

1 **Rice Galaxy: an open resource for plant science**

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23

24 **Abstract**

25 *Background*

26 Rice molecular genetics, breeding, genetic diversity, and allied research (such as rice-pathogen  
27 interaction) have adopted sequencing technologies and high density genotyping platforms for genome  
28 variation analysis and gene discovery. Germplasm collections representing rice diversity, improved  
29 varieties and elite breeding materials are accessible through rice gene banks for use in research and  
30 breeding, with many having genome sequences and high density genotype data available. Combining  
31 phenotypic and genotypic information on these accessions enables genome-wide association analysis,  
32 which is driving quantitative trait loci (QTL) discovery and molecular marker development. Comparative  
33 sequence analyses across QTL regions facilitate the discovery of novel alleles. Analyses involving DNA  
34 sequences and large genotyping matrices for thousands of samples, however, pose a challenge to non-  
35 computer savvy rice researchers.

36 *Findings*

37 We adopted the Galaxy framework to build the federated Rice Galaxy resource, with shared datasets,  
38 tools, and analysis workflows relevant to rice research. The shared datasets include high density  
39 genotypes from the 3,000 Rice Genomes project and sequences with corresponding annotations from  
40 nine published rice genomes. Rice Galaxy includes tools for designing single nucleotide polymorphism  
41 (SNP) assays, analyzing genome-wide association studies, population diversity, rice-bacterial pathogen  
42 diagnostics, and a suite of published genomic prediction methods. A prototype Rice Galaxy compliant to  
43 Open Access, Open Data, and Findable, Accessible, Interoperable, and Reproducible principles is also  
44 presented.

45 *Conclusions*

46 Rice Galaxy is a freely available resource that empowers the plant research community to perform state-  
47 of-the-art analyses and utilize publicly available big datasets for both fundamental and applied science.

48 **Keywords**

49 Rice, Breeding, workflow, genomes, high-density genotypes, reproducibility, SNP, GWAS, Galaxy project

50 **Findings**

51 *Background*

52 With the decreasing cost of genome sequencing, rice molecular geneticists, breeders and diversity  
53 researchers are increasingly adopting genotyping technologies as routine components in their  
54 workflows, generating large datasets of genotyping and genome sequence information. Concurrently  
55 international consortia have made re-sequencing or high density genotyping data from representative  
56 diversity collections publically available. These include, but are not limited to the medium-depth (15-20x  
57 coverage) resequencing data of the 3,010 accessions from the 3K Rice Genome (3K RG) Project (~1 – 2  
58 million SNPs per accession) [1,2] and the 700,000 SNP Affymetrix array data for the 1,445 accessions of  
59 the High Density Rice Array (HDRA) germplasm collections [3]. The corresponding accessions are  
60 available at non-profit prices from the Genetic Resource Center (GRC) of the International Rice Research  
61 Institute (IRRI) for phenotyping, allowing subsequent Genome-Wide Association Studies (GWAS).  
62 Analysis of such datasets is a challenge to rice researchers due to (1) the fairly large data matrix and the  
63 compute-intensive algorithms that requires specialized computing infrastructure (a fairly large RAM,  
64 powerful CPU, and large disk space), and (2) the relative difficulty in using Open Source / free software  
65 tools for analysis, which are commonly provided without graphical user interface and require proper  
66 installation in a Linux operating system environment.

67 On the computational side, public web resources with specialized tools already exist, and are  
68 maintained at different institutions. The Rice SNP-Seek database [4,5], largely developed and hosted by  
69 IRRI, contains phenotypic, genotypic, and passport information for over 4,400 rice accessions from large  
70 scale rice diversity projects such as the 3K RG and the HDRA collections. SNP-Seek ([http://snp-  
seek.irri.org](http://snp-<br/>71 seek.irri.org) ) currently contains phenotype data for 70 different morphological and agronomic traits

72 and stores SNPs and small indels discovered by mapping the 3K RG accessions to four published rice  
73 draft genome assemblies, collectively resulting in the discovery of ~11M new SNPs and ~0.5M new  
74 indels. While SNP-Seek focused on delivery of prior analyzed content rather than providing an analysis  
75 platform, Gigwa [6] ( <http://gigwa.southgreen.fr/gigwa/> ), hosted at the South Green portal [7]  
76 (<http://www.southgreen.fr/>), is a scalable and user-friendly web-based tool which provides an easy and  
77 intuitive way to explore large amounts of genotyping data from next-generation sequencing (NGS)  
78 experiments. Gigwa allows for filtering of genomic and genotyping data from NGS analyses based not  
79 only on variant features, including functional annotations, but also on genotype patterns to explore the  
80 structure of genomes in an evolutionary context for a better understanding of the ecological adaptation  
81 of organisms. Gramene [8] is a curated, open-source, integrated data resource for comparative  
82 functional genomics in crops and model plant species that, among other species, includes rice. Data and  
83 analysis tools are available as portals at the Gramene site (<http://gramene.org/>). In these resources  
84 mentioned, the analyses methodologies are custom-built by the respective projects.

85 There are other freely available web-based bioinformatics and breeding informatics software tools,  
86 optimized for plant species other than rice, including Araport (<https://www.araport.org/>) for  
87 Arabidopsis, Cassavabase (<https://cassavabase.org/>) for cassava, and The Triticeae Toolbox (T3,  
88 <https://triticeaetoolbox.org/>) for wheat and barley. While these tools are very useful, they are  
89 species/crop specific and custom-built for the specialized requirements of their respective communities  
90 (such as project datasets), making adoption in rice challenging for at least two reasons: (1) the need to  
91 produce curated rice datasets that work seamlessly with the software system (e.g. genome-browser  
92 ready data, curated genes, published QTLs from biparental crosses and GWAS and markers associated to  
93 traits), and (2) the need for a dedicated software development team to customize the application for  
94 rice-specific data and analyses.

95 The ability of software to automate repetitive analyses task is attractive for data analysts, and the public  
96 sharing of the analytical methodology (as opposed to just the raw data and the results) enhances  
97 reproducibility and is being supported by academic communities of practice such as FORCE11  
98 (<https://www.force11.org> ). Many research groups working with NGS data have a high demand for  
99 computing infrastructure and their complex analyses often comprise several steps using different  
100 software tools (pipeline). The deployment of these different software tools is a big challenge to small  
101 institutions without dedicated scientific computing support staff. There is no single solution to address  
102 these challenges. Our approach to help overcome them is the integration of a range of these different  
103 bioinformatics tools into the Galaxy bioinformatics system. Galaxy [9] is a web-based analysis  
104 workbench and workflow management system initiated at the Penn State University. It includes a  
105 collection of software packages which can be operated via a web browser on a public server. Galaxy is a  
106 mature community effort, supported by various high-powered institutions, is relatively easy to deploy  
107 and maintain, and thus well-suited to serve low and moderately resourced institutions such as IRRI. The  
108 graphical user interface of Galaxy means that no knowledge of code is needed, thus facilitating  
109 bioinformatics analyses by researches without computational expertise.

110 We built a suite of federated Galaxy resources and tools, which we collectively named **Rice Galaxy**  
111 (Figure 1). Rice Galaxy contains shared software tools and datasets tailored to the needs of rice  
112 researchers and breeders, providing computing resources through an easy-to-use interface, and  
113 allowing reproducibility and publication of analytical methodology and results.

