

Bioinformatics Workflow and Applications Using the PoPLAR Gateway

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Introduction

Thanks to advances made by Next Generation Sequencing (NGS) technology, a large volume of genetic data is now accessible for analysis. From raw data to published results, an efficient and automated pipeline for the analysis of genetic data will revolutionize modern research. Individual programs can be optimized and placed in a science gateway for researchers to customize their pipelines. In particular, the addition of reliable high performance computing (HPC) programs to the PoPLAR Gateway opens the doors to computational abilities even for scientists with little to no programming experience or access to their own HPC resources.

Materials

We are currently using the Beacon super-computer. The 256GB of memory per node allows for tests with large databases. The PoPLAR Gateway is under development. This is an example screenshot of the login screen.

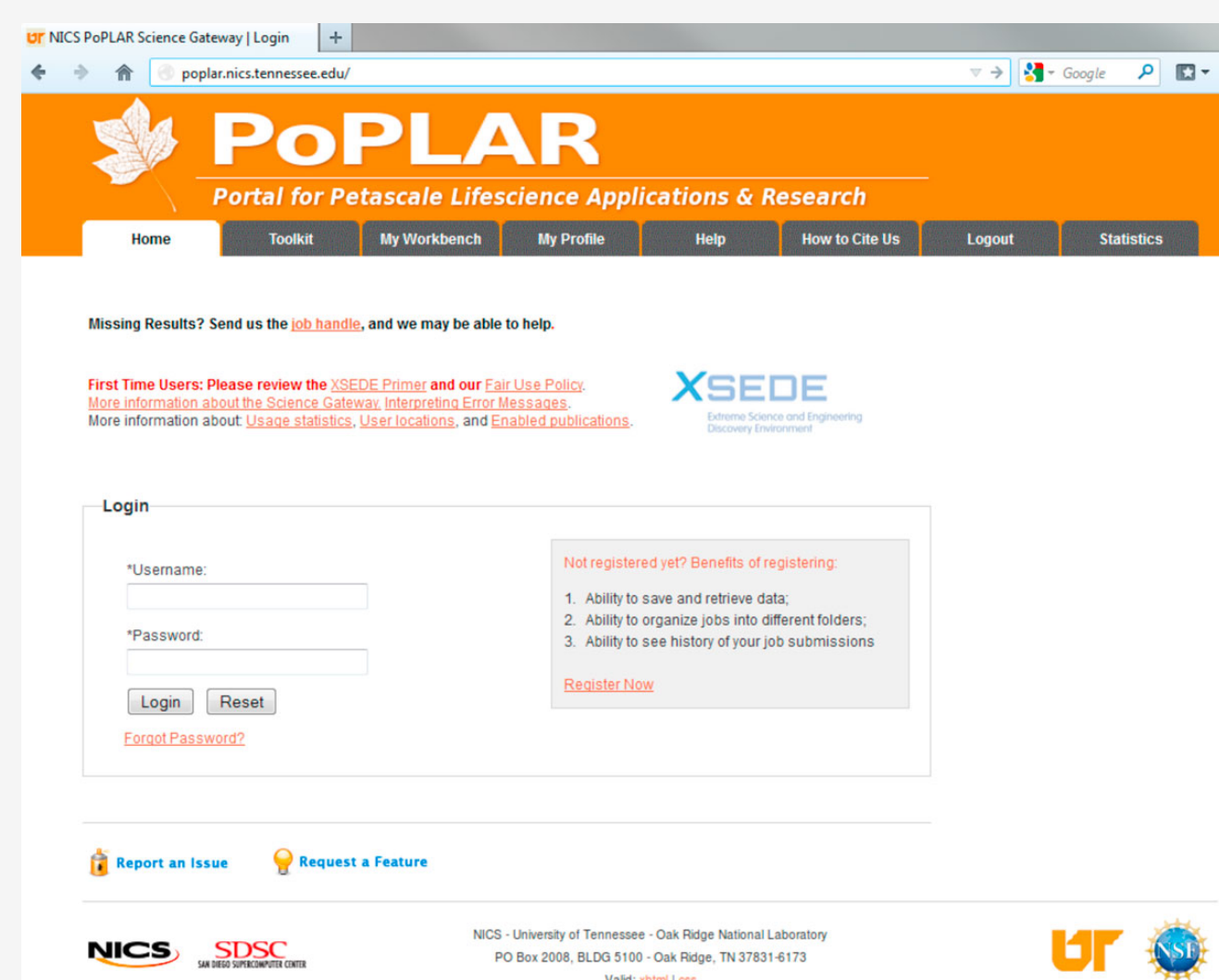
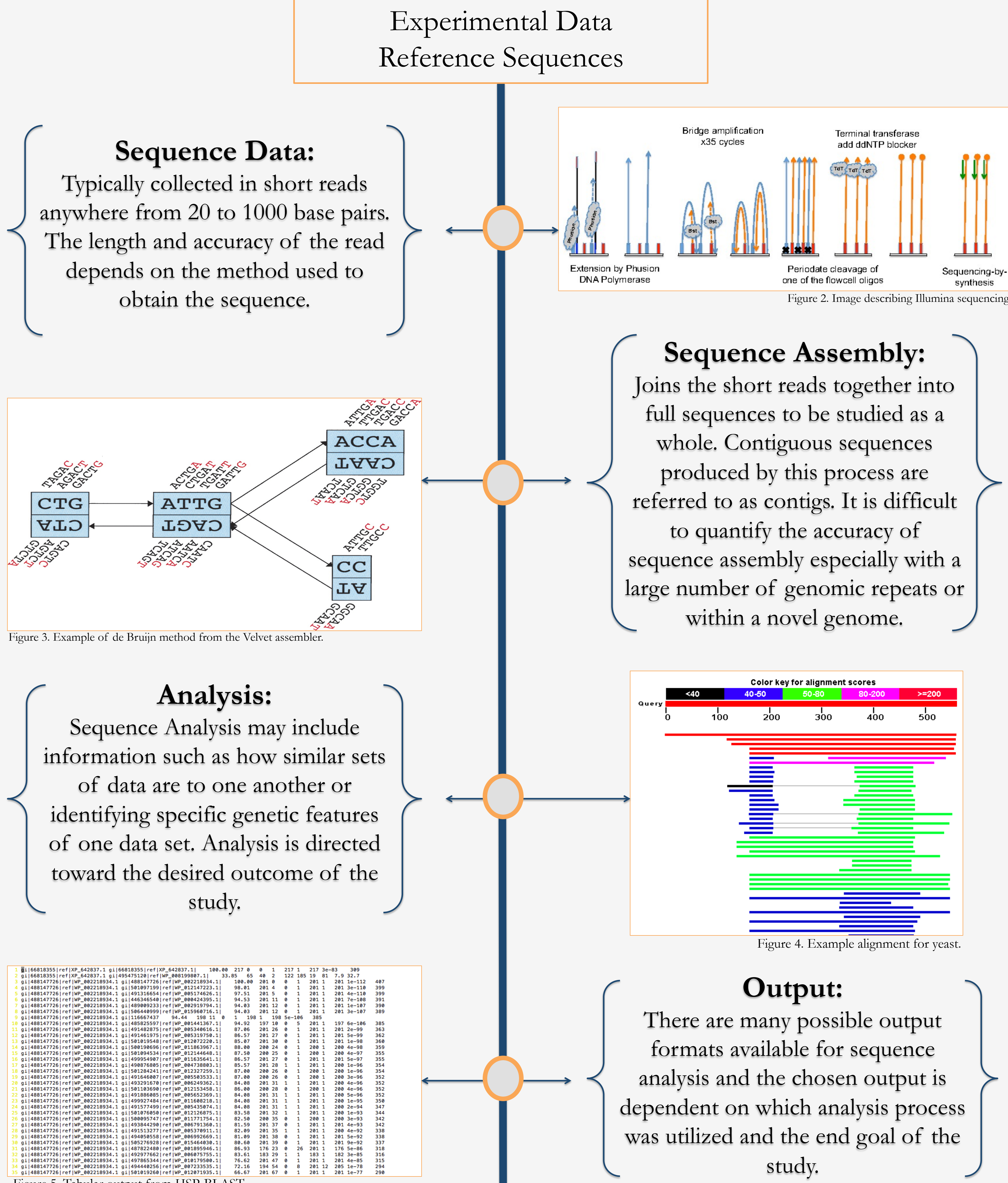
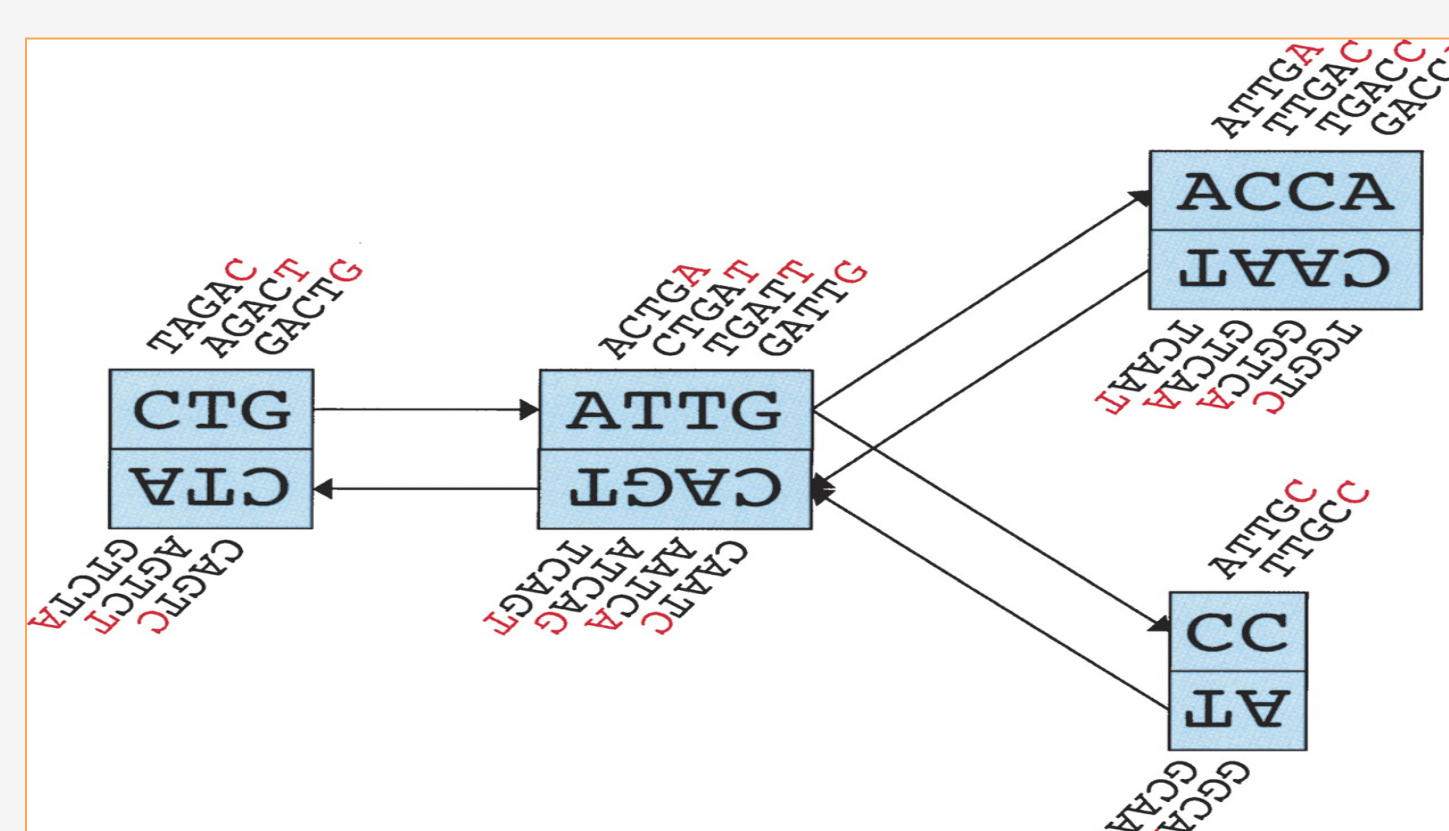
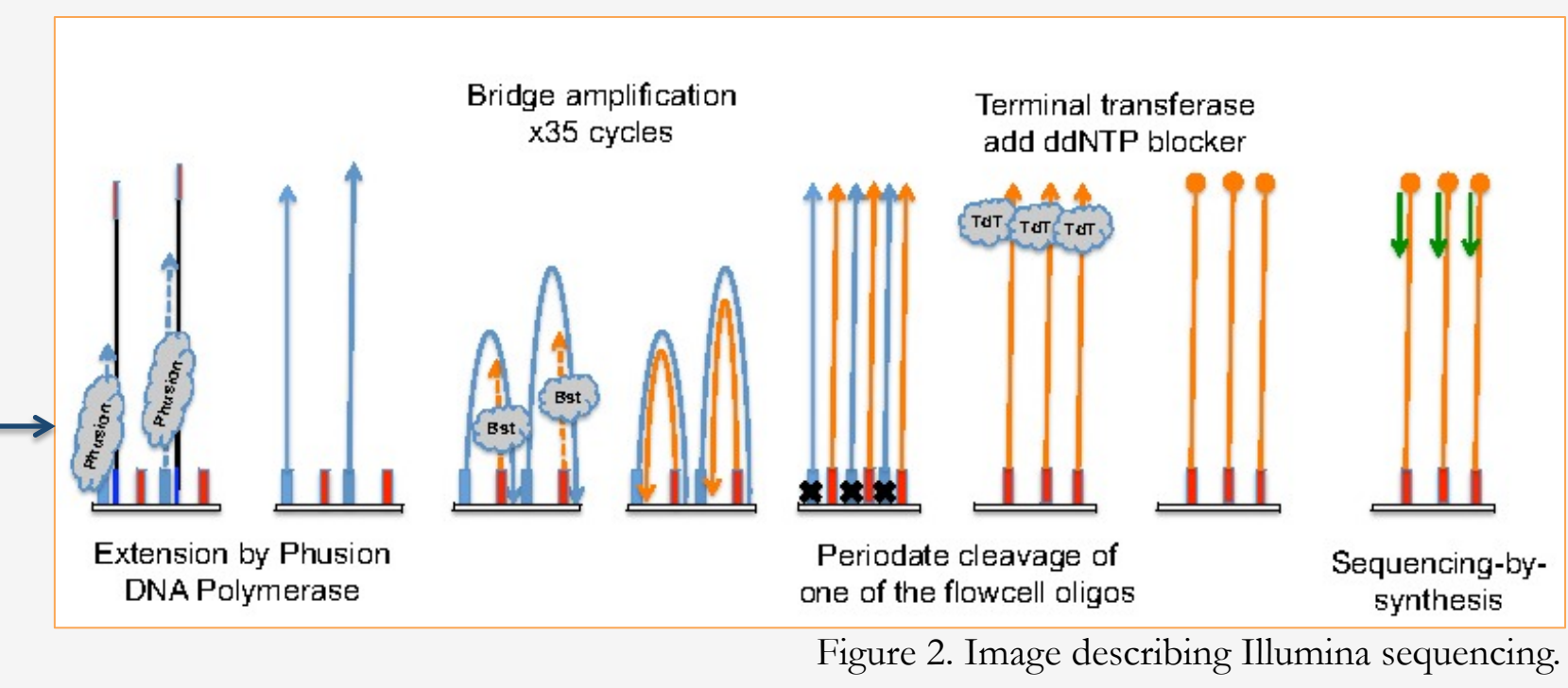


