A Proposal for Beast 2.0

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Vision

To provide tools for computational science that are

- *easy to use*, that is, well documented, have intuitive user interfaces with small learning curve.
- *open access*, that is, open source, open xml format, facilitating reproducability of results, runs on many platforms.
- *easy to extend*, by having extensibility in design.

Scope

Efficient testing of probabilistic hypotheses for sequence data analysis involving tree models.

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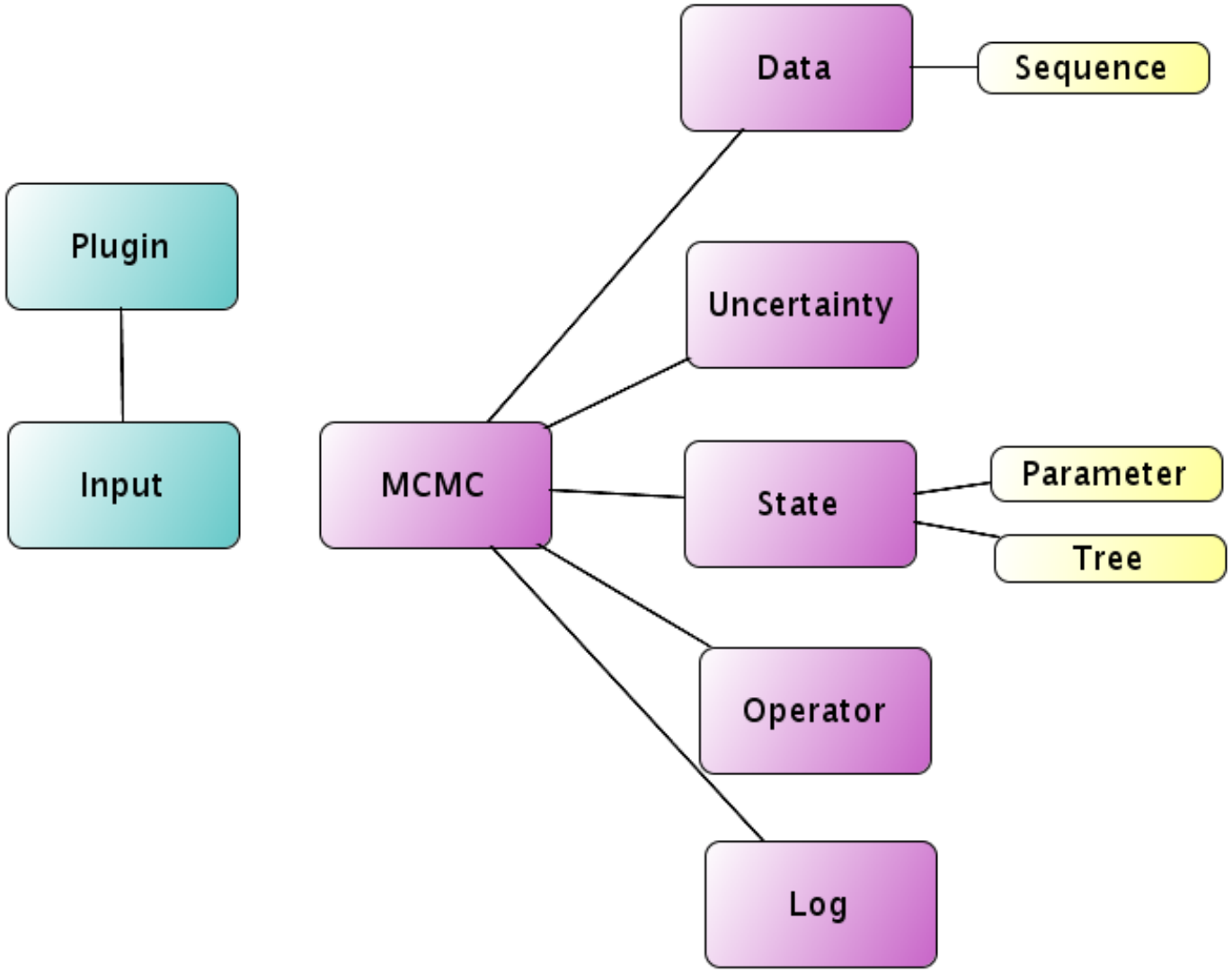
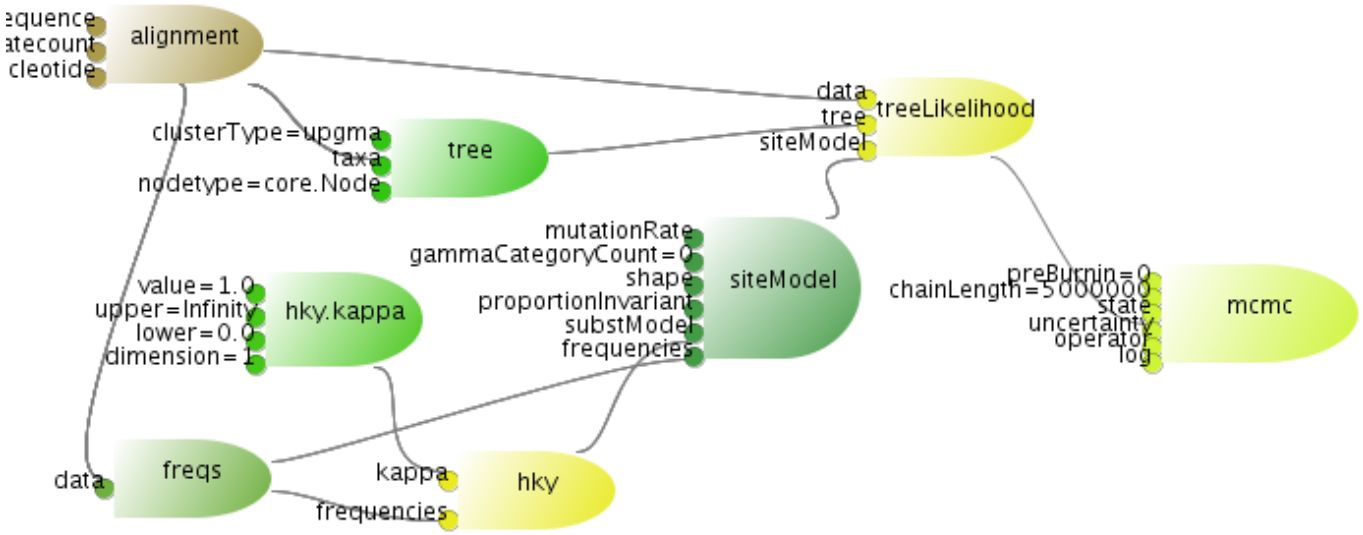
Core