114 The Rice Galaxy federated resources are hosted at:

- 115 • IRRI Galaxy @ International Rice Research Institute: <http://galaxy.irri.org>
- 116 • Rice Galaxy (common) Toolshed: <http://52.76.88.51:8081/>

117 *DISCUSSION*

118 **1. Built-in / interoperable rice data**

119 The Rice Galaxy system is customized to provide rice-specific genomic and genotypic data. Of primary  
120 importance is the gold-standard *japonica* variety reference genome (Nipponbare IRGSP release 1.0) [10],  
121 to which the reference gene models and most of the SNPs published have been anchored. In addition,  
122 eight medium to high quality published genomes from various sequencing projects and the respective  
123 genome annotations for each are installed as alternative genome builds and are available as drop-down  
124 menu choices in Rice Galaxy. These include four high-quality builds from *indica*-type varieties Minghui  
125 63 and Zhengshan 97 [11], IR 8 (GenBank: MPPV00000000.1), Shuhui 498 [12], as well as an aus-type  
126 variety N 22 (GenBank: LWDA00000000.1), as well as four medium to low quality genomes, two *indica*  
127 (IR 64 , [13] and 93-11, [14] ) and two aus-type rice genomes (DJ 123, [13] and Kasalath, [15]). While  
128 these references were selected to represent diversity, they further represent variety groups that display  
129 agronomically important characteristics, such as heat and drought tolerance, disease resistance,  
130 submergence tolerance, adaptation to low-phosphorus soil, wide adaptability, good grain quality,  
131 aerobic (upland) adaptation and deep roots [16-18]. Even though these genomes are highly similar to  
132 each other, they each contain unique regions (from 12.3 Mbp to 79.6 Mbp) that may harbor genes  
133 restricted to these variety-groups [5]. With the availability of several reference genomes, it becomes  
134 relatively straightforward to custom design SNP assays that are either of broad utility across varietal  
135 groups or specific to single groups.

136 Rice Galaxy includes genotyping data of the 3k RG (such as the 3K RG 3024 accessions x 4.8M filtered  
137 SNPs, 440K core SNPs, 1M GWAS-ready SNPs, and 2.3M indels) useful for GWAS, region-specific  
138 diversity analyses, and single locus allele mining in the shared data library.

## 139 **2. Toolkits Built (and detailed discussion of each toolkit)**

140 *SNP assay design: Lift-over of SNPs from one genome to another*

141 SNPs discovered relative to the gold-standard reference genome (Nipponbare IRGSP 1.0, [10]) are  
142 commonly used in QTL mapping (either by GWAS or biparental cross). In order to develop robust

143 markers associated with the trait of interest, however, a SNP assay that works in the target varietal  
144 groups is needed. Consequently there is a need to “lift-over” SNPs from one genome to another (for  
145 example from Nipponbare *japonica* to an *indica* varietal group represented by IR 64). The workflow is as  
146 follows: (1) Get flanking sequences surrounding the target SNP in source genome (the main reference  
147 Nipponbare), (2) align these flanking sequences to target genome of variety of interest to verify if it hits  
148 a unique region in the target genome of similar location from the source genome, allowing some  
149 mismatches but not allowing multiple region hits, and (3) identify the flanking sequences surrounding  
150 the lifted-over SNP in the context of the target genome, for SNP assay design. The shared workflow is  
151 published in Rice Galaxy as [SNP lift-over].

### 152 *3k RG data access*

153 Rice Galaxy provides access to the raw variant call format (VCF) files of each accession in the 3K RG  
154 project via connection (as data source in Rice Galaxy) to the 3,000 rice genomes at Amazon Web  
155 Services (AWS) Public Data (<https://aws.amazon.com/public-datasets/3000-rice-genome/>), with tools  
156 allowing region-specific download. In Rice Galaxy, tools in the [Get Data / FROM 3KRG] section allows  
157 listing of the accessions in the 3K RG and retrieval of genotype data for a selected accession of interest  
158 from the 3K RG collection. The subset genome region of interest (chromosome name – base start – base  
159 end) can be specified and extracted from the VCF of the accession of interest stored in AWS Public  
160 Datasets.

161 In addition, we developed an original Rice Galaxy component called Rapid Allelic Variant extractor  
162 (RAVE), which allows simultaneous extraction of genotyping data from several accessions of the internal  
163 3K RG resource. It relies on the PLINK software [20], which efficiently builds a user-adjusted genotyping  
164 submatrix from a compressed PLINK binary biallelic genotype table (bed file + bim, fam files). Users can  
165 customize the genotyping dataset vertically by choosing a subpopulation (*indica*, *japonica*, *aromatic*,  
166 *aus*, *tropical*, *temperate*, etc.) or setting a list of varieties, and horizontally by restricting variations with a

167 list of genomic regions, or a list of gene names. Additionally, users can filter the SNP positions by  
168 specifying thresholds for missing data or minor allele frequency (MAF). The extracted VCFs can be  
169 directly generated by Rice Galaxy, stored as output into the history pane of the Galaxy interface, and can  
170 be reformatted to Hapmap, a versatile file format for further analyses such as marker (SNP) design,  
171 GWAS analyses, or visualization in within a JBrowse [21] genome browser (Vcf2jbrowse component).  
172 External SNP datasets can also be imported into Rice Galaxy and merged with 3k accessions in order to  
173 compare and look at the closest genotypes using SNIPlay [22] workflow.

#### 174 *GWAS analysis using TASSEL*

175 Using this feature, it is relatively easy to construct a genotyping matrix for a subset of accessions from  
176 the 3K RG and connect associated phenotypic information to perform GWAS analyses online, with  
177 outputs being decorated with various graphical enhancements. For the 3K RG accessions, the subset 1M  
178 GWAS and 440K Core SNPs that is usable for GWAS is already available as shared dataset in Rice Galaxy  
179 (Figure 2). Researchers working on the 3K RG panel can generate new phenotyping data from their  
180 respective experiments, upload the phenotype data into Rice Galaxy, and then perform GWAS using the  
181 TASSEL bioinformatics tool [23]. The GWAS Rice Galaxy workflow implementing TASSEL and Multi-Locus  
182 Mixed-Model package for association studies is shared from SNIPlay at Rice Galaxy (Figure 3).

183 Aside from GWAS with 3K RG datasets, researcher-generated marker and phenotype data (outside of 3K  
184 RG) can also be uploaded to Rice Galaxy for GWAS analysis.

#### 185 *Genomic selection using Oghma genome prediction tool*

186 Genomic selection (GS) is a promising breeding technique with potential to improve the efficiency and  
187 speed of the breeding process in rice [24]. With the intent of enabling the GS analysis process used on  
188 the 2 datasets in the Spindel et al. [24] study, (encoding data, filtering data to keep informative markers,  
189 creating a model from training set, evaluating the model and finally, performing the prediction itself),  
190 and to automate the analysis pipeline, the relevant packages (`methods`, `fpc`, `cluster`,



191 `vegan`, `pheatmap`, `pROC`, `randomForest`, `miscTools`, `pRF`, `e1076`,  
192 `rrBLUP`, and `glmnet`) for the R Statistical language (<https://www.r-project.org/>) were installed in  
193 Rice Galaxy and the tool suite was collectively named Oghma (Operators for Genome decipHering by  
194 Machine learning). Quality control tool (based on PLINK) and imputation tool using Beagle [25]  
195 (<https://faculty.washington.edu/browning/beagle/beagle.html>) were also installed. Four phenotype  
196 prediction/classifier methods (rrBLUP, random forest, SVM and lasso) were identified as relevant and  
197 deployed as tools in Rice Galaxy (Figure 4).

198 Figure 5 shows the overall GS analysis workflow using Oghma. Genotypes are encoded through [encode]  
199 tool. For the training set, an encoded genotype and the corresponding phenotype files are used by a  
200 classifier tool to train a model, which can be used with another encoded genotype file to predict trait  
201 values (the genomic prediction). It is important to note that (1) both genotype for training and  
202 genotype to predict must have the same markers (and thus, genotype files must have the same number  
203 of columns) to make a prediction, and (2) the "evaluation" option of the classifier tool can have any  
204 value except 1 (it is recommended to keep the default value = 0).