Figure 1. Screenshot of PoPLAR login screen.

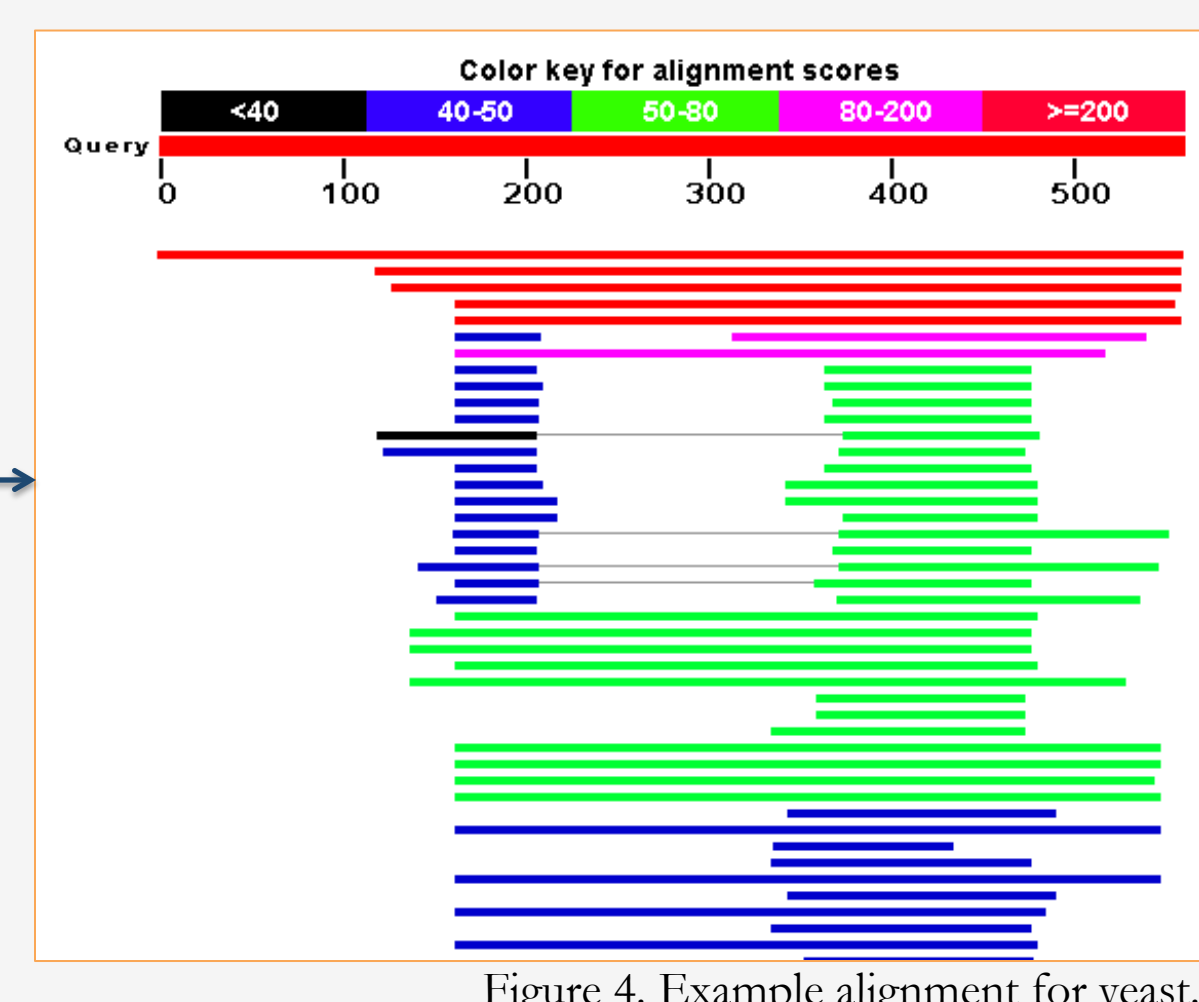
Workflow



Sequence Data:
Typically collected in short reads anywhere from 20 to 1000 base pairs. The length and accuracy of the read depends on the method used to obtain the sequence.



Sequence Assembly:
Joins the short reads together into full sequences to be studied as a whole. Contiguous sequences produced by this process are referred to as contigs. It is difficult to quantify the accuracy of sequence assembly especially with a large number of genomic repeats or within a novel genome.



Analysis:
Sequence Analysis may include information such as how similar sets of data are to one another or identifying specific genetic features of one data set. Analysis is directed toward the desired outcome of the study.

