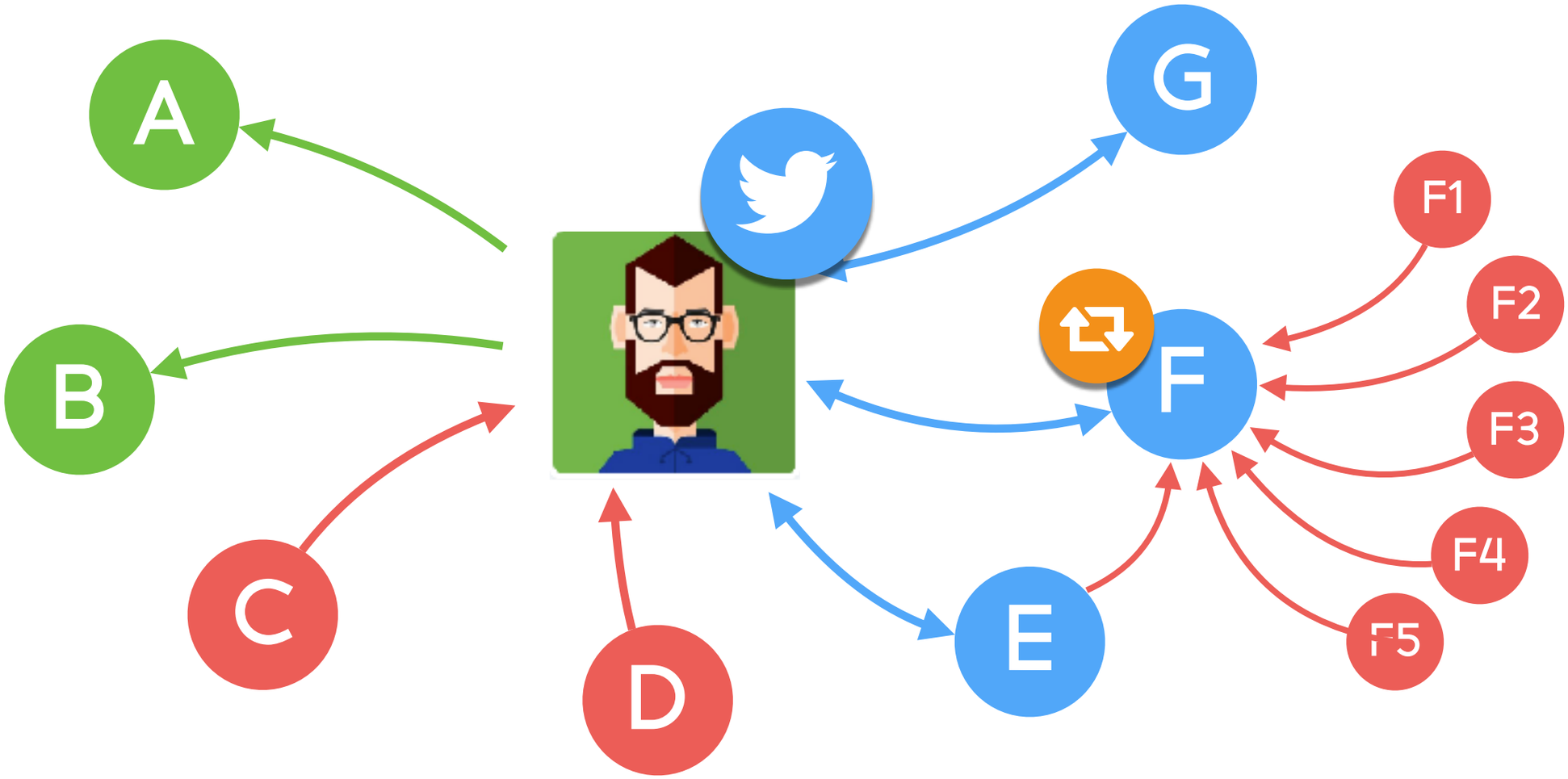
FOLLOWERS – FOLLOWING



FOLLOWERS – FOLLOWING



FOLLOWERS – FOLLOWING



EVERYBODY CAN SEE YOUR PROFILE

TWITTER CHEATSHEET – 1

140 characters in one tweet including picts and links.
Better use 120 to allows RT