205 A big challenge when using machine learning approaches for genomic prediction is the optimization of  
206 the model based on training data, specifically setting the best parameters of the methods mentioned  
207 prior. Oghma was designed to automate the optimization of the parameter(s) of the classifiers on the fly  
208 (as opposed to manual tweaking), thus allowing users without experience of machine learning to easily  
209 optimize a model for their own data. Oghma includes some tools to evaluate prediction accuracy to  
210 allow the user to choose the most accurate method on their data by performing a cross-validation with  
211 a user-uploaded training set. Two metrics, the coefficient of determination ( $R^2$ ) and the correlation  
212 between predicted and observed phenotype, and a visualization (scatterplot of predicted vs observed)  
213 have been implemented to evaluate the methods. The [computeR2] and [plotPrediction] tools are used  
214 to compute  $R^2$  and visualize the accuracy of prediction. These tools both take the true phenotypes and

215 the predicted outputs as inputs (take note that both predictions and phenotypes data must be in the  
216 same order), and return the computed  $R^2$  or the scatterplot display of true phenotype vs prediction.  
217 Oghma can be used to evaluate a classifier (Figure 6). Like the general GS workflow, genotype and  
218 phenotype are used as input for any classifier, but the "evaluation" option must be set to 1. Fold for  
219 cross-validations are designed through the [fold] tool, which take as input the encoded file. These folds  
220 are used as extra argument by the classifier tools. The chosen classifier tool produces a file, which is not  
221 a model but the prediction of the test set for each cross-validation. This output is used as input, along  
222 with the phenotypes and folds, by [evaluation], which output some performances index ( $R^2$  and  
223 correlation). Although it does give a real indication of performances, trying to predict the training set  
224 (i.e. using the same genotype file in the pipeline described above), or at the least, showing if the  
225 classifier is not under-fitting the data.

226 We installed several classifiers in Oghma to allow users to test the best one(s) suited for their dataset, as  
227 our literature survey shows that no method seems to outperform the others on all genomic prediction  
228 tasks. It was noticed that Random Forest was the most accurate and the most stable classifier on Spindel  
229 dataset [24], thus we set this as default in Oghma. An original aggregation method is also implemented  
230 in Oghma, aggregating outputs of multiple classifiers to improve prediction. This tool takes as input the  
231 prediction of  $n$  classifiers and tries to aggregate them through weighted mean of the prediction (weight  
232 optimized by genetic algorithm) or regression (multiple type of regression have been implemented,  
233 based on decision tree, SVM and Random Forest). Limited testing shows that this approach is promising,  
234 matching Random Forest in some cases, especially with a meta-SVM, with polynomial or linear model, as  
235 aggregation method, but still needs some improvement as the accuracy remains unstable when  
236 evaluated through cross-validation (data not shown). The aggregation method can also be evaluated  
237 using the aforementioned evaluation tools.

238 *Diversity and population structure analysis of end-user datasets*

239 SNP datasets - such as those extracted from the 3K RG resource after a filtering by the RAVE module or  
240 custom sets directly uploaded in Rice Galaxy environment (Figure 7) can be processed for a complete  
241 exploration and large scale analysis thanks to the SNIPlay Rice Galaxy workflow (Figure 8). The workflow  
242 is available through the instance, requiring a VCF file as input. This workflow allows various analyses: (i)  
243 SNP annotation by snpEff (<http://snpeff.sourceforge.net/>) wrapper preconfigured for RGAP release 7.0  
244 [26] (<http://rice.plantbiology.msu.edu/>) gene models (ii) variant filtration using PLINK wrapper, (iii)  
245 general statistics such as Transition-Transversion ratio, levels of heterozygosity and missing data for  
246 each variety using VCFtools, (iv) SNP density analysis, (v) diversity indices calculation in sliding windows  
247 along the genome using VCFtools (Pi, Tajima's D, FST if subpopulations provided), (vi) linkage  
248 disequilibrium, (vii) population structure by sNMF ([http://membres-](http://membres-timc.imag.fr/Olivier.Francois/snmf/index.htm)  
249 [timc.imag.fr/Olivier.Francois/snmf/index.htm](http://membres-timc.imag.fr/Olivier.Francois/snmf/index.htm)), (viii) Principal Component Analysis and Identity By State  
250 (IBS) clustering of varieties by PLINK, and (ix) SNP-based distance phylogenetic tree by FastME  
251 (<http://www.atgc-montpellier.fr/fastme/>). Most key steps are decorated with sophisticated  
252 visualizations using a dedicated plugin. Visualization can be displayed by clicking on the [visualization]  
253 icon.

254 In practice, this workflow can be processed for many applications such as the identification of possible  
255 introgression events, the identification of putative genomic regions involved in the control of qualitative  
256 trait through a FST approach, the investigation for potential duplicates in the 3K RG accessions dataset  
257 and custom datasets, or the estimate of closest varieties of new sequenced accessions, by ranking a list  
258 of varieties from the database most closely matching the given sample. It can be used also for the close  
259 inspection of genomic region of interest after a GWAS analysis, through a linkage disequilibrium focus or  
260 the haplotyping of candidate genes.

261 *Uniqprimer module*

262 Uniqprimer is a workflow for comparative genomics-based diagnostic primer design, developed from a  
263 pipeline used in-house at Colorado State University to develop novel species and subspecies-level  
264 diagnostic tools for bacterial plant pathogens including pathovars of *Xanthomonas translucens* [27],  
265 geographical variants of rice-associated *Xanthomonas* spp. [28-30], and the genetically diverse rice  
266 pathogen *Pseudomonas fuscovaginae* [31]. Uniqprimer is now deployed in Rice Galaxy for user-friendly  
267 diagnostic primer design from draft or complete pathogen genomes. The user inputs multiple bacterial  
268 genomes from diagnostic target species as well as non-target species (i.e. “include” and “exclude”  
269 genome files), and the tool performs comparative alignment, primer design, and primer validation to  
270 output a list of primers that are specific to the target genomes (Figure 9). The uniqprimer standalone  
271 program is written in Python and is available at the Southgreen github repository  
272 (<https://github.com/SouthGreenPlatform/Uniqprimer> ), along with the detailed documentation for  
273 developers and end-users.

### 274 **3. Rice Galaxy OA: a Prototype for Open Access**

275 IRRI, as a member center of the Consultative Group for International Agricultural Research (CGIAR,  
276 <https://www.cgiar.org/>), complies with the CGIAR policy on Open Access and Open Data  
277 (<https://www.cgiar.org/how-we-work/accountability/open-access/> ). In collaboration with Indiana  
278 University in the United States and National Institute of Advanced Industrial Science and Technology in  
279 Japan, and carried out through grants from the National Science Foundation (NSF) in the US and the  
280 MacArthur Foundation through the Research Data Alliance (RDA - <https://www.rd-alliance.org/>), the  
281 team undertook a prototyping effort to bring the Rice Galaxy system to maximum compliance with the  
282 CGIAR policy.

283 The basis for the design to add open access to Rice Galaxy is a foundational technical idea emerging  
284 from activities occurring in the international RDA. This idea acknowledges that for open data access to  
285 be broadly realized, all meaningful data objects must have a globally unique and persistent identifier

286 (PID). Globally unique means the name is not shared with other objects on a global scale. An identifier is  
287 persistent when the PID itself cannot be destroyed, and when the relationship between the identifier  
288 and the data object it points to is permanent. Through an international working group in RDA, a team of  
289 researchers is advancing the notion of PID Kernel Information, which injects a tiny amount of carefully  
290 selected metadata into a PID record. This technique has the potential to stimulate an entirely new  
291 ecosystem of third party services that can process the billions of expected PIDs. The key challenge of this  
292 working group is to determine which from amongst thousands of relevant metadata are suitable to  
293 embed in the PID record.

294 Our design draws on earlier work by us in data provenance capture and representation [32-34] and  
295 employs a hands-off technique (*data provenance capture*) to gather information about a researcher's  
296 rice genomics analysis as the analysis is running. Through this technique, information acquired while the  
297 analysis is running is compiled and combined with pre-analysis information that is available at the  
298 beginning of the analysis workflow. Such information includes who performed the analysis, when it was  
299 performed, and under what conditions.