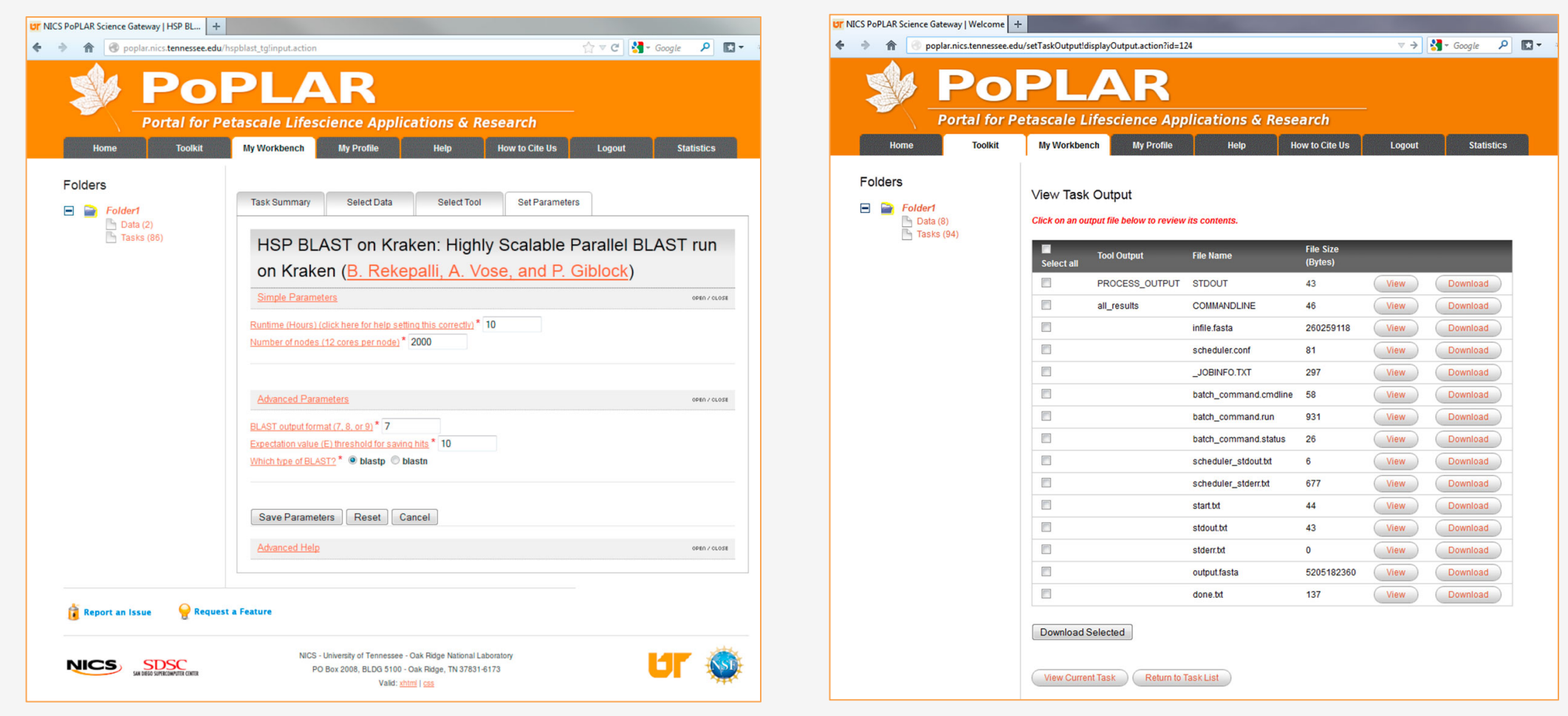
Figure 5. Tabular output from HSP-BLAST.