Data
Sequence
Plugin
Uncertainty
Input
MCMC
State
Parameter
Tree
Operator
Log

Phylosophy

Everything is a plug-in



Plug-ins provide...

- connection with with other plug-ins/values through 'inputs'
- validation
- documentation
- 'XML parsing'

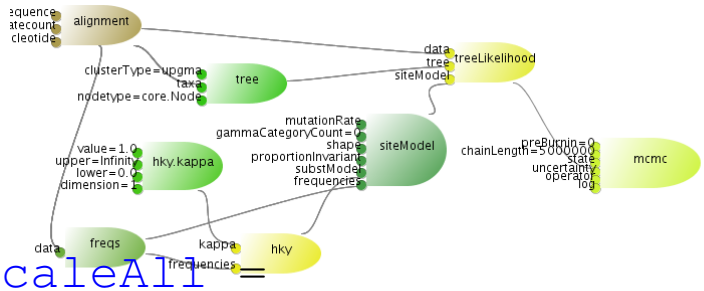
Plugin class

```
@Description("Description␣goes␣here")
public class Plugin {
    public void initAndValidate(State state)

    public String getCitations()

    public String getID()
    public void setID(String sID)

    public void store(int nSample)
    public void restore(int nSample)
} // class Plugin
```

HKY Plugin


```
@Description("HKY85 (Hasegawa, Kishino & Yano, 1985) substitution
public class HKY extends 'Plugin' {
    public Input<Frequencies> m_freqs = new Input<Frequencies>("f
    public Input<Parameter> m_kappa = new Input<Parameter>("kappa

    @Override public void initAndValidate(State state) throws Exc
        initialiseEigen();
    }

    public void getTransitionProbabilities(double distance, doubl
        ...
    }
    @Override public void store(int nSample) {}
    @Override public void restore(int nSample) {
        updateMatrix = true;
        updateIntermediates = true;
    }
    @Override public String getCitation() {
        return "Hasegawa, M., Kishino, H and Yano, T. 1985. Datin
    }
} // class HKY
```

Inputs



Simple primitives

```
public Input<Boolean> m_pScaleAll =
    new Input<Boolean>("scaleAll",
        "if true, all elements of a parameter (not tree) are scal
        new Boolean(false));
```

Other plugins

```
public Input<Frequencies> m_freqs =
    new Input<Frequencies>("frequencies",
        "frequencies nucleotide letters");
```

Multiple inputs

```
public Input<List<Parameter>> m_pParameters =
    new Input<List<Parameter>>("parameter",
        "parameter, part of the state",
        new ArrayList<Parameter>());
```

Input validation

Default: OPTIONAL (see previous slide)

If input is REQUIRED:

```
public Input<Parameter> m_kappa =
    new Input<Parameter>("kappa",
        "kappa parameter in HKY model",
        Validate.REQUIRED);

public Input<List<Operator>> m_operators =
    new Input<List<Operator>>("operator",
        "operator for generating proposals in MCMC state space",
        new ArrayList<Operator>(), Validate.REQUIRED);
```

If input is XOR:

```
public Input<Tree> m_pTree =
    new Input<Tree>("tree",
        "if specified, all tree branch length are scaled");
public Input<Parameter> m_pParameter =
    new Input<Parameter>("parameter",
        "if specified, this parameter is scaled"
        , Validate.XOR, m_pTree);
```

State

- State is explicit in XML & as object (unlike Beast 1)
- Contains parameters and trees
- Operators work on the state

```
public double proposal(State state) throws Exception {...}
```

- Uncertainty calculated given state

```
public double calculateLogP(State state) throws Exception {...
```

- State can be interrogated on value of parameters/trees

```
state.getParameter(/**Parameter**/ p)
state.getTree(/**Tree**/ t)
```

Store/Restore

BEAST 1: push model

- Model
- Event handling
- Framework and plug-ins responsible
- Elegant, undocumented, requires lots of Panadol

BEAST 2: pull model

- store/restore
- sample number provided to prevent multiple (re)stores
- MCMC only tells its 'uncertainties' to store/restore, plug-ins responsible