300 There have been earlier approaches to capture provenance of Galaxy workflows. Geocks *et al* [35]  
301 developed a history panel for users to facilitate reproducibility. Gaignard *et al*. [36] proposes the SHARP  
302 toolset, a semantic web (i.e. linked data) approach of harmonizing provenance collected from both the  
303 Galaxy and Taverna workflow systems. Kanwal *et al*. [37] captured the activity of a workflow (called a  
304 *provenance trace*) including the version of analysis tools run, the software parameters used, and the  
305 data objects produced at each workflow step. This work also targets increased reproducibility of past  
306 workflow instances. Missier *et al*. [38] proposes the "Golden Trail" architecture to describe and store  
307 workflow runtime provenance retrieved from Galaxy. The golden trail of provenance that is collected  
308 can be used to construct a virtual experiment view of past workflow runs. The four research  
309 contributions described further underline the need for the capture of provenance from workflow

310 systems. They propose different but equally important uses of data provenance, that is, to facilitate the  
311 improvement of science through reproducibility and construction of virtual views of an experiment once  
312 it has completed.

313 Our design for Rice Galaxy Open Access (OA) shares similarities with these other techniques, however its  
314 end goal is different, which is to advance open access, hence making Rice Galaxy consistent with CGIAR's  
315 open access policy. To do this, we focus on each piece of data and information deemed valuable that  
316 emerges from workflow runs deemed to be of importance. This particular data and information must be  
317 retained and shared with others, while being subject to reasonable restrictions. This is a highly selective  
318 approach to provenance capture, and one that makes our work unique. We briefly outline the solution  
319 here and identify resources for those interested in pursuing the topic in more detail.

320 The architecture of Rice Galaxy OA (Figure 10A) utilizes the Handle system [39] and two standards  
321 emerging from the Research Data Alliance, RDA PID Type [40] and the Data Type Registry [41]. It  
322 additionally uses storage and compute resources provisioned through the NSF funded project, Pacific  
323 Rim Applications and Grid Middleware Assembly (PRAGMA).

324 A researcher interacts with the open access enhanced Rice Galaxy system as follows:

- 325 (1) Researcher performs an analysis in Rice Galaxy
- 326 (2) Data objects (input data, output data, information such as configuration parameters) are  
327 extracted from Rice Galaxy OA into a PRAGMA Data Repository Database (MongoDB) (Figure  
328 10A),
- 329 (3) The data objects are assigned Persistent Identifiers, the PID Kernel Information is assigned into  
330 the PID record at this time, and a landing page created for each (Figure 10B).
- 331 (4) Data objects can be downloaded from the Data Identity server and re-loaded to the Rice Galaxy  
332 server for full faithful reproduction of the analysis

333 The resulting system appears to be promising and addresses a number of the recommendations from  
334 CGIAR. The Rice Galaxy OA system is a user transparent means of harvesting digital objects from  
335 applications and assigning PIDs to scientific outcomes. The architecture is modular and built with default  
336 PID information types and metadata using RDA products (Figure 10A). Although this proof-of-concept  
337 prototype successfully demonstrates the feasibility of this approach, there remains some future work.  
338 The community needs to provide feedback on which data and information products are most important  
339 to retain and make available. Additionally, not all workflow runs are important to a researcher as they  
340 could be system tests or new workflow tests. Thus, how a researcher identifies the items he/she wishes  
341 to make available to others and when, remains an important consideration for this system. For more  
342 information, points of contact to the team, the underlying software for Rice Galaxy OA, and the link to  
343 the prototype server can be found at <https://github.com/Data-to-Insight-Center/RDA-PRAGMA-Data-Service/wiki/Welcome-to-PRAGMA-Data-Service-Prototype> .

#### 345 **4. Rice Galaxy architecture discussion**

346 We deployed IRRRI Galaxy in an AWS EC2 instance (t2.large instance 2 vCPU, 4 GiB RAM) for the  
347 production server deployment in the cloud with Linux Ubuntu release 12.04.2 LTS (GNU/Linux 3.2.0-40-  
348 virtual x86\_64) using Galaxy release 14 as described in the Galaxy documentation.  
349 External data from the 3K RG Project files stored in the 3K RG AWS Simple Storage Service (S3) Public  
350 Data resource hosted at <http://s3.amazonaws.com/3kricegenome/> (or s3:// 3kricegenome/) is accessed  
351 using AWS S3 Command Line Interface, a command line tool utility in AWS that provides an interface to  
352 access AWS S3 objects (CLI, <https://docs.aws.amazon.com/cli/latest/reference/s3/> ). First, Rice Galaxy  
353 connects to the 3K RG AWS bucket using s3API and allows the objects inside the bucket to be  
354 transparent to Galaxy. VCF files (and the accompanying index files) are downloaded to Rice Galaxy using  
355 the S3 CLI with the `aws s3 cp` command, executed as:

```
356     aws -profile user s3 cp
357     s3://3kricegenome/REFERENCE/VCF_FILE.snp.vcf.gz* .
```

358 The subset region of the VCF file (chromosome:start-end) is then extracted using BCftools  
359 (<http://samtools.github.io/bcftools/>) wrapped in Rice Galaxy and exported to the history pane as  
360 bgzipped, indexed BCF file, which can then be converted back to VCF using [VCFTOOLS] in Rice Galaxy.  
361 Standard methods for tool wrapper development and deployment were followed. All tool wrapper XMLs  
362 developed specifically for Rice Galaxy are deposited and shared in a project-specific Rice Galaxy toolshed  
363 repository at <http://52.76.88.51:8081/> (Figure 11) and will also be deposited in the central Galaxy  
364 toolshed (<https://toolshed.g2.bx.psu.edu/>). All developments and testing of Rice Galaxy and Rice Galaxy  
365 Toolshed were done in Docker containers hosted in virtual machines at the Advanced Science and  
366 Technology Institute, Department of Science and Technology of the Philippine Government (ASTI –  
367 DOST) prior to final deployment to the AWS instance.

368 This resource will empower the rice research community to benefit from publicly available datasets (e.g.  
369 3K RG) and materials (seed/accessions), to enhance or even drive their own respective institutional  
370 genetic/genomic/breeding efforts. The Rice Galaxy instance (data, tools, computing resources) is free for  
371 use by all.

372 In addition to the integration of these tools, new Galaxy wrappers and visualization plugins are being  
373 developed for visualizing chromosomes and their information (SNP density, structural variants,  
374 translocations) either in linear or circular mode, using recent web technologies (Ideogram.js [42] ,  
375 BioCircos.js [43], respectively).

376 Finally, a Docker container of Rice Galaxy is under development so that it can be easily shared and  
377 deployed through the Galaxy Docker flavor initiative ([https://github.com/bgruening/docker-galaxy-](https://github.com/bgruening/docker-galaxy-stable)  
378 [stable](https://github.com/bgruening/docker-galaxy-stable) ).

379 **Conclusion**



380 Rice Galaxy is a federated Galaxy resource specialized for rice genetics, genomics, and breeding. The  
381 resource empowers the rice research community to utilize publicly available datasets (3K RG), materials  
382 (seed/accessions), and their own data, allowing complex data analyses to be performed even without  
383 investment in their own computational infrastructure and software development team. Rice research –  
384 related tools are also hosted in Rice Galaxy (i.e. Uniqprimer rice pathogen diagnostic design).  
385 Rice Galaxy is freely accessible to all and we invite the rice research community to participate in  
386 enriching the tools hosted by the resource. It can serve as a repository for data, analyses results, and  
387 new bioinformatics tools coming from institutions that have used the publicly available rice diversity  
388 panels from 3K RG, or have developed rice genomic/genetic analyses tools that they wish to share to the  
389 community, and a computing infrastructure for small institutes without in-house computing capability.

