

LIMS zur digitale Erschließung und Bewahrung pflanzengenetischer Ressourcen am IPK- Gatersleben



Matthias Lange
12. Juni 2018

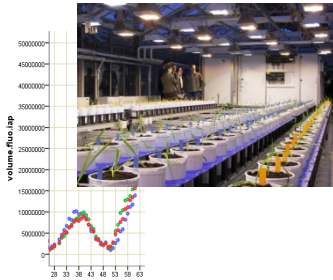


IPK – Leibniz-Institut für Pflanzengenetik und Kulturpflanzenforschung



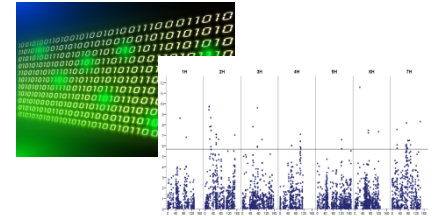
IPK Forschungsschwerpunkte

Anpassung und Nachhaltigkeit



**Pflanze-Umwelt
Interaktion**

Bereitstellung und Nutzarmachung



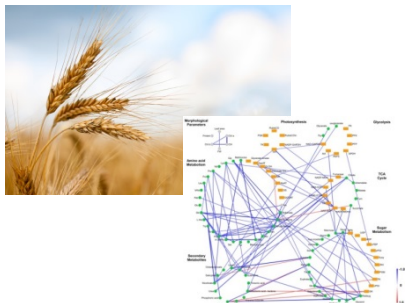
**Erschließungs-
konzepte für
PGR**

**Biodiversität
der
Kulturpflanzen**

**Wachstum
und
Stoffwechsel**

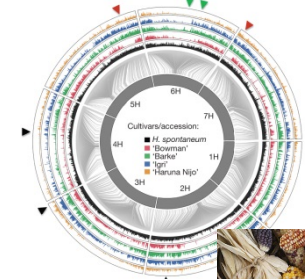
**Genom-
diversität
und Evolution**

**Pflanzliche
Leistung**

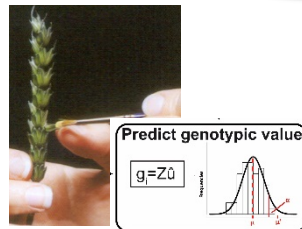


**Pflanzliche
Reproduktions-
mechanismen**

**Genetische
Vielfalt**



**Züchtungs-
technologien**



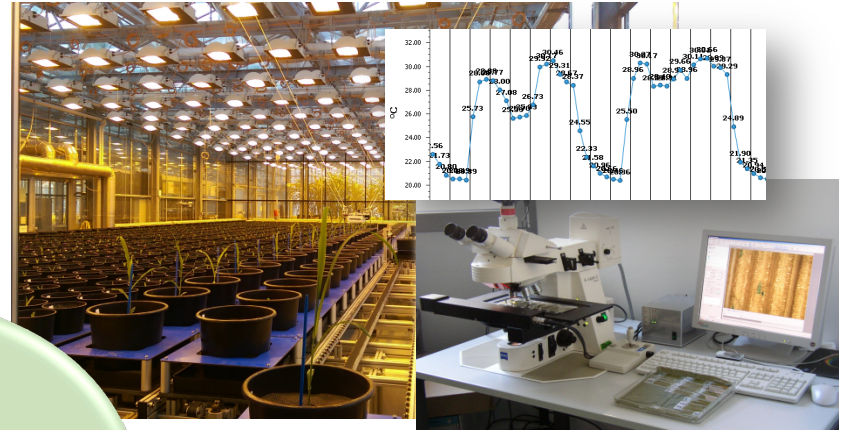
Datenspektrum



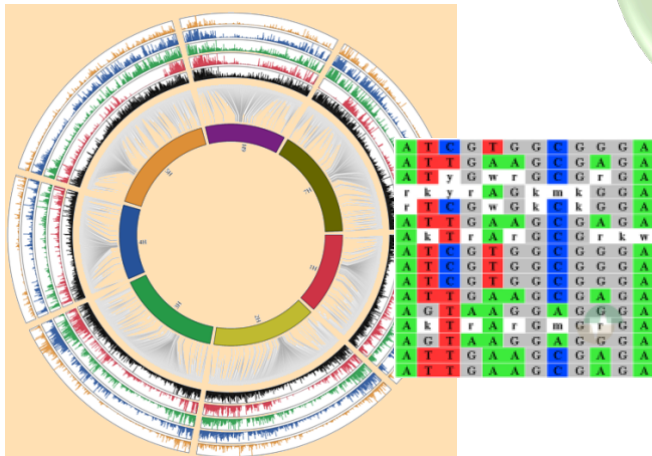
Handschriftliche Aufzeichnungen
Feldbonituren, Lagermanagement