@ use the handle to mention
others in your tweets.

hashtag = used to group tweets
and conversations by topics

RT RT @username : re-post someone else's
tweet in your thread

TWITTER CHEATSHEET – 2

REPLY

tweet in response to an other tweet
and start a conversation

.@

if tweet starts with an handle, only this person will see the tweet in his thread. Add a character before the @ to make it public

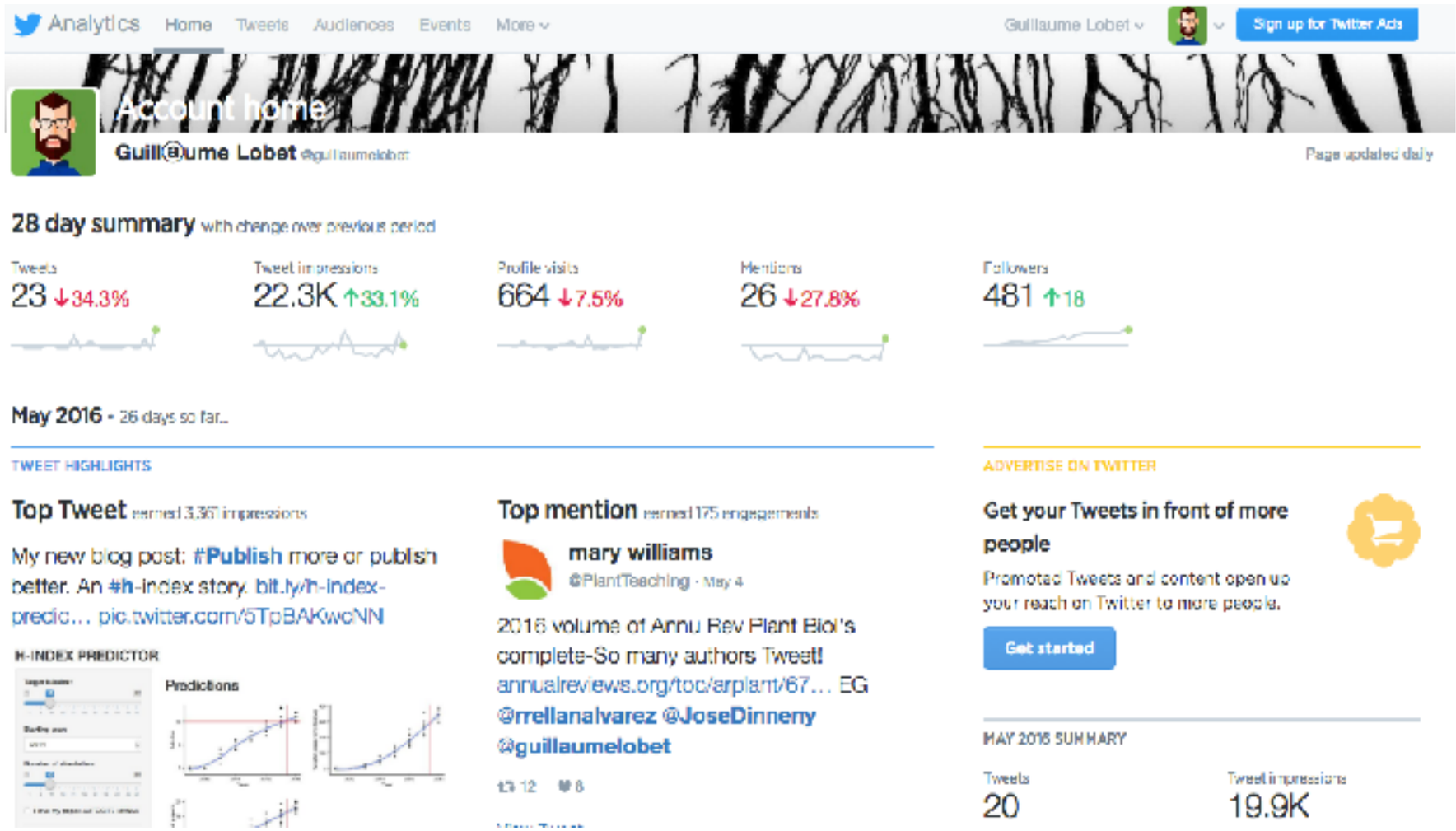
LIKE

flag an interesting tweet. Used to be stars...