#### 390 **Availability and requirements**

391 Project name: RICE GALAXY

392 Project home page: <https://github.com/InternationalRiceResearchInstitute/RiceGalaxy>

393 Operating system(s): Linux Ubuntu release 12.04.2 LTS

394 Programming language: Python

395 Other requirements: R release 3.2.3 and following packages: methods, fpc, cluster, vegan, pheatmap,  
396 pROC, randomForest, miscTools, pRF, e1076, rrBLUP, glmnet ;TASSEL release 5.2.40; plink v1.90b3k;  
397 JBrowse 1.14.1; snpEff 4.3T; sNMF 1.2 (and as R package LEA); FastME 2.0

398 License: Rice Galaxy tools are released under GNU GPL. All software from external sources is bound by  
399 their respective licenses.

400 Any restrictions to use by non-academics: Rice Galaxy tools are without restriction to non-academics. All  
401 software from external sources is bound by their respective non-academic restrictions

402 Code availability: Tool wrappers at Rice Galaxy Toolshed (<http://52.76.88.51:8081/> ). Rice Galaxy is  
403 available at IRRI Github (<https://github.com/InternationalRiceResearchInstitute/RiceGalaxy>).

404 **Availability of supporting data**

405 3,000 Rice Genomes Project at Gigascience database (<http://gigadb.org/dataset/200001> )

406 3K RG BAM and VCF files available from Amazon Public data and ASTI-DOST IRODs site, instructions at

407 <http://iric.irri.org/resources/3000-genomes-project> .

408 SNP sets and morpho-agronomic characterization from 3K RG at SNP-Seek download site (<http://snp->

409 [seek.irri.org/ download.zul](http://snp-irri.org/download.zul) )

410 **Availability of supporting source code and requirements**

411 Project name: Uniqprimer

412 Project home page: <https://github.com/SouthGreenPlatform/Uniqprimer>

413 Operating system(s): Linux OS

414 Programming Language: Python

415 Other requirements: MUMmer 3

416 License: GNU GPL

417 Project name: PRAGMA Data Service

418 Project home page: repository <https://github.com/Data-to-Insight-Center/RDA-PRAGMA-Data->

419 [Service/wiki/Welcome-to-PRAGMA-Data-Service-Prototype](https://github.com/Data-to-Insight-Center/RDA-PRAGMA-Data-Service/wiki/Welcome-to-PRAGMA-Data-Service-Prototype)

420 Operating system(s): Platform independent

421 License: Apache License 2.0

422 **Declarations**

423 **Abbreviations**

424 3K RG:3,000 Rice Genomes;HDRA: High Density Rice Array; SNP: single nucleotide polymorphism; GWAS:

425 Genome-Wide Association Studies; RAM:random access memory; CPU: central processing unit;

426 IRRI:International Rice Research Institute;NGS: next-generation sequencing;QTL:quantitative trait loci;

427 IRGSP:International Rice Genome Sequencing Project; RGAP:Rice Genome Annotation Project;KASP:

428 Kompetitive Allele Specific PCR; VCF : variant call format ;AWS: Amazon Web Services; RAVE: Rapid  
429 Allelic Variant extractor; MAF: minor allele frequency;TASSEL: Trait Analysis by aSSociation, Evolution  
430 and Linkage; GS:genomic selection;Oghma: Operators for Genome decipHering by MACHine learning;  
431 rrBLUP:ridge regression best linear unbiased predictor; SVM:support vector machine; FST:fixation index;  
432 NSF:National Science Foundation;CGIAR: Consultative Group for International Agricultural Research;  
433 RDA: Research Data Alliance;PID:persistent identifier;OA:open access; PRAGMA:Pacific Rim Applications  
434 and Grid Middleware Assembly; EC2:elastic computing cloud; CLI: command line interface; S3: Simple  
435 Storage Service; API: Python Application Programming Interfaces; XML: eXtensible Markup Language;

#### 436 **Competing interests**

437 The author(s) declare that they have no competing interests.

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442 NSF OCI 1234983, the RDA/US-sponsored adoption program funded by the MacArthur Foundation, and  
443 the AIST ICT International Collaboration Grant.

#### 444 **Authors' contributions**

445 VJ and AD equally contributed to create Rice Galaxy. NB contributed the genomic prediction tools. AD,  
446 GD, PL, and MR contributed the RAVE and SNIPLAY tools. JD, JRM, JPP created the development Rice  
447 Galaxy cloud instances hosted at DOST-ASTI. LM created the SNP-Seek interfaces. LT, JL, JEL contributed  
448 the Uniqprimer tool. GZ, KR, BP, and JH contributed the Rice Galaxy Open Access, MT, NA, and TK  
449 contributed to funding acquisition and writing, RM coordinated the conceptualization of the project and  
450 the writing process.

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454 architecture.

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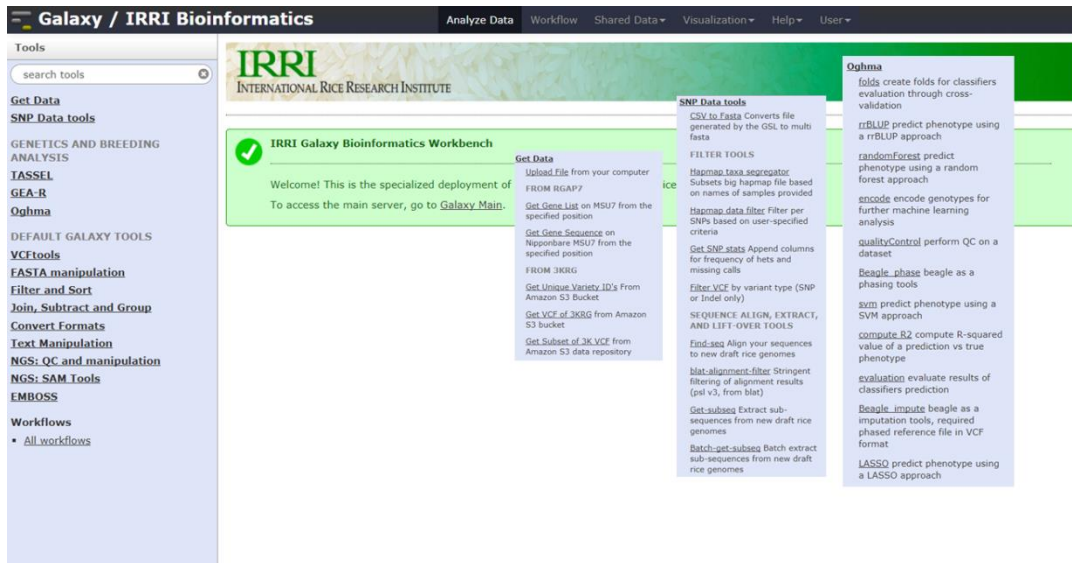
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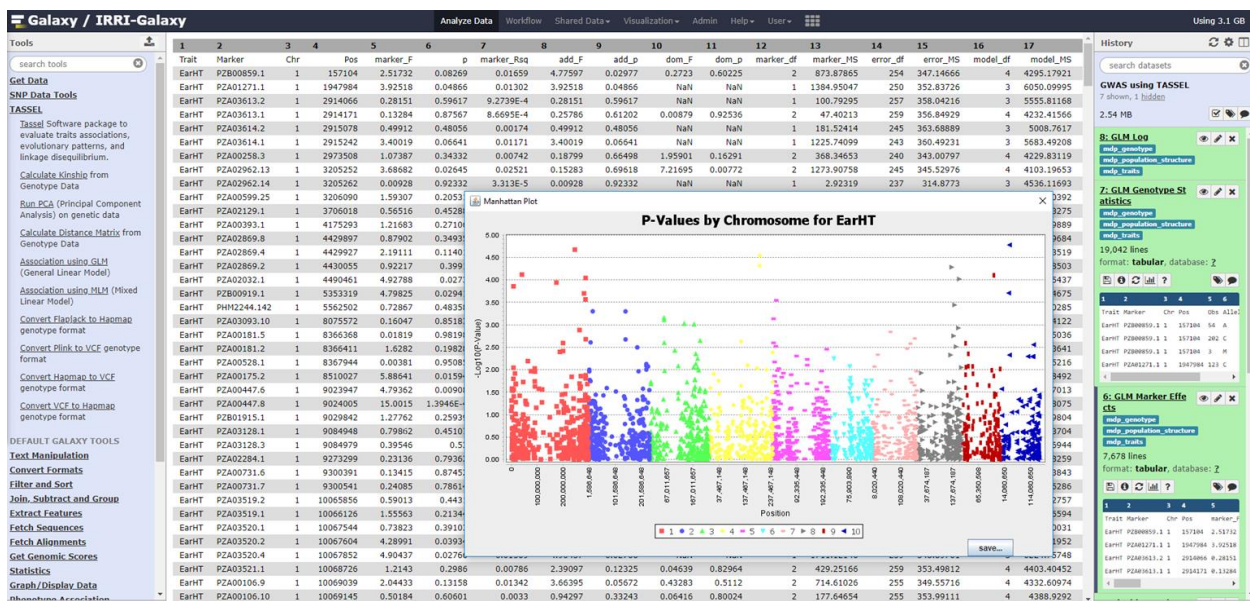
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571  
 572 Figure 1. Rice Galaxy @ IRR with customized analyses tools for genetics, breeding, and custom data  
 573 sources (i.e. 3,000 Rice Genomes project).  
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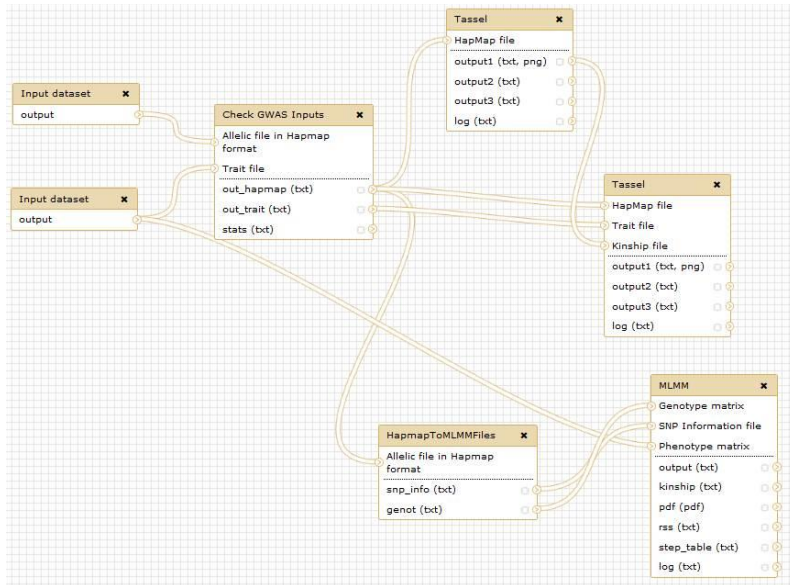