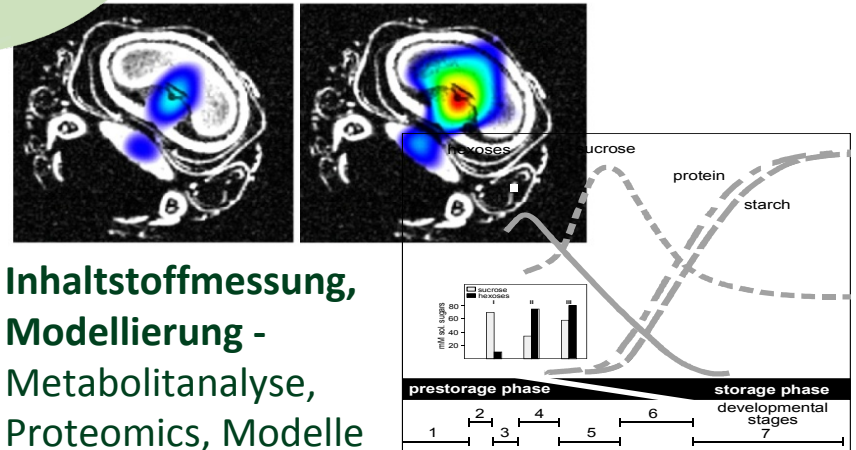
**Biodiversität
der
Kulturpflanzen**



**Automatisierte/Hochdurchsatz
Phenotypisierung - Heterogene
Sensorikplattformen**

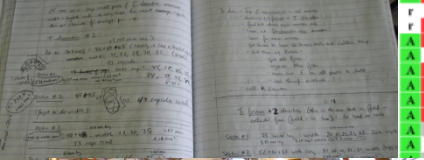
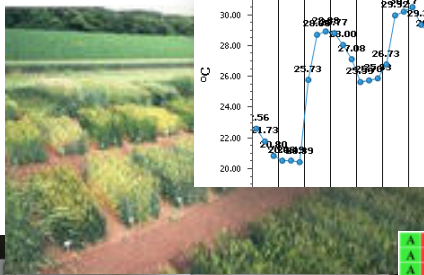
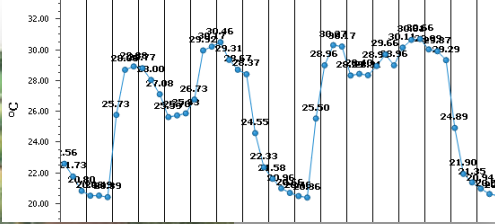


**Genotypisierung – Genome und Marker
Daten**

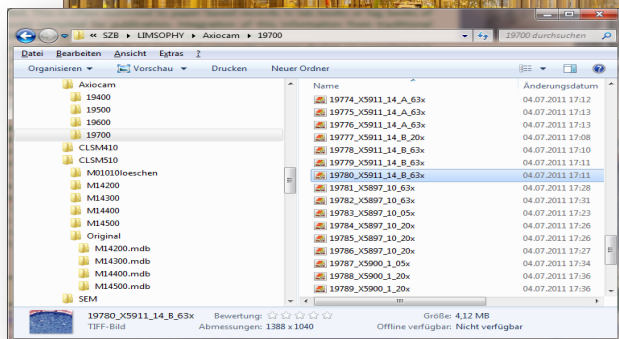
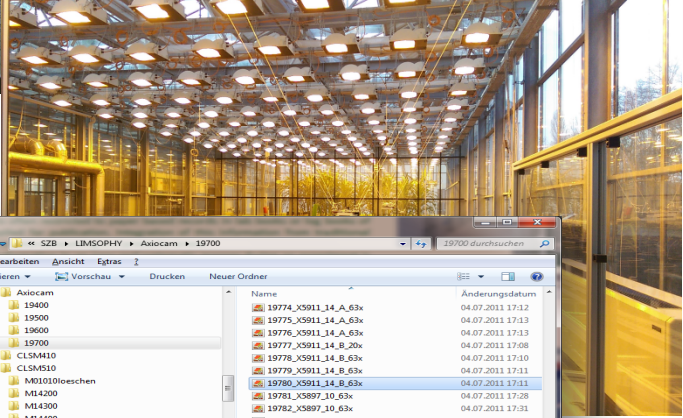
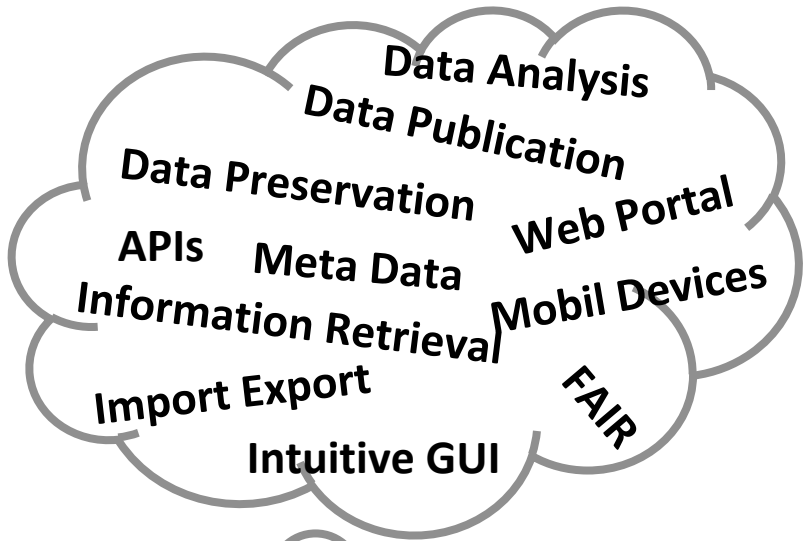