DM

Direct message, for private conversations.
Only for people who follow each others

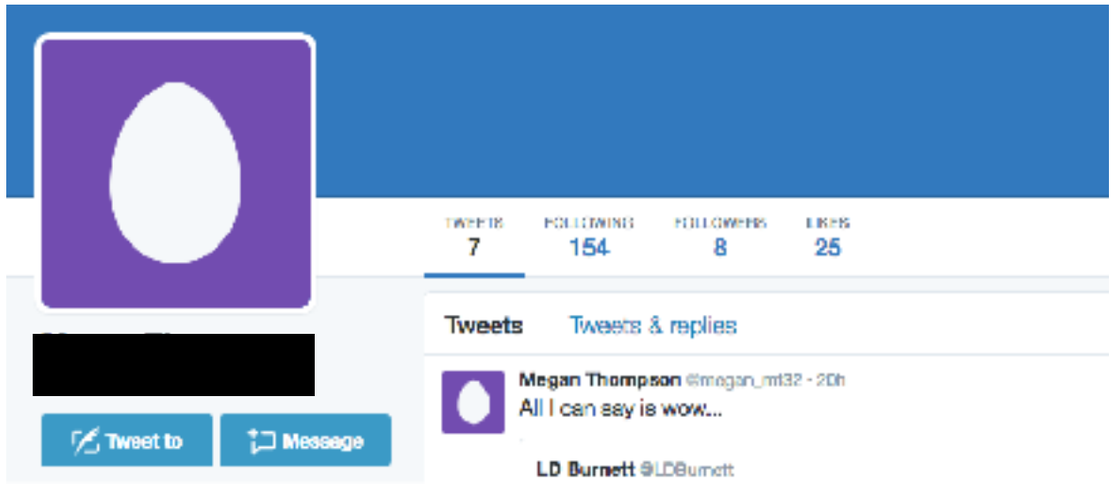
TWITTER ANALYTICS



https://analytics.twitter.com/user/username

TIPS AND TRICKS

GET RID OF THE EGG!