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577 Figure 2. Genome-Wide Association Studies analysis (implemented by TASSEL software) in Rice Galaxy.

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579

580 Figure 3. Genome-Wide Association Studies analysis workflow in SNIPlay as implemented in Rice Galaxy.

581

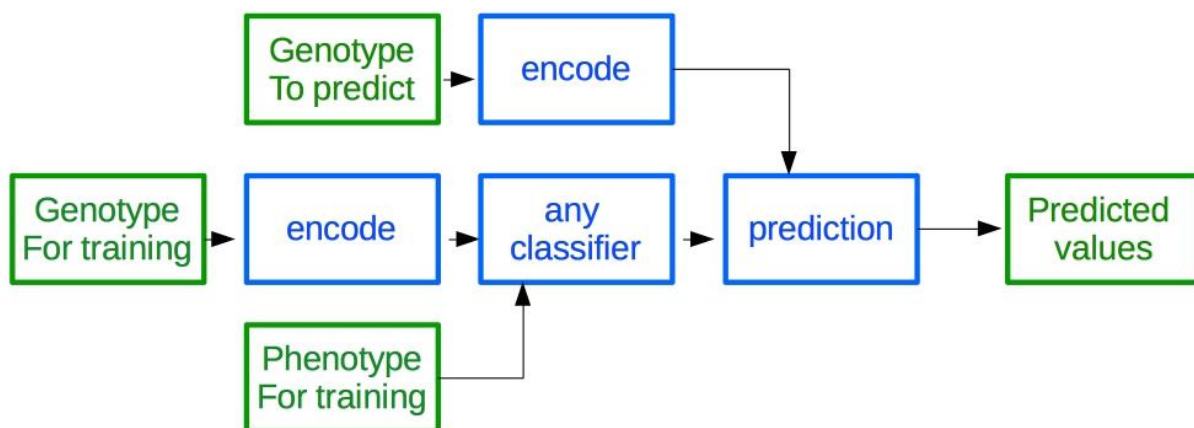
The screenshot shows the Galaxy / IRRi Bioinform interface. The top navigation bar includes 'Galaxy / IRRi Bioinform', 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', 'Help', and 'User'. On the left, a 'Tools' sidebar lists various tools under the 'Oghma' category, including 'folds', 'rrBLUP', 'randomForest', 'encode', 'qualityControl', 'Beagle\_phase', 'svm', 'compute R2', 'evaluation', 'Beagle\_impute', and 'LASSO'. On the right, a green banner reads 'IRRI Galaxy Bioinformatics Workbench' with a checkmark icon, followed by a welcome message: 'Welcome! This is the specialized deployment of Galaxy at the International Rice Research Institute (IRRI). To access the main server, go to [Galaxy Main](#).'

582

583 Figure 4. Oghma genomic prediction and selection tools in Rice Galaxy with various classifier tools

584 installed.

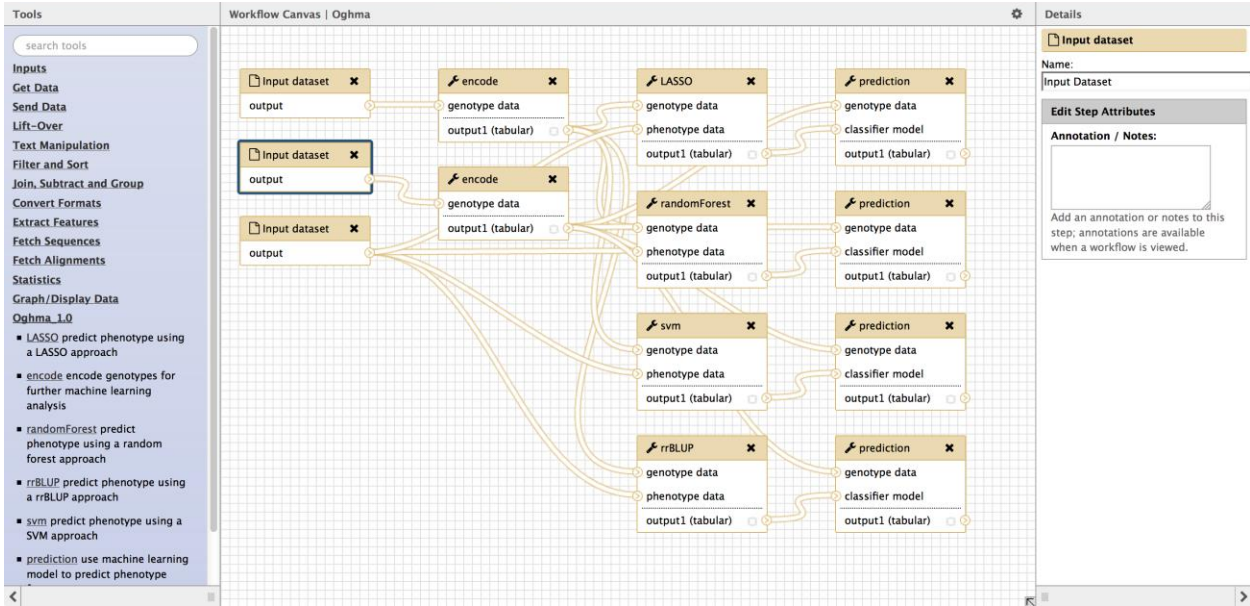
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587 A. Overview of the Genomic Selection analyses workflow as implemented in Oghma tool suite.