**Inhaltstoffmessung,
Modellierung -
Metabolitanalyse,
Proteomics, Modelle**

Die Herausforderung: LIMS/ELN als zentrale Datenmanagement-Infrastruktur



A DNA sequence alignment grid showing letters A, T, C, G in various colors (red, green, blue) on a grid.



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Vorgehensweise LIMS-Einführung am IPK

Entscheidung Institutsleitung zum Bedarf

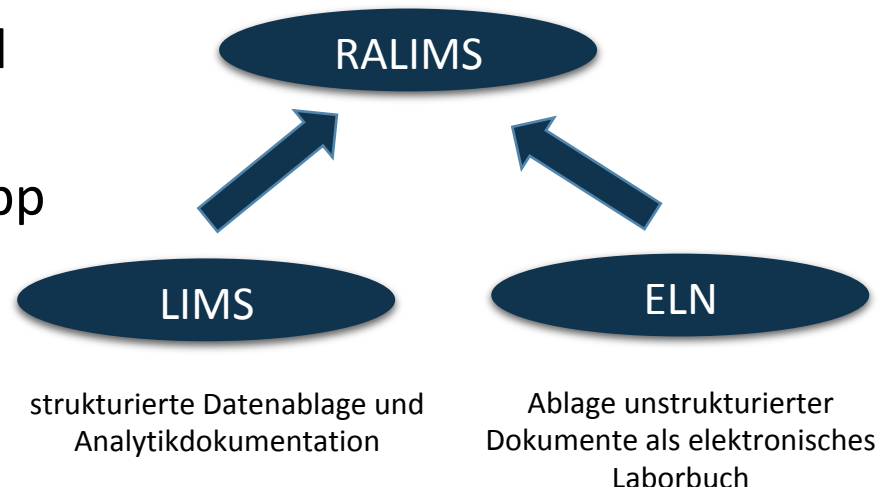
Finanzierung Projektgruppe LIMS über 12 Monate

Eigenschaften IPK-LIMS-System

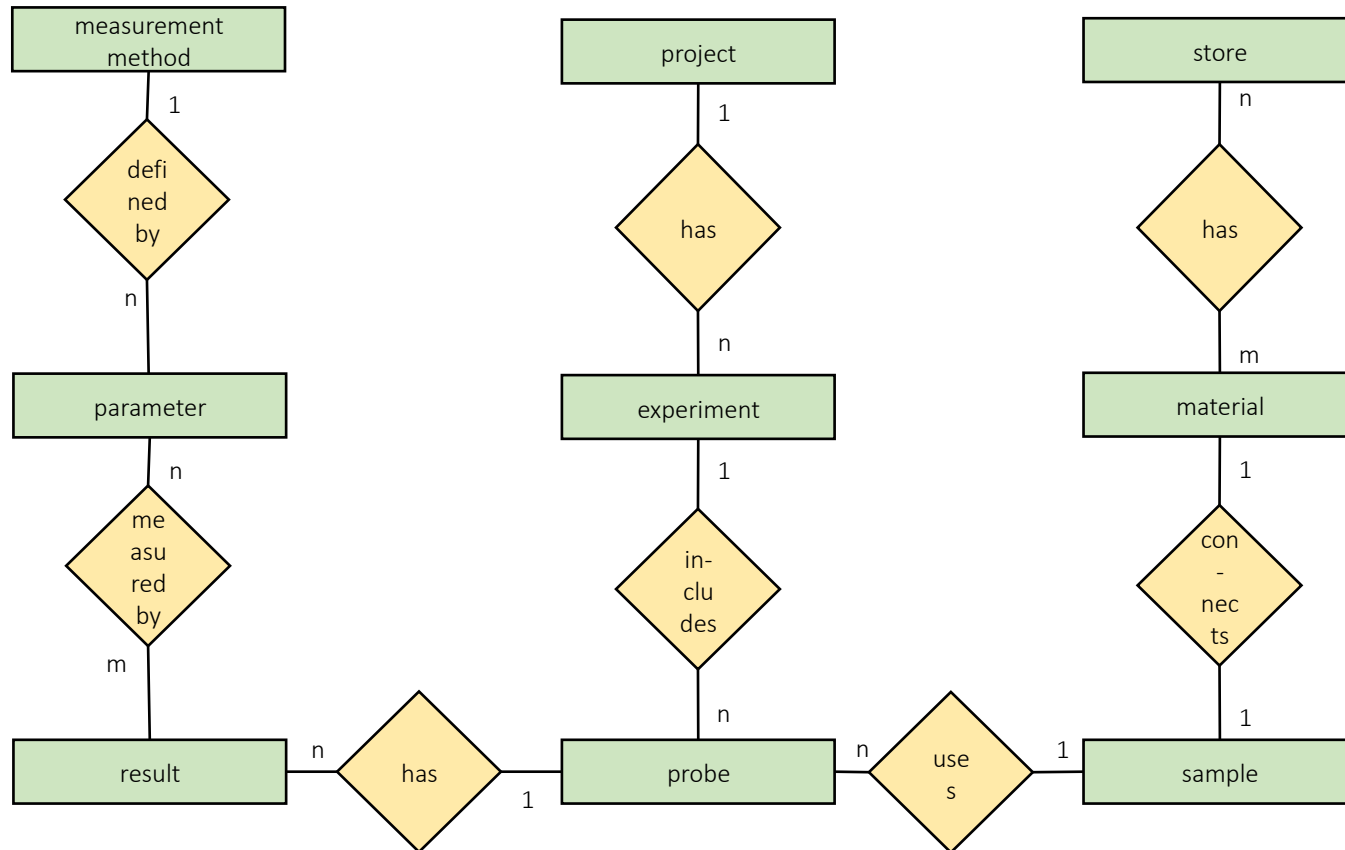
- Kombination aus LIMS und ELN
- Kombination relationale Datenbank und externer Speicher
- Anpassbare, tabellarische Nutzeroberfläche
- Frei programmierbare Import- und Exportschnittstellen
- Zentrale Installation als Remote App (MS-Windows Server)
- Erweiterbares Datenschema
- Auditierung und Datenschutz