PROFILE

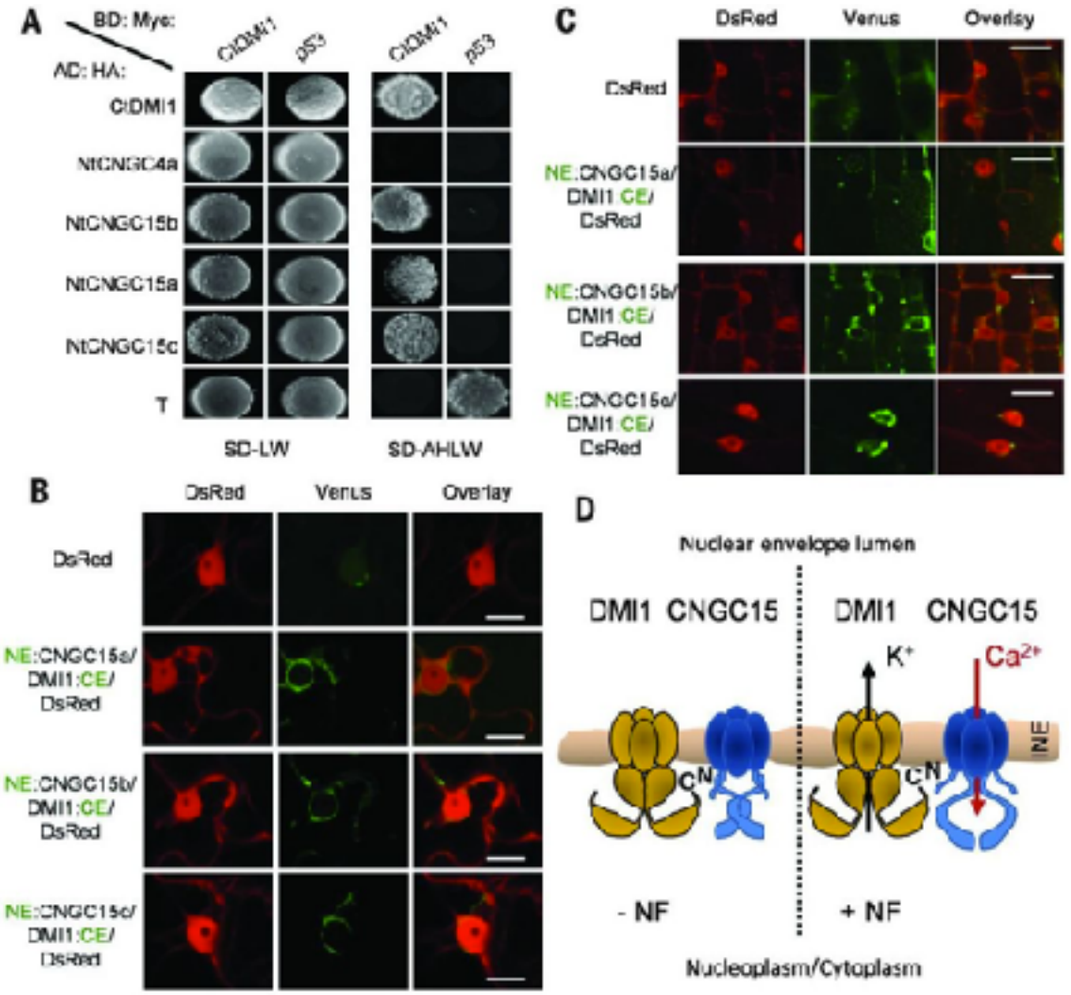
Your **picture**.
– Can be changed

Your **name**.
- Can be changed