588

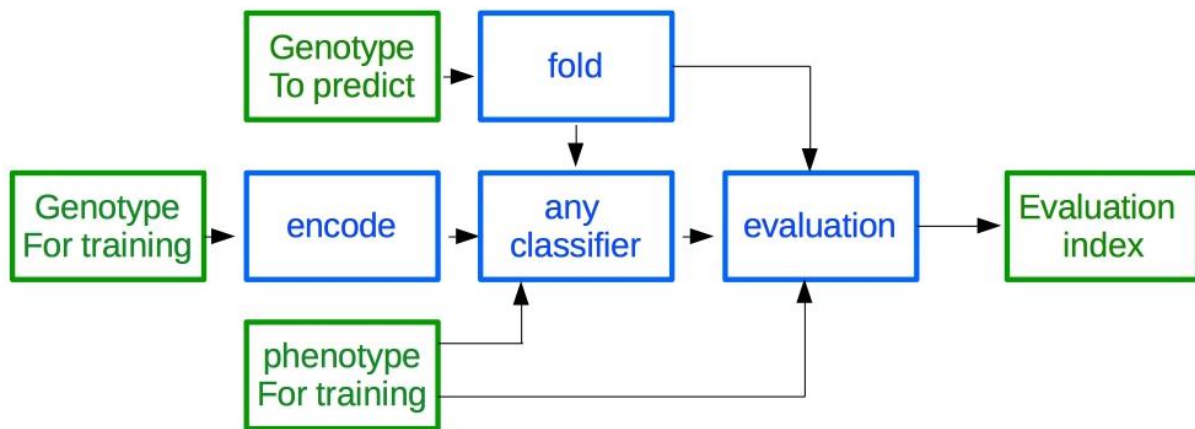


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590 B. Rice Galaxy workflow for genome prediction using Oghma tool suite.

591 Figure 5: Genomic Selection analyses workflow as implemented by Oghma tool suite.

592

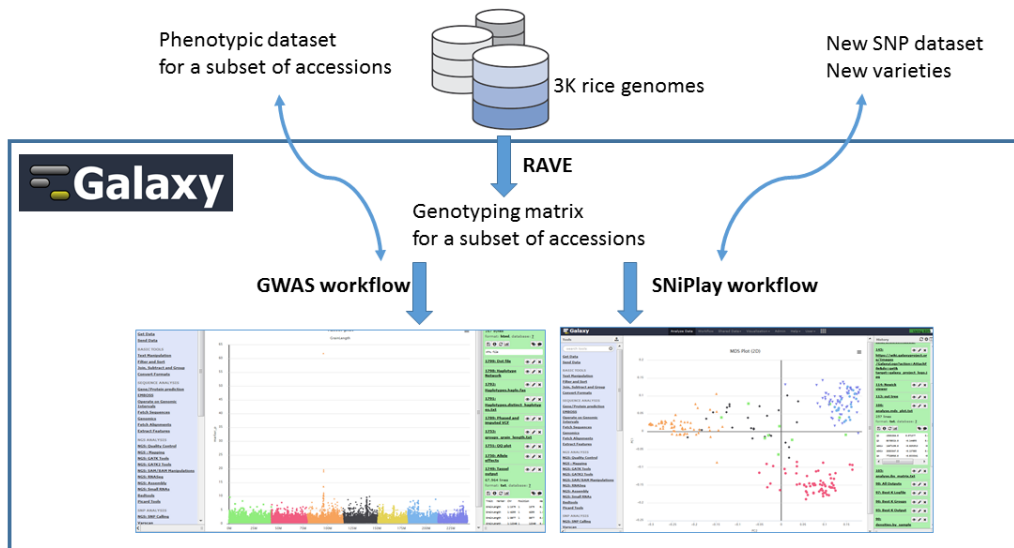


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595 Figure 6. Workflow for classifier evaluation in the genome prediction tool suite implemented by Oghma.

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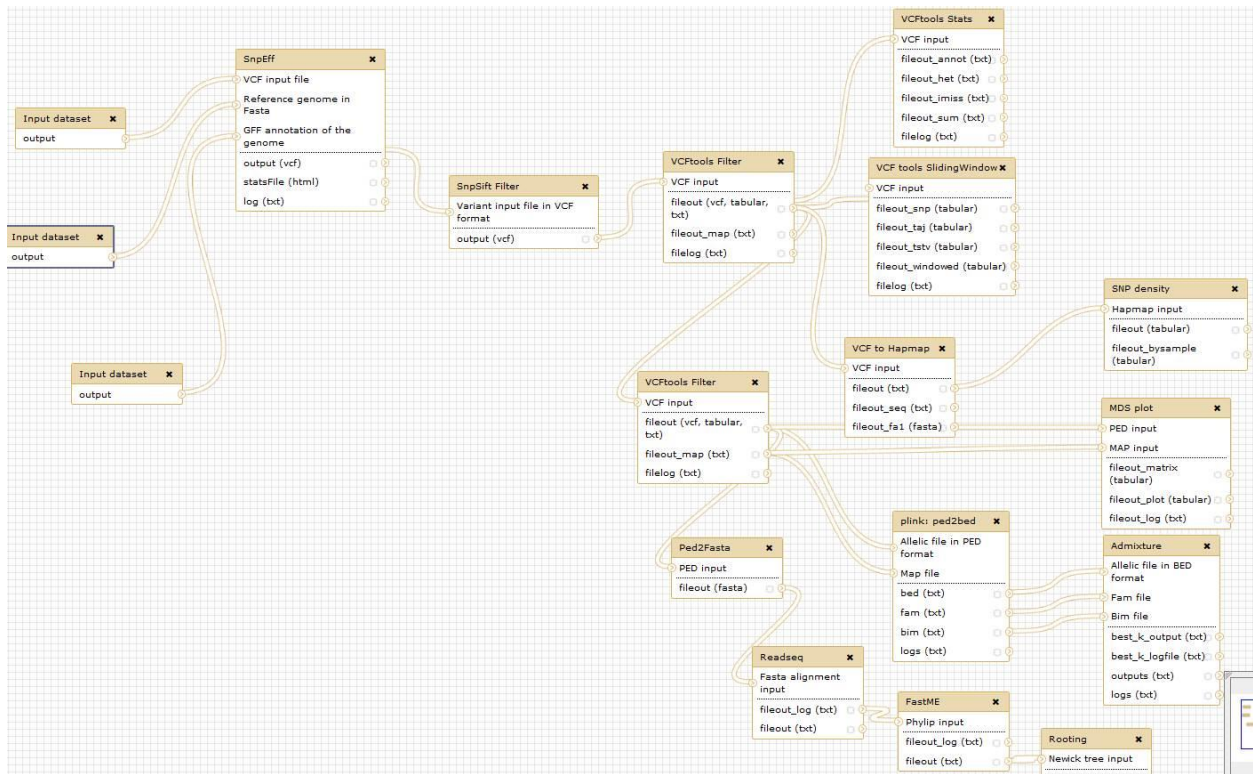
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598 Figure 7. Overview schematic showing the integration of the 3K Rice Genomes project genotyping

599 database and rapid extraction of subset SNPs by RAVE module for use by analyses workflows installed in