A · A · C
Infotray AG



LIMS Datenstruktur – Nachhaltig durch Einfachheit



LIMSOPHY Module

- Gruppiert in Funktionskategorien
- Tabellarische Darstellung von Allgemein zu Details
- Individuelle Ansichten, Layouts und Berechtigungen
- Copy/Paste Integration in Standardsoftware
- Auditierung, Archivierung
- Offline-fähig

The screenshot displays the Limsophy software interface. At the top, there is a menu bar with options: Edit, View, Favourites, Layouts, Tools, Modules, Window, and ?. Below the menu bar is a toolbar with various icons. The main window is titled 'Methods' and features the IPK logo in the top right corner.

The 'Methods' section contains a table with the following data:

Name	Methods Typ	Archive Status
Elementar Analyse		aktiv
ELISA		aktiv
Extraktion von DNA		aktiv
Fettsäuren		aktiv
Flow cytometric analysis of le...	Flow cytometric...	aktiv
Flow cytometric analysis of s...	Flow cytometric...	aktiv
Flow cytometric Pufferprotok...		aktiv

Below the 'Methods' table is a detailed view for a selected method, showing fields for Name, Methods Typ, Archive Status, File, and Responsible. The 'Methods Version' section contains a table with the following data:

Versi...	Description	File	Released on	Released by	Status of Version	Comment
3		alle Präp.protokolle für Same...	08/09/2011	WEIGELT	Freigegeben	
2		alle Präp.protokolle für Samen.d...	05/05/2011	SHARBEL	Ersetzt	
1		Protocols for the Flow Cytometry...	03/05/2011	SHARBEL	Ersetzt	

At the bottom right of the interface, there is a 'Processing Mode' field with the value 'Limsophy : LANGE@genophen'.

LIMSOPHY LIMS für strukturierte Daten

- Tabellen und Attributen
- Generische Ergänzungen (EAV)
- Datentypen
 - Wahrheitswerte
 - Text
 - Zahlen
 - Diskrete Werte
 - Dateireferenzen
 - Binärdaten

The screenshot displays the LIMSOPHY LIMS software interface. The main window shows a table of samples with columns for 'Nr.', 'Linie', 'Generation', 'Genotype', 'Datei', 'Pflanzdatum', 'Wachstumsdau.', 'Saatgut', and 'Result - Val.'. Below this, a detailed table shows 'Bestückung' (A-H) with columns for 'Proben-Nr.', 'Leaf', 'Leaf..mm..', 'Proben-Nr.', 'Leaf', 'Leaf..mm..', and 'Prot'. To the right, a line graph plots 'Biomass' (y-axis, 0.0 to 9.0) against 'Pflanzdatum' (x-axis, 18.09.2011 to 10.04.2011). The graph shows two data series: one in red and one in purple. Below the graph, a table shows 'Anzahl' and 'Datei-Referenzen'. On the left, a microscopic image shows three plant leaves, with the middle one being larger and more developed than the others.