- Make it meaningful

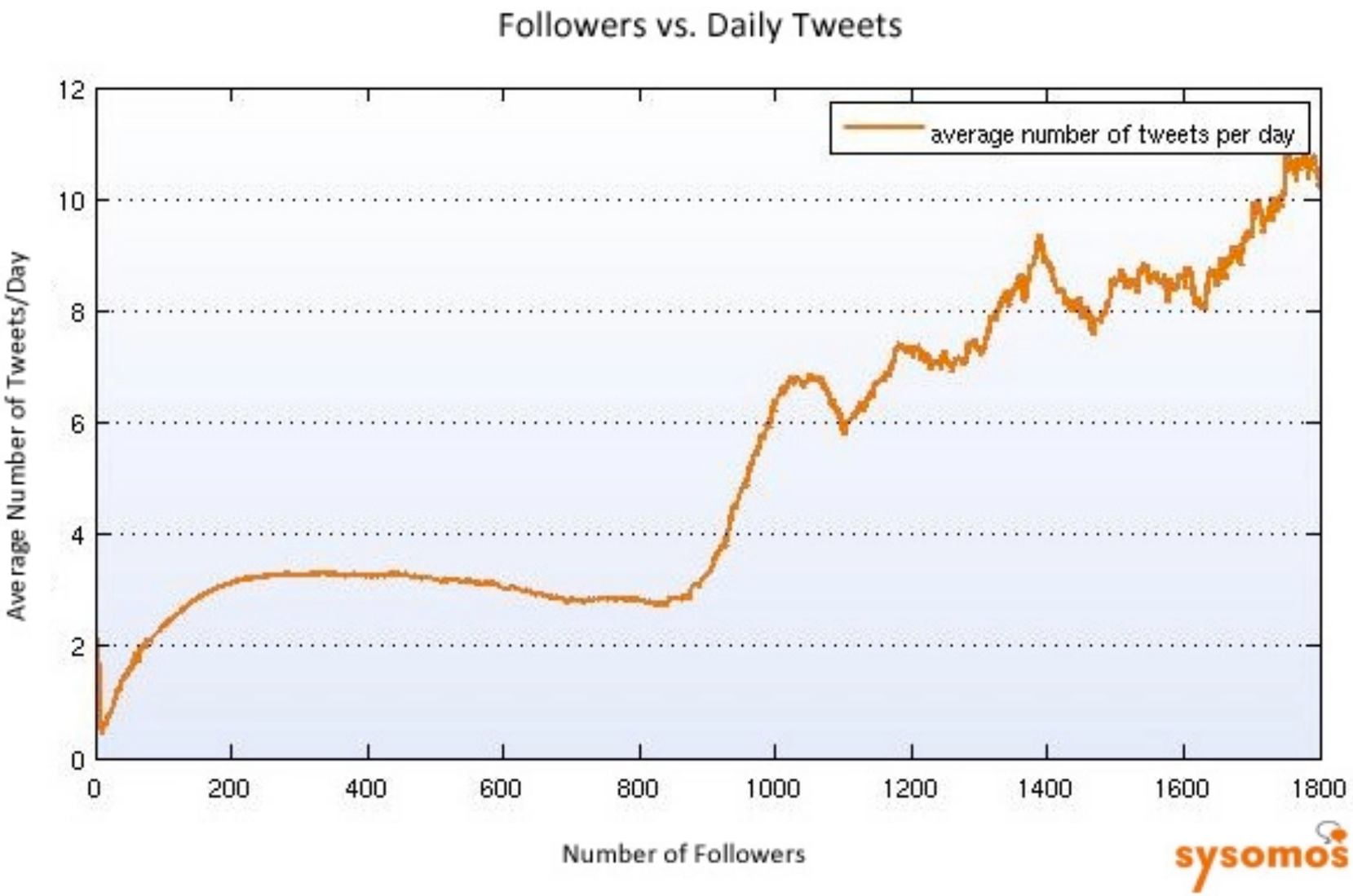
Your **handle.**
- **Cannot be changed**
- Make it easy
- Use your name