Query	Subject	Score	E-value	Bits
1	1	100.00	0.00	100.00
2	2	99.99	0.01	99.99
3	3	99.98	0.02	99.98
4	4	99.97	0.03	99.97
5	5	99.96	0.04	99.96
6	6	99.95	0.05	99.95
7	7	99.94	0.06	99.94
8	8	99.93	0.07	99.93
9	9	99.92	0.08	99.92
10	10	99.91	0.09	99.91
11	11	99.90	0.10	99.90
12	12	99.89	0.11	99.89
13	13	99.88	0.12	99.88
14	14	99.87	0.13	99.87
15	15	99.86	0.14	99.86
16	16	99.85	0.15	99.85
17	17	99.84	0.16	99.84
18	18	99.83	0.17	99.83
19	19	99.82	0.18	99.82
20	20	99.81	0.19	99.81
21	21	99.80	0.20	99.80
22	22	99.79	0.21	99.79
23	23	99.78	0.22	99.78
24	24	99.77	0.23	99.77
25	25	99.76	0.24	99.76
26	26	99.75	0.25	99.75
27	27	99.74	0.26	99.74
28	28	99.73	0.27	99.73
29	29	99.72	0.28	99.72
30	30	99.71	0.29	99.71
31	31	99.70	0.30	99.70
32	32	99.69	0.31	99.69
33	33	99.68	0.32	99.68
34	34	99.67	0.33	99.67
35	35	99.66	0.34	99.66
36	36	99.65	0.35	99.65
37	37	99.64	0.36	99.64
38	38	99.63	0.37	99.63
39	39	99.62	0.38	99.62
40	40	99.61	0.39	99.61
41	41	99.60	0.40	99.60
42	42	99.59	0.41	99.59
43	43	99.58	0.42	99.58
44	44	99.57	0.43	99.57
45	45	99.56	0.44	99.56
46	46	99.55	0.45	99.55
47	47	99.54	0.46	99.54
48	48	99.53	0.47	99.53
49	49	99.52	0.48	99.52
50	50	99.51	0.49	99.51
51	51	99.50	0.50	99.50
52	52	99.49	0.51	99.49
53	53	99.48	0.52	99.48
54	54	99.47	0.53	99.47
55	55	99.46	0.54	99.46
56	56	99.45	0.55	99.45
57	57	99.44	0.56	99.44
58	58	99.43	0.57	99.43
59	59	99.42	0.58	99.42
60	60	99.41	0.59	99.41
61	61	99.40	0.60	99.40
62	62	99.39	0.61	99.39
63	63	99.38	0.62	99.38
64	64	99.37	0.63	99.37
65	65	99.36	0.64	99.36
66	66	99.35	0.65	99.35
67	67	99.34	0.66	99.34
68	68	99.33	0.67	99.33
69	69	99.32	0.68	99.32
70	70	99.31	0.69	99.31
71	71	99.30	0.70	99.30
72	72	99.29	0.71	99.29
73	73	99.28	0.72	99.28
74	74	99.27	0.73	99.27
75	75	99.26	0.74	99.26
76	76	99.25	0.75	99.25
77	77	99.24	0.76	99.24
78	78	99.23	0.77	99.23
79	79	99.22	0.78	99.22
80	80	99.21	0.79	99.21
81	81	99.20	0.80	99.20
82	82	99.19	0.81	99.19
83	83	99.18	0.82	99.18
84	84	99.17	0.83	99.17
85	85	99.16	0.84	99.16
86	86	99.15	0.85	99.15
87	87	99.14	0.86	99.14
88	88	99.13	0.87	99.13
89	89	99.12	0.88	99.12
90	90	99.11	0.89	99.11
91	91	99.10	0.90	99.10
92	92	99.09	0.91	99.09
93	93	99.08	0.92	99.08
94	94	99.07	0.93	99.07
95	95	99.06	0.94	99.06
96	96	99.05	0.95	99.05
97	97	99.04	0.96	99.04
98	98	99.03	0.97	99.03
99	99	99.02	0.98	99.02
100	100	99.01	0.99	99.01

Figure 5. Tabular output from HSP-BLAST.

Future Goals

In the future, the PoPLAR Gateway will be a comprehensive resource for the manipulation and analysis of genetic data. It will allow scientists to compete with the large amount of data generated by today's biological research, and create a user-friendly environment that accommodates rather than hinders those with little computational experience.



References

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<http://www.bio.davidson.edu/courses/>



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