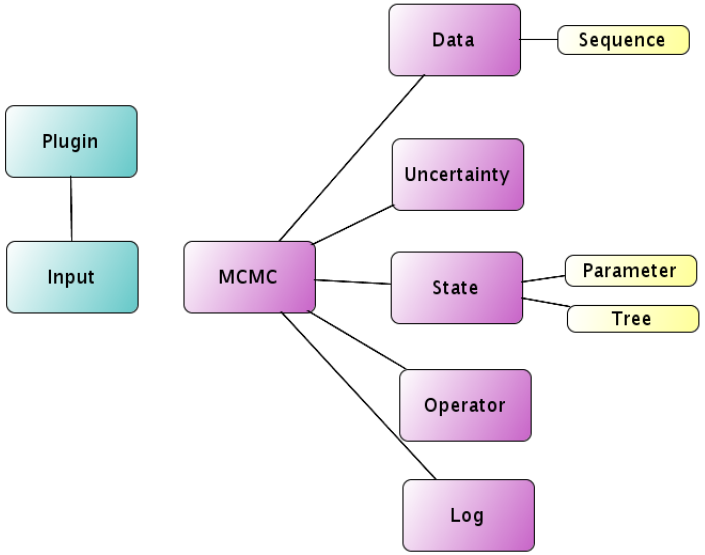
XML

```
<mcmc id="mcmc" chainLength="5000000">
    <state>
        <parameter id="hky.kappa" value="1.0" lower="0.0"/>
        <tree spec='util.ClusterTree' id='tree' clusterType='upgma'>
           <input name='taxa' idref='alignment'/>
        </tree>
    </state>

    <uncertainty id='likelihood' idref="treeLikelihood"/>

    <operator spec='ScaleOperator' scaleFactor="0.5" weight="1">
        <parameter idref="hky.kappa"/>
    </operator>
    <operator spec='ScaleOperator' scaleFactor="0.5" weight="1">
        <tree idref="tree"/>
    </operator>
    <operator spec='Uniform' weight="10">
        <tree idref="tree"/>
    </operator>
    <operator spec='SubtreeSlide' weight="5" gaussian="true" size="1.0">
        <tree idref="tree"/>
    </operator>
    <operator id='narrow' spec='Exchange' isNarrow='true' weight="1">
        <tree idref="tree"/>
    </operator>
    <operator id='wide' spec='Exchange' isNarrow='false' weight="1">
```

XML parsing/writing provided by the framework XML

Reserved elements

<mcmc >
<uncertainty >
<operator >
<log >
<data >
<sequence >
<state >
<parameter >
<tree >




```
<beast version='2.0' namespace='x.y.z:' >
<map name='elementName' >x.y.z.Class </map>
```

XML


```
<!-- The HKY substitution model (Hasegawa, Kishino & Yano, 1985)          -->
<input spec='HKY' id="hky">
    <parameter name='kappa' idref='hky.kappa'/>
    <input id='freqs' name='frequencies' spec='Frequencies'>
        <input name='data' idref='alignment'/>
    </input>
</input>

<!-- site model                                                            -->
<input spec='SiteModel' id="siteModel">
    <input idref='freqs' name='frequencies'/>
    <input name='substModel' idref='hky'/>
</input>

<input spec='TreeLikelihood' id="treeLikelihood">
    <input name='data' idref="alignment"/>
    <input name='tree' idref="tree"/>
    <input name='siteModel' idref="siteModel"/>
</input>
```

XML


```
    <!-- The sequence alignment (each sequence refers to a taxon above).         -->
    <!-- ntax=6 nchar=768                                                         -->
    <!-- npatterns=69                                                             -->
    <data id="alignment" dataType="nucleotide">
        <sequence taxon="human">
AGAAATATGTCTGATAAAAGAGTTACTTTGATAGAGTAAATAATAGGAGCTTAAACCCCCTTATTTCTACTAGGACTATGAGAATCGAAC
        </sequence>
        <sequence taxon="chimp">
AGAAATATGTCTGATAAAAGAATTACTTTGATAGAGTAAATAATAGGAGTTCAAATCCCCTTATTTCTACTAGGACTATAAGAATCGAAC
        </sequence>
        <sequence taxon="bonobo">
AGAAATATGTCTGATAAAAGAATTACTTTGATAGAGTAAATAATAGGAGTTTAAATCCCCTTATTTCTACTAGGACTATGAGAGTCGAAC
        </sequence>
        <sequence taxon="gorilla">
AGAAATATGTCTGATAAAAGAGTTACTTTGATAGAGTAAATAATAGAGGTTTAAACCCCCTTATTTCTACTAGGACTATGAGAATTGAAC
        </sequence>
        <sequence taxon="orangutan">
AGAAATATGTCTGACAAAAGAGTTACTTTGATAGAGTAAAAAATAGAGGTCTAAATCCCCTTATTTCTACTAGGACTATGGGAATTGAAC
        </sequence>
        <sequence taxon="siamang">
AGAAATACGTCTGACGAAAGAGTTACTTTGATAGAGTAAATAACAGGGGTTTAAATCCCCTTATTTCTACTAGAACCATAGGAGTCGAAC
        </sequence>
    </data>
```

XML

Reserved attributes:

```
<input id='myId'
      idref='otherId'
      name='inputName'
      spec='x.y.z.MyClass' />
```

Resolving plug-in class:

- specified in spec attribute
- if not, get from element2class map
- if not, use element name (and hope it shows up in the namespace somewhere).

XML

Resolving input name:

- specified in name attribute

```
<input name="xyz" >
```

- if not, use (non-reserved) attribute name

```
<input xyz="3" >
```

- if not, use element name

```
<xyz value="3" >
```

- if input, use 'value' when there is text content, but no element content

```
<input>3</input>
```

XML

Resolving input value:

- if idref is specified, use the referred object

```
<input idref="other" >
```

- specified in value attribute

```
<xyz value="3" >
```

- if not, use value of (non-reserved) attribute

```
<input xyz="3" >
```

- if not, use text content when there is text content, but no element content

```
<input>3</input>
```

XML

Parsing rules: Processing non reserved attributes

```
<input otherAttribute="xyz" />
```

equals

```
<input >
  <input name='otherAttribute' value='xyz' />
</input>
```

Processing non reserved element names

```
<myElement />
```

==

```
<input spec='myElement' name='myElement' />
```

unless 'spec' is a specified attribute, then that overrides, likewise for 'name'

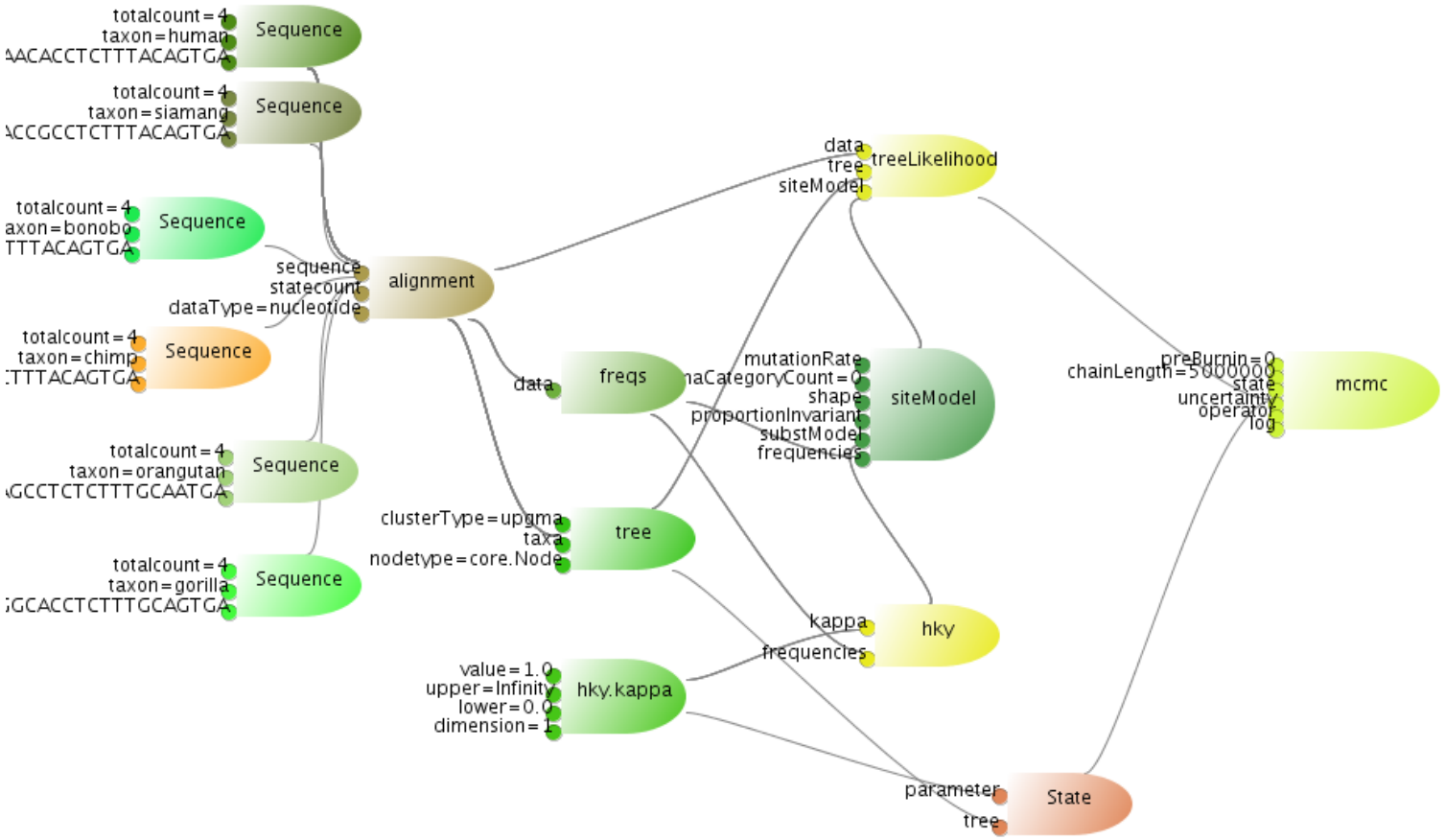
Processing of text content (only when there are no enclosing elements)

```
<input name='data' >xyz </input>
```

==

```
<input name='data' value='xyz'/ >
```

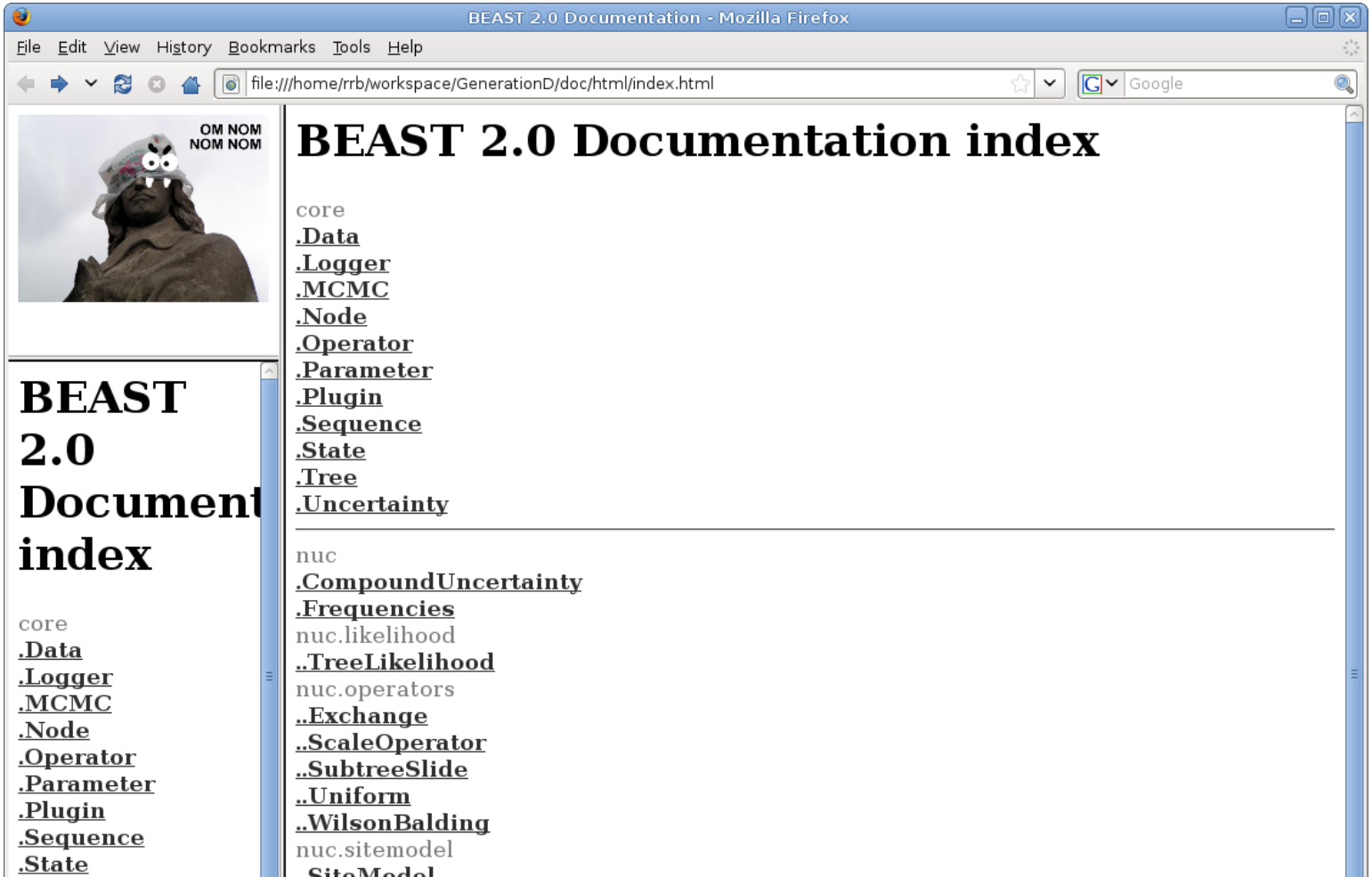
Model builder



Documentation

XML documentation provided through

- @Description annotation on plug in
- Tooltip text on inputs
- getCitation method
- Input validation rules



Documentation

BEAST 2.0 Documentation - Mozilla Firefox

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file:///home/rrb/workspace/GenerationD/doc/html/index.html

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nuc
.CompoundUncerta
.Frequencies
nuc.likelihood
..TreeLikelihood
nuc.operators
..Exchange
..ScaleOperator
..SubtreeSlide
..Uniform
..WilsonBalding

BEAST 2.0 Documentation: nuc.substitutionmodel.HKY

Specifies transition probability matrix for a given distance

HKY85 (Hasegawa, Kishino & Yano, 1985) substitution model of nucleotide evolution.

Reference:

Hasegawa, M., Kishino, H and Yano, T. 1985. Dating the human-ape splitting by a molecular clock of mitochondrial DNA. Journal of Molecular Evolution 22:160-174.

Inputs:

kappa

type: core.Parameter
kappa parameter in HKY model
Required input

frequencies

type: nuc.Frequencies
frequencies of characters
Required input

Documentation

BEAST 2.0 Documentation - Mozilla Firefox

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file:///home/rrb/workspace/GenerationD/doc/html/index.html

BEAST 2.0 Documentation: nuc.substitutionmodel.HKY

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java author annotation

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BEAST 2.0 Documentation: core.Uncertainty

implemented by the following
nuc.CompoundUncertainty
nuc.likelihood.TreeLikelihood
snap.likelihood.SnAPPrior
snap.likelihood.SnAPTreeLikelihood

Not documented!!!

Inputs:

<none>

BEAST 2.0


```
~> java -cp bin app.BeastMCMC

Usage: BeastMCMC [options] <Beast.xml>
where <Beast.xml> the name of a file specifying a Beast run
and the following options are allowed:
-seed <int> : sets random number seed (default 127)
-threads <int> : sets number of threads (default 1)
```

BEAST 2.0

HKY + nucleotide data, 'random' initial tree
2000 samples in debug mode, scaling if required, auto optimise on, same logging, operators. etc.
testMCMC.xml – great apes

```
6 taxa
768 sites
69 patterns
10M samples  single thread
        Beast 1.6/java  Beast1.6/native Beast 2.0
real    3m55.056s       3m38.670s       2m31.794s
user    3m54.839s       3m38.670s       2m32.162s
sys     0m0.392s        0m0.428s        0m0.476s
```

BEAST 2.0

testMCMC.xml –

```
46 taxa
1363 sites
199 patterns
500K samples

Beast1.6/native core
real    1m56.097s
user    1m58.683s
sys     0m0.332s

Beast 2.0 + auto
real    0m56.843s
user    0m59.264s
sys     0m0.428s
```

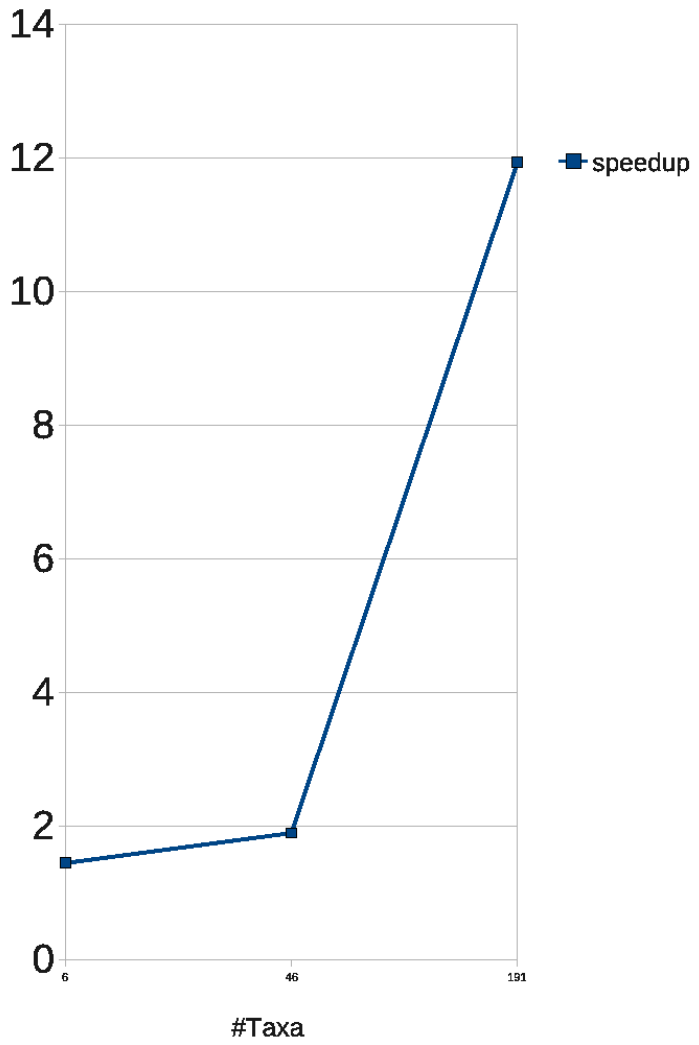
BEAST 2.0

testMCMC.xml –

```
191 taxa
606 sites
228 patterns
100K samples

Beast1.6/native
real    8m32.418s
user    8m33.060s
sys     0m0.476s

Beast 2.0
real    0m43.962s
user    0m46.051s
sys     0m0.432s
```



Summary Beast 2.0

Extensibility

- Everything is a plug-in
- Plug-in implementation:
  - Add @Description annotation
  - Specify Inputs
  - Implement initAndValidate
  - Optional: getCitation, store, restore
- Get xml-parsing, Input validation, xml-documentation for free
- Store/restore more transparent
- Explicit state object

Documentation

- Framework 'forces' proper documentation habits
- Automatic documentation generation

Performance

- Up to 1 order of magnitude better performance