LIMSOPHY: ELN Funktionalität

- Elektronisches Laborbuch
- Unstrukturierte Daten
- Vorlagenbasierten Ausfüllen von Laborprotokollen

The screenshot displays the LIMSOPHY software interface, which is used for laboratory information management and electronic lab notebooks (ELN). The main window is titled 'RALIMS' and features a menu bar with options like 'Bearbeiten', 'Sicht', 'Favoriten', 'Layouts', 'Extras', 'Module', and 'Fenster'. Below the menu is a toolbar with various icons for file operations and navigation.

The interface is divided into several sections:


- Proben (Experiments):** A table listing various experiments with columns for 'Experiment', 'Beschreibung', 'Probenotyp', 'Erfass-Transaktion - D...', and 'Probenstatus'. One experiment, 'RNR6 Experiment 14' with the description 'PCR gen. DNA', is highlighted in blue.
- Detail View:** A detailed view of the selected experiment, showing fields for 'Projekt-Nr.', 'Uproj-Nr.', 'Exp-Nr.', 'Proben-Nr.', 'Probenstatus', 'Beschreibung', 'Auftraggeber', and 'Adresse Auftraggeber'. Below this is a section for 'Beurteilung' (Evaluation) and a 'PCR Protokoll Touchdown Taq' table.
- PCR Protokoll Touchdown Taq:** A table detailing the PCR protocol steps, including components and their volumes, and a table of cycle parameters.
- Thumbnail View:** A window showing a gel electrophoresis image with a thumbnail of the gel. The image shows a single band, indicating a successful PCR amplification. The thumbnail window includes metadata such as 'User: 9', 'Exp. Time: 0:16 sec', 'Upper: 255', 'Lower: 0', 'Int.: 0', and 'Date: 21.03.2012, Time: 12:06:51'.
- Ergebnisse (Results):** A table at the bottom showing the results of the PCR TD Taq experiment, with columns for 'Parameter', 'Thumbnail (Dat...)', 'Ergebnis - Wert', and 'Date'.

Akzeptanzerhöhung durch Erstellung nutzerspezifische Frontends

Limsofhy

Bearbeiten | Sicht | Favoriten | Layouts | Extras | Module | Fenster ?

Lemnatec_Aufträge



Datenimport | Ergebnisse | Studien

Laden aller Lemnatec_Experimente

1. Wählen Sie bitte das benötigte Lemnatec-Projekt aus und beschreiben Sie Ihr Experiment !

LTA 6-well-tray

LTC 2-pot-config

LTA 12-well-tray

LTC 4-pot-config

LTA single pot

LTC single pot

LTB single pot

2. Importieren Sie ihr CSV-Sheet und speichern Sie ihre Daten im Limsofhy


Datenimport (1. Teilimport)

Datenimport (2. Teilimport)

Speichern

3. Bitte markieren Sie die gewünschten Proben für den Export

Datenexport_Lemnatec



Anlage

- ▶ LTA 6-well-tray
- LTA 12-well-tray
- LTA single pot
- LTB single pot
- LTC 2-pot-config
- LTC 4-pot-config
- LTC single pot

Numm.../...	Experiment der Anlage	Beginn	Ende	Verantwortlicher	Experimentstatus
▶ 3118	1634AJ_LTA			Dr. Astrid Junker	in Bearbeitung

Assay-Informationen

Ereignisse | Zusätzliche Information | Keywords | Personen | Bereiche | Publikationen

Datensatz für Ereignisse hinzufügen

Name	Beschreibung des Ereignisses	Dateien in der ...
▶ Ereignis	27.08.2016 Carrier stuck in the morn...	
Ereignis	29.08.2016 FluorCam measuremen...	
Datum des Erei...	27.08.2016	
Datum des Erei...	29.08.2016	

Proben (Experimente)

PlantID	Measurement I...	Treatment	Species (...)	Genotyp (...)	Variety	Well/Position	Stc
▶ 1634AJ0...	1634AJ		Zea mays	ZEA 3115		A1	
1634AJ0...	1634AJ		Zea mays	ZEA 3115		A2	
1634AJ0...	1634AJ		Zea mays	ZEA 3115		B1	
1634AJ0...	1634AJ		Zea mays	ZEA 3115		B2	
1634AJ0...	1634AJ		Zea mays	ZEA 3115		C1	
1634AJ0...	1634AJ		Zea mays	ZEA 3115		C2	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		A1	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		A2	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		B1	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		B2	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		C1	
1634AJ0...	1634AJ		Zea mays	ZEA 1136		C2	
1634AJ0...	1634AJ		Zea mays	ZEA 752		A1	