Your **bio**.
- Can be changed
- Make it informative

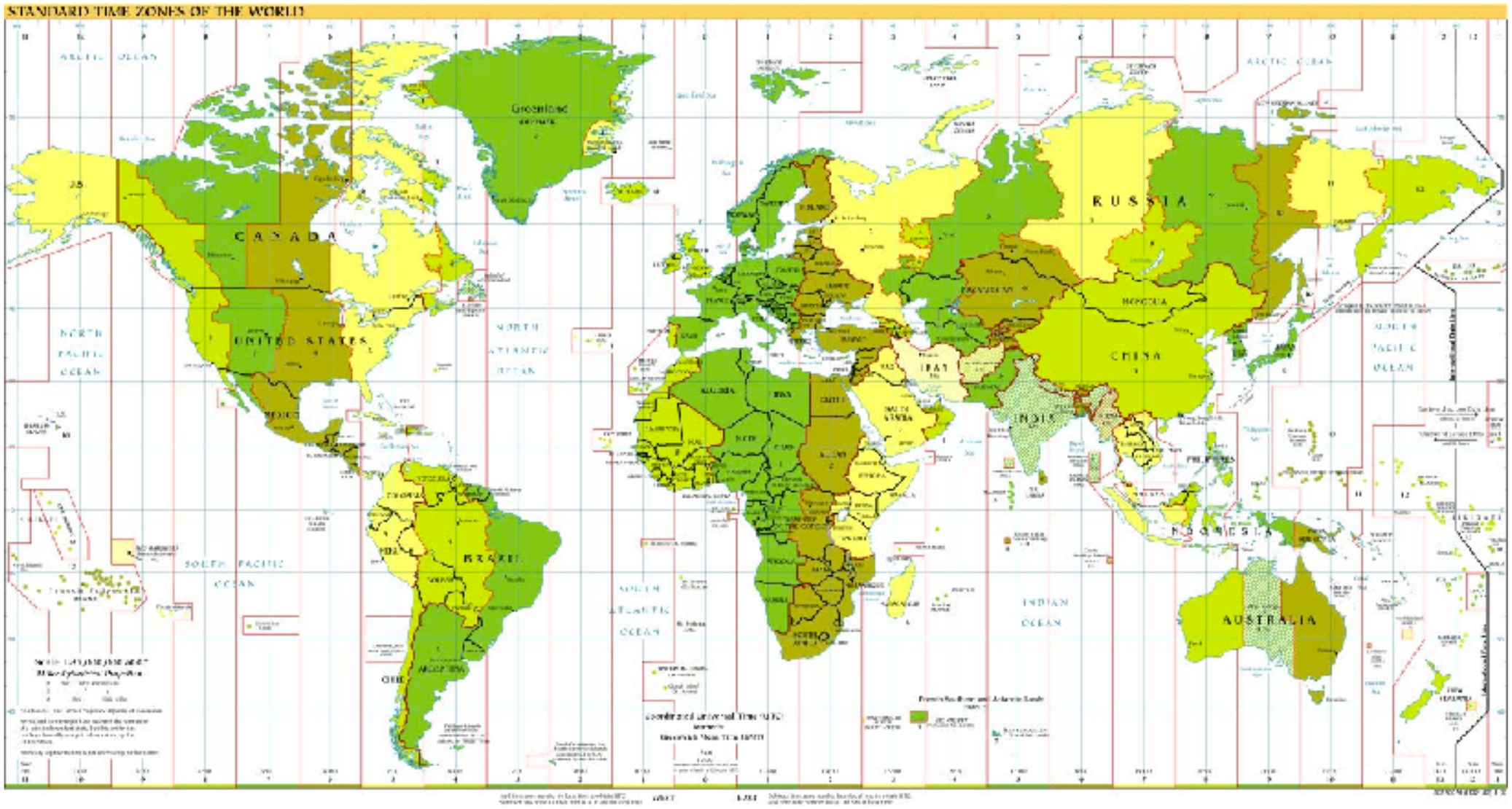
TWEETS DEFINE FOLLOWERS



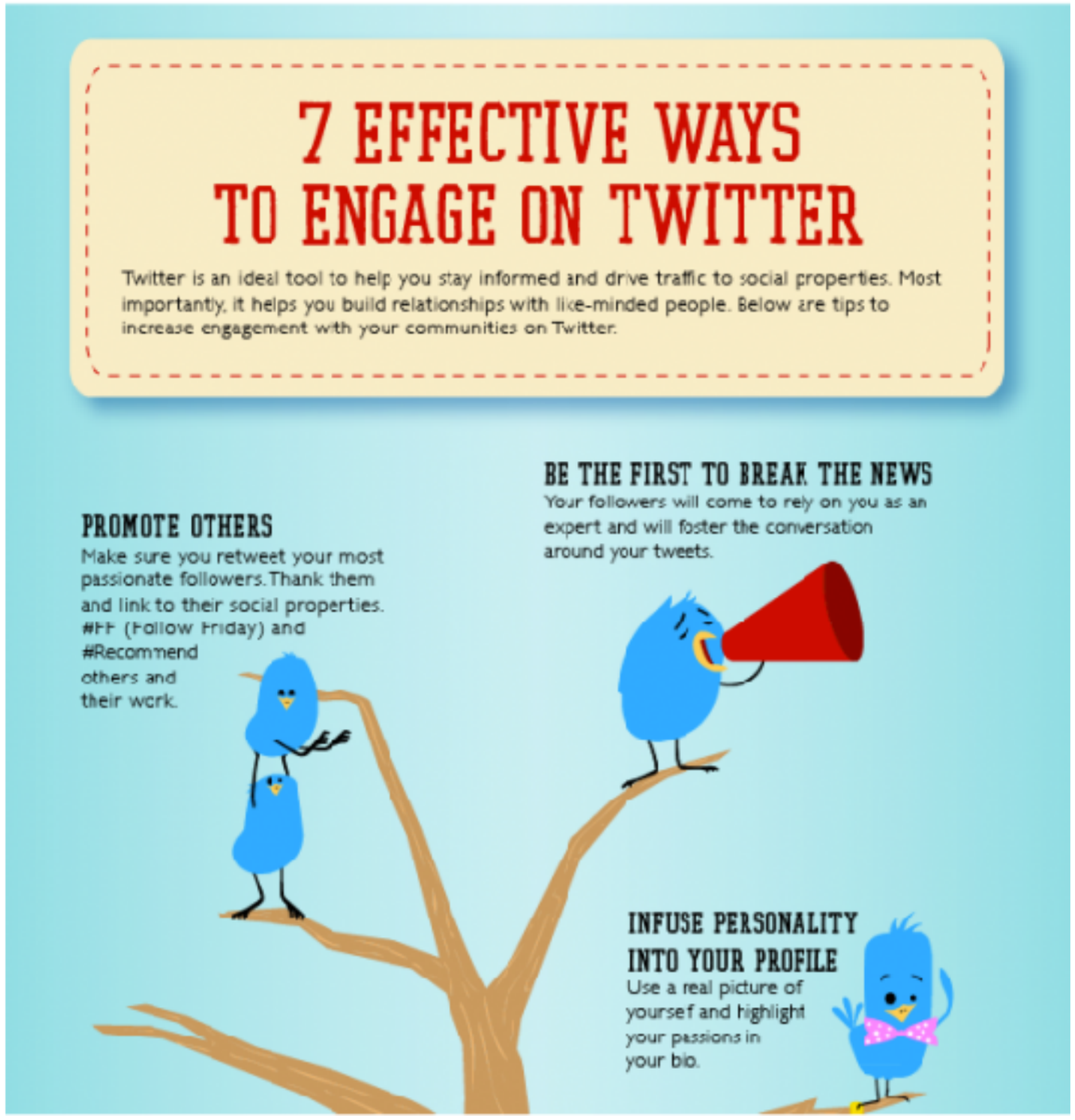
TWEETS DEFINE FOLLOWERS



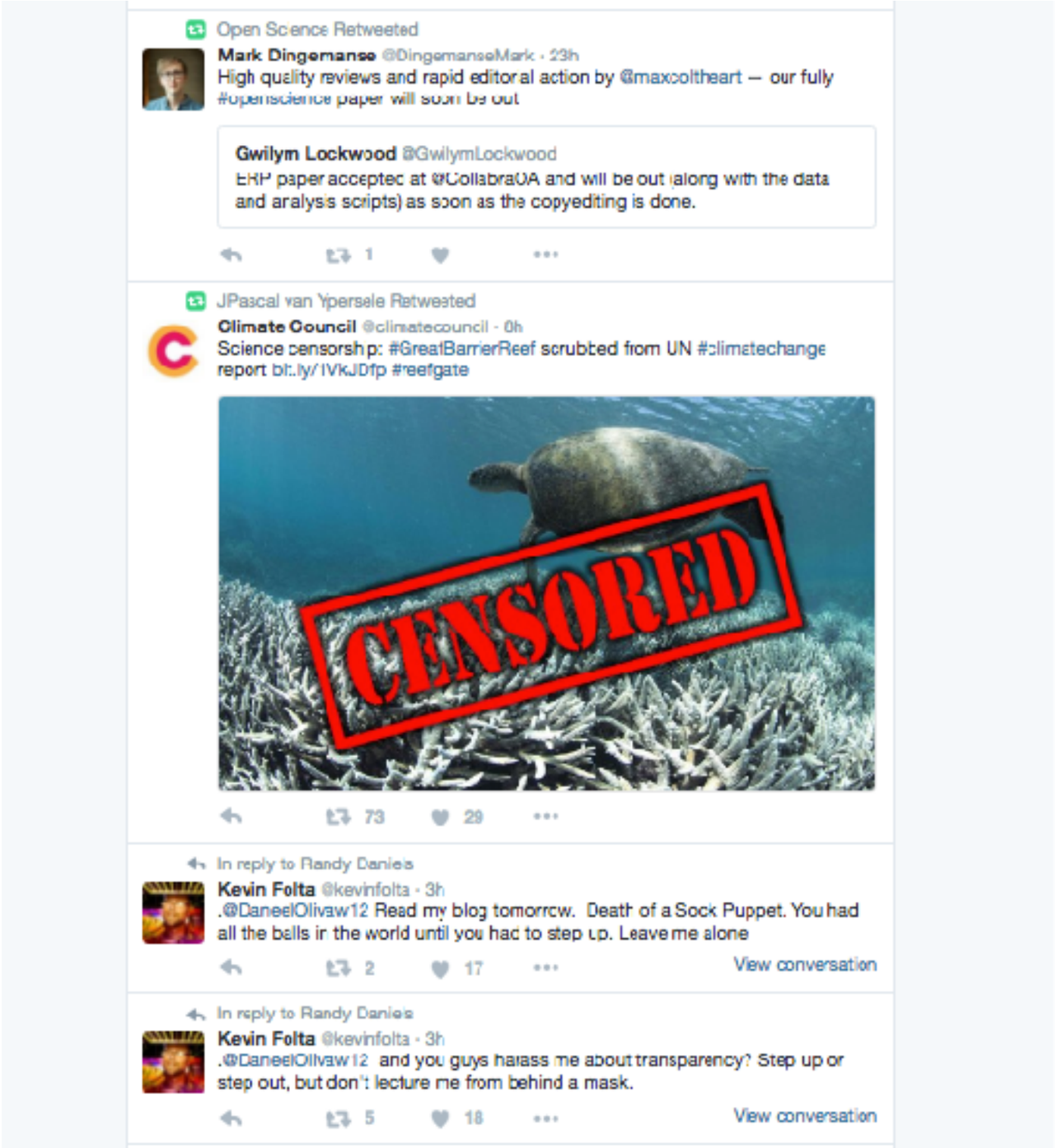
PLAN YOUR TWEETS FOR LARGER AUDIENCE



ENGAGE WITH OTHER PEOPLE BE NICE !



ADD IMAGES FOR BETTER IMPACT



USE URL SHORTENERS

https://www.dropbox.com/s/8z2a4gv8q2phamw/20160527_social_media.pdf?dl=0

http://bit.ly/lobet-social-media

