

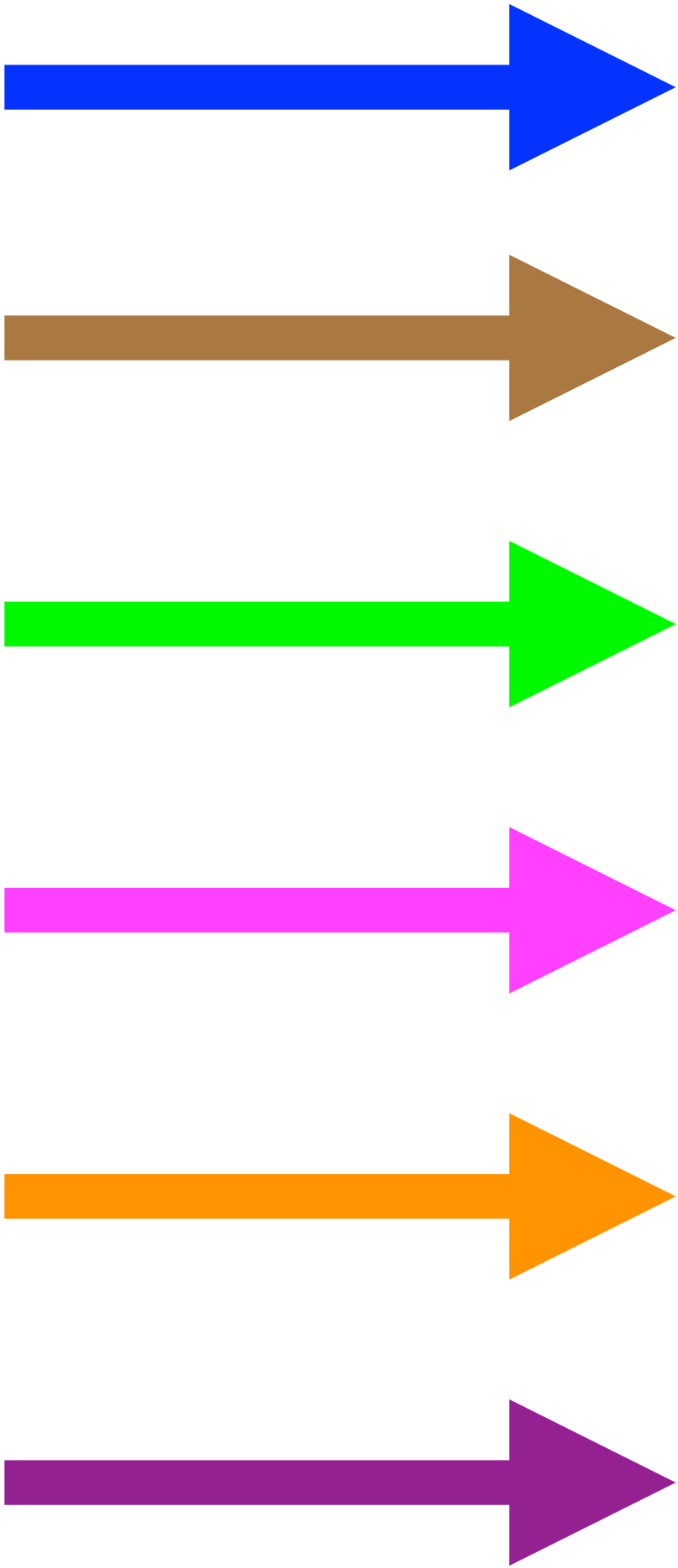
Replicarexchange



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