Parameter

	Prüfmethode	Parameter	Ergebnis - Wert	Einheit	Kommentar
▶ <input type="checkbox"/>	01. Carrier-Konf...	seeding date	22.08.2016		
<input type="checkbox"/>	01. Carrier-Konf...	pot	6-well tray		
<input type="checkbox"/>	01. Carrier-Konf...	Covering	no cover		
<input type="checkbox"/>	09. Experiment...	Replicate	6		
<input type="checkbox"/>	02. IsaTab Stud...	Characteristics(Assay s...	22.08.2016		
<input type="checkbox"/>	02. IsaTab Stud...	Characteristics(Assay d...	10		
<input type="checkbox"/>	02. IsaTab Stud...	Characteristics(Growth ...	small LemnaTec phyt...		
<input type="checkbox"/>	03. Rooting Pro...	Rooting medium germi...	substrate 2 (Klasman...		
<input type="checkbox"/>	03. Rooting Pro...	Container type germin...	6-well tray		
<input type="checkbox"/>	03. Rooting Pro...	Container dimension g...	3x3	cm	
<input type="checkbox"/>	03. Rooting Pro...	Number of plants per c...	1		
<input type="checkbox"/>	06. Aerial condi...	start of light period post...	06:00		
<input type="checkbox"/>	06. Aerial condi...	end of light period post ...	22:00		
<input type="checkbox"/>	08. Watering	Irrigation type germinat...	automated		

Bearbeitungsmod DE | Limsofhy : LANGE@genophen

Projektspezifische Web-Portale

The screenshot shows a web browser window displaying the BRIDGE portal. The browser's address bar shows the URL: `apex.ipk-gatersleben.de/apex/f?p=164:14:427942456578::NO::`. The page features a green header with the 'BRIDGE' logo and a navigation menu on the left with options like Project, Data, Progress, Report, APIs, and Contact. The main content area contains a table with the following data:

Accenumb internal	Last Lims Import	Treatments & Measurements	Fullbotname	Annuality
HOR_16273	17-MAR-2017	comments: It could also be a convar3/not con.2 with spike.Only one spike has branching or could be a con. 3	Hordeum sp.	spring type
HOR_16223	17-MAR-2017	comments: In one of spikes the ending of some of central glumes looks like a new spiklet	Hordeum sp.	spring type
HOR_10801	17-MAR-2017	awns_length: 21.5	Hordeum vulgare L. convar. distichon (L.) Alef. var. nutans (Rode) Alef.	spring type
HOR_10812	17-MAR-2017	awns_length: 13.5	Hordeum vulgare L. convar. distichon (L.) Alef. var. erectum (Rode) Alef.	spring type
HOR_3087	17-MAR-2017	awns_length: 22.5	Hordeum vulgare L. convar. vulgare var. hybernum Viborg	winter type
HOR_11126	17-MAR-2017	awns_length: 15.5	Hordeum vulgare L. convar. distichon (L.) Alef. var. erectum (Rode) Alef.	spring type
HOR_11128	17-MAR-2017	awns_length: 16.5	Hordeum vulgare L. convar. distichon (L.) Alef. var. erectum (Rode) Alef.	spring type
HOR_11137	17-MAR-2017	awns_length: 15.5	Hordeum vulgare L. convar. distichon (L.) Alef. var. erectum (Rode) Alef.	spring type

Status

Querschnittsaufgaben

- Lagerungsverwaltung
- Chemikalien, Gefahrstoffe
- GVO
- Fotoarchiv

Projektdatenmanagement

- Laborbuch/Versuchsprotokollierung
- Primärdatenkatalogisierung und -verwaltung
- Ablage und Organisation von quantifizierten Messdaten
- Migration obsoleter Datenbanken und Informationssystemen
- Laboraufträge und Datenauslieferung
- Projektspezifische Web-Portale

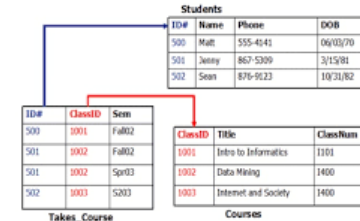
	GESAMT	2017	2016	2015	2014	2013	2012	2011
Proben	2.328.506	1.109.390	162.663	176.540	618.046	48.110	86.444	127.313
Dateien	1.714.149	297.623	261.095	456.352	317.274	178.196	190.319	13.290
Ergebnisse	4.664.003	2.218.708	487.989	353.080	123.6092	96.220	17.288	254.626
Aktive Nutzer (pro Jahr)		160	131	101	54	70	42	nicht mehr verfügbar

Arbeitsschwerpunkte Datenmanagement

• IT-Infrastructure

- Laboratory Information Management System: LIMSOPHY
- Scalable Storage Management System: HSM
- Scalable Hardware: Oracle Data Appliance
- Database Technology: relational, noSQL
- Frontend Technologies (OS-native, Web, Mobile Devs)

Relational DBMS



• FAIR Data Management

- Data Sharing and Publication: DataCite
- Unique Researcher Identifier: ORCID-DE
- Search Engines, Registries, Repositories: diverse
- RESTful API's: Breeding API
- Research Data Management Plans: ongoing