WHAT TO DO:

- Create 2 groups
- Choose a name for the group / twitter account
- Define the *editorial* lines
- Create the twitter account (www.twitter.com)
- Personalise the profile page
- Start tweeting

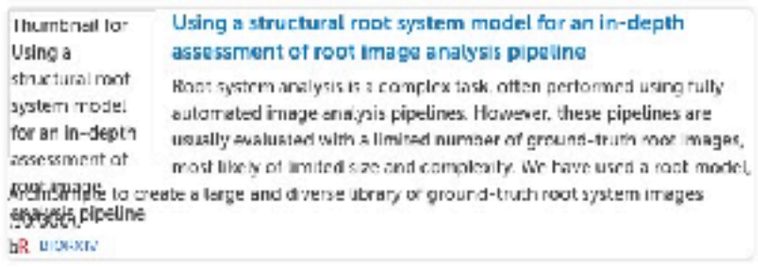
SAVE YOUR TWEETS ON STORIFY

As seen on plantmodelling.xyz

Twitter reviewing + response

Live reviewing but Larry M York of a bioRxiv pre-print + reply from Guillaume Lobet

by Guillaume Lobet a year ago 73 Views



Larry M. York @LarryMattYork — Follow

Replying to @guillaumelobet

Interesting and useful. concept of synthetype a bit confusing. simulation parameter set is more like a genotype 1/n

6:15 PM - Sep 16, 2016

1

Larry M. York @LarryMattYork — Follow

Replying to @LarryMattYork @guillaumelobet

the 10 outcomes of that simulation parameter set are more like phenotypes as influenced by 'environmental' conditions 2/n

6:19 PM - Sep 16, 2016

2

https://storify.com