600 Rice Galaxy.

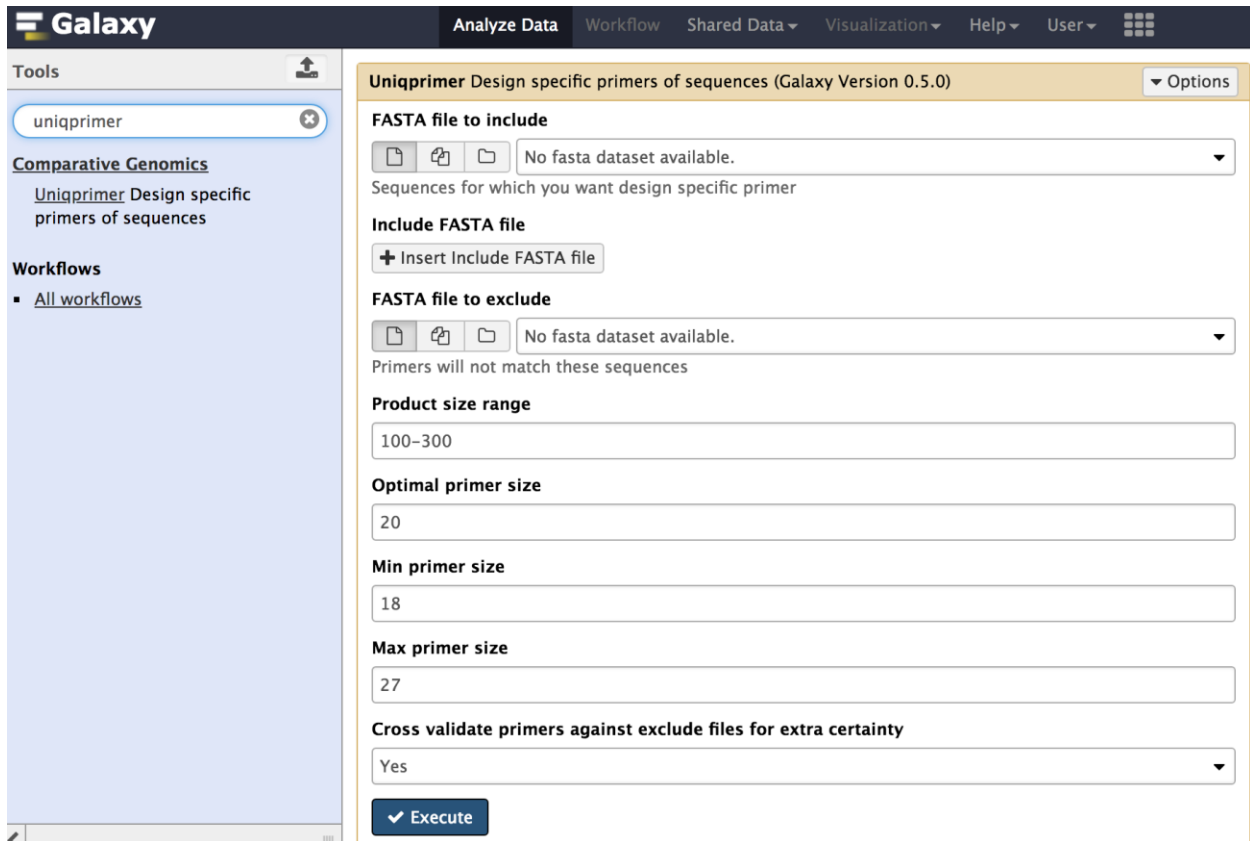
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603 Figure 8. Rice Galaxy SNiPlay workflow for diversity and population structure analyses using various  
604 software tools.

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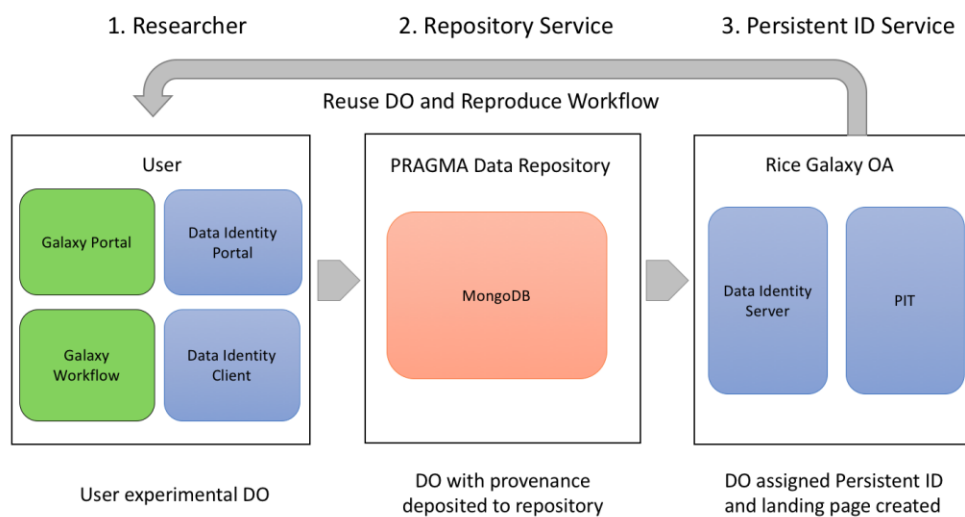


606

607 Figure 9. Uniqprimer comparative genomics-based diagnostic primer design tool for microbial pathogen

608 detection installed in Rice Galaxy.

609



610

611 A. The underlying software infrastructure for the components of Rice Galaxy Open Access.

**Figure 10A: Galaxy Workflow and mlm.json File**

The Galaxy workflow includes the following tools and outputs:

- HapMap file (input/output)
- Tassel (input: HapMap file, Trait file, Kinship file; outputs: output1 (txt, png), output2 (txt), output3 (txt), log (txt))
- mlm.json file (JSON metadata)

```

{
  "a_galaxy_workflow": "true",
  "annotation": "",
  "format-version": "0.1",
  "name": "MLM",
  "steps": [
    {
      "annotation": "",
      "id": 0,
      "input_connections": {},
      "inputs": [
        {
          "description": "",
          "name": "Hapmap file"
        }
      ],
      "name": "Input dataset",
      "outputs": [],
      "position": {
        "xact": 295.5,
        "yep": 138.5
      },
      "tool_errors": null,
      "tool_id": null,
      "tool_state": "{}",
      "tool_version": null,
      "type": "data_input",
      "user_outputs": []
    },
    {
      "id": 1
    }
  ]
}
    
```

**Figure 10B: IRRI Data Repository beta**

The interface shows search results for the workflow. The results table is as follows:

Creator	DO Name	Timestamp	Actions
kunalan	kunalan_glm_2018-04-27-20:19:36	2018-04-27-20:19:36	Download Data Object, Download Metadata Object
luoyu	luoyu_glm_2018-04-27-20:47:29	2018-04-27-20:47:29	Download Data Object, Download Metadata Object
luoyu	luoyu_mlm_2018-04-30-18:42:26	2018-04-30-18:42:26	Download Data Object, Download Metadata Object
luoyu	luoyu_glm_2018-04-30-19:53:18	2018-04-30-19:53:18	Download Data Object, Download Metadata Object

The selected entry (luoyu\_mlm\_2018-04-30-18:42:26) is shown in detail below:

**MLM DO Metadata**

luoyu\_mlm\_2018-04-30-18:42:26  
 11723/362b15b1-9334-4f0d-8e6d-8fb3d8d55e45  
 DO Name: luoyu\_mlm\_2018-04-30-18:42:26  
 Creator: luoyu  
 Timestamp: 2018-04-30-18:42:26

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613 B. Digital Object flow in Rice Galaxy Open Access. A Galaxy analysis workflow (exported as JSON file) is  
 614 deposited to the DO repository, and the data identity server publishes the deposited DO + meta-data for  
 615 discoverability.

616 Figure 10. The components (A) and the flow of Digital Objects from upload to discoverability (B) in the  
 617 prototype Rice Galaxy Open Access.

618

**Figure 11: Galaxy Tool Shed Categories**

The interface shows a list of tool categories with the following details:

Name	Description	Repositories
EIB Hackathon 2018	tools from 2018 Hackathon	7
File Conversion	tools for converting file formats	1
Genomic Selection	tools for the genomic selection project	6
GWAS	gwas tools	1
Sequence	repositories for design, validation and analyses of sequences	2
SNP Calling	tools for SNP Discovery	2

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620

621 Figure 11. Rice Galaxy Toolshed with the various available tools.

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