• Defined Processes and Communication

- Minimum Information Standards: MIAPPE, MCPD
- Standards: material naming, IDs, file formats, storage paths
- Lab-Processes and policies: sequencing, chemicals, ...
- User Training and Support

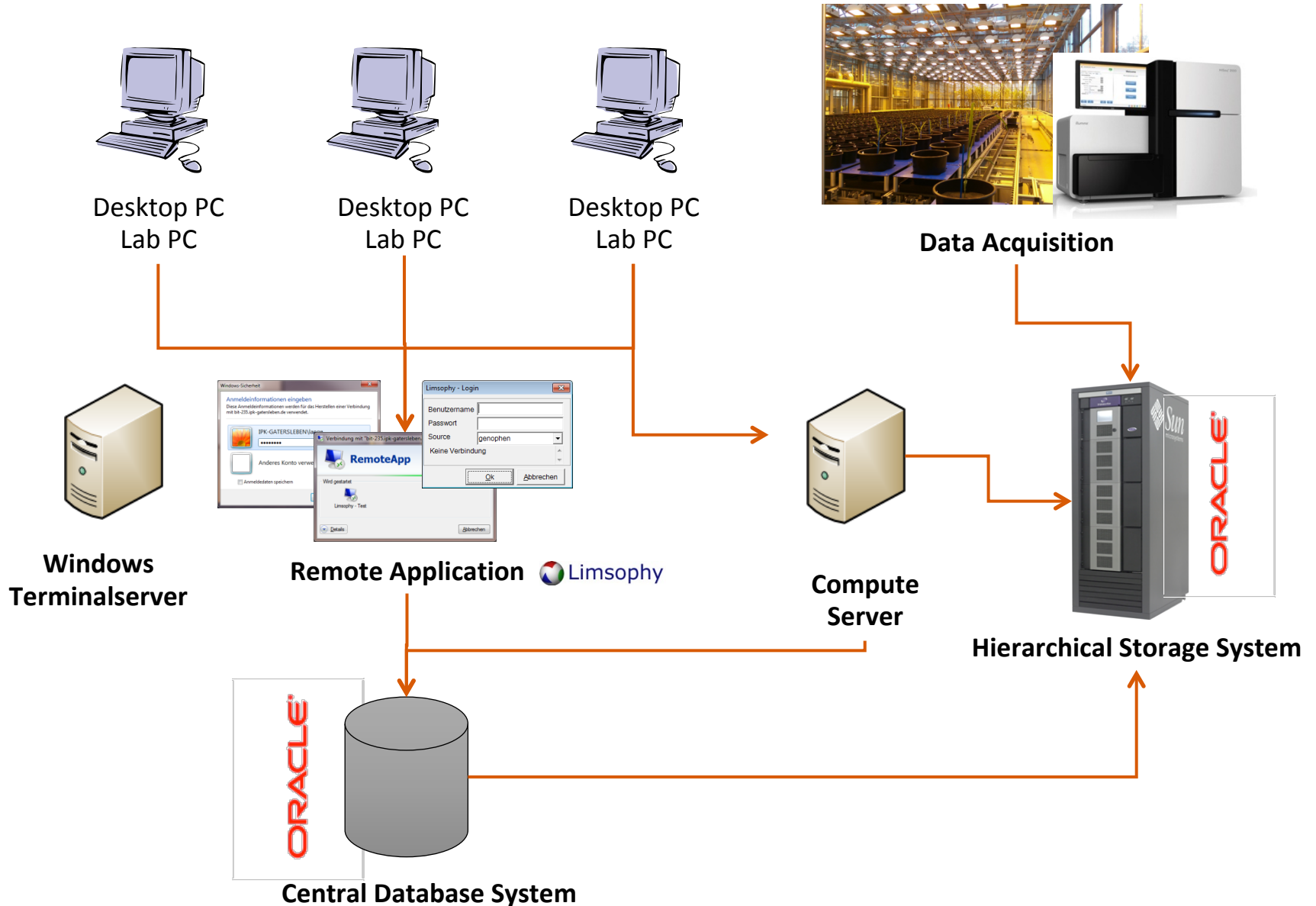




Danke für Ihre Aufmerksamkeit



Architektur der IPK LIMS-Dateninfrastruktur



LIMS als Basis für FAIR Data Management

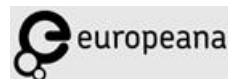
Infrastructure:



Data
Publication:



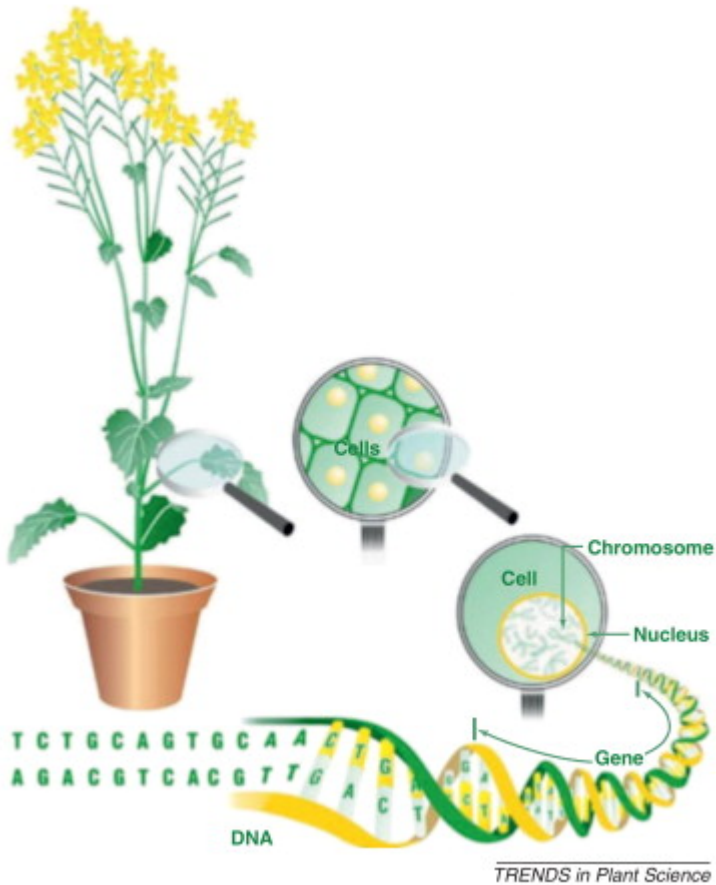
Plant Genetic Resources
and Biodiversity:



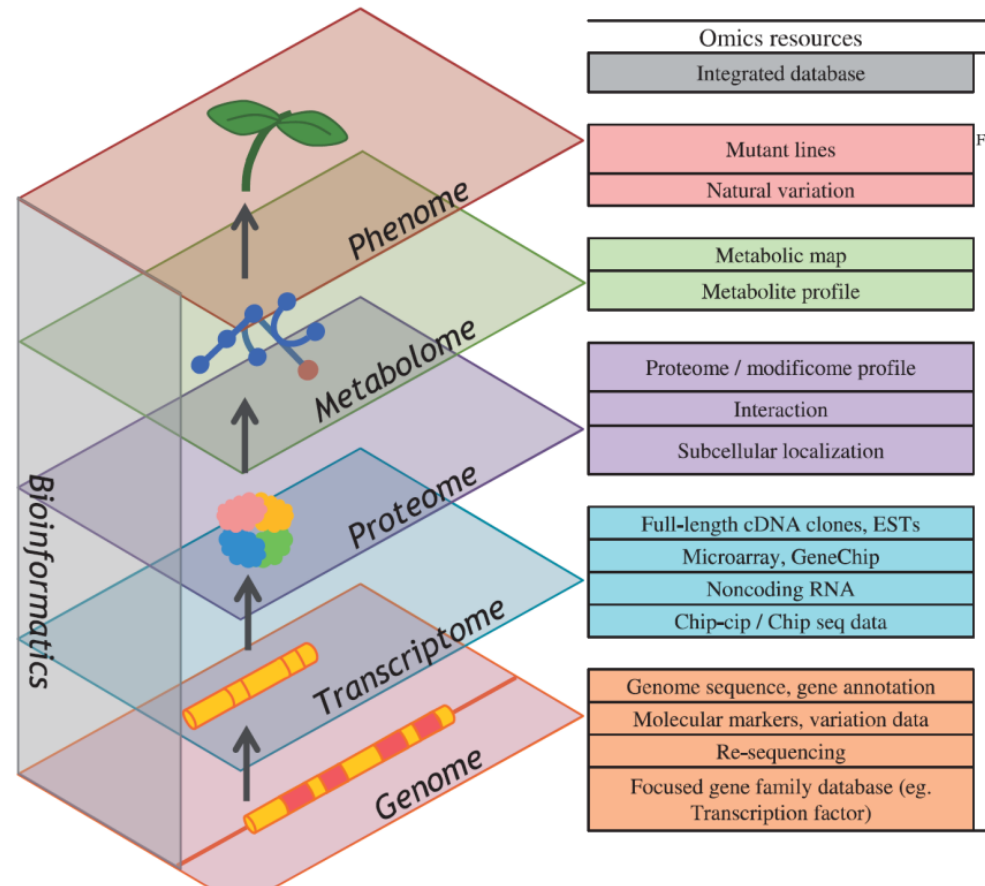
Plant Phenotyping
Networks & Standards:



“Vom Gen zum Phen”



(R. Furbank, M. Tester, Trends in Plant Science, 2011)



(K. Mochida K. Shinozaki, Plant Cell & Physiology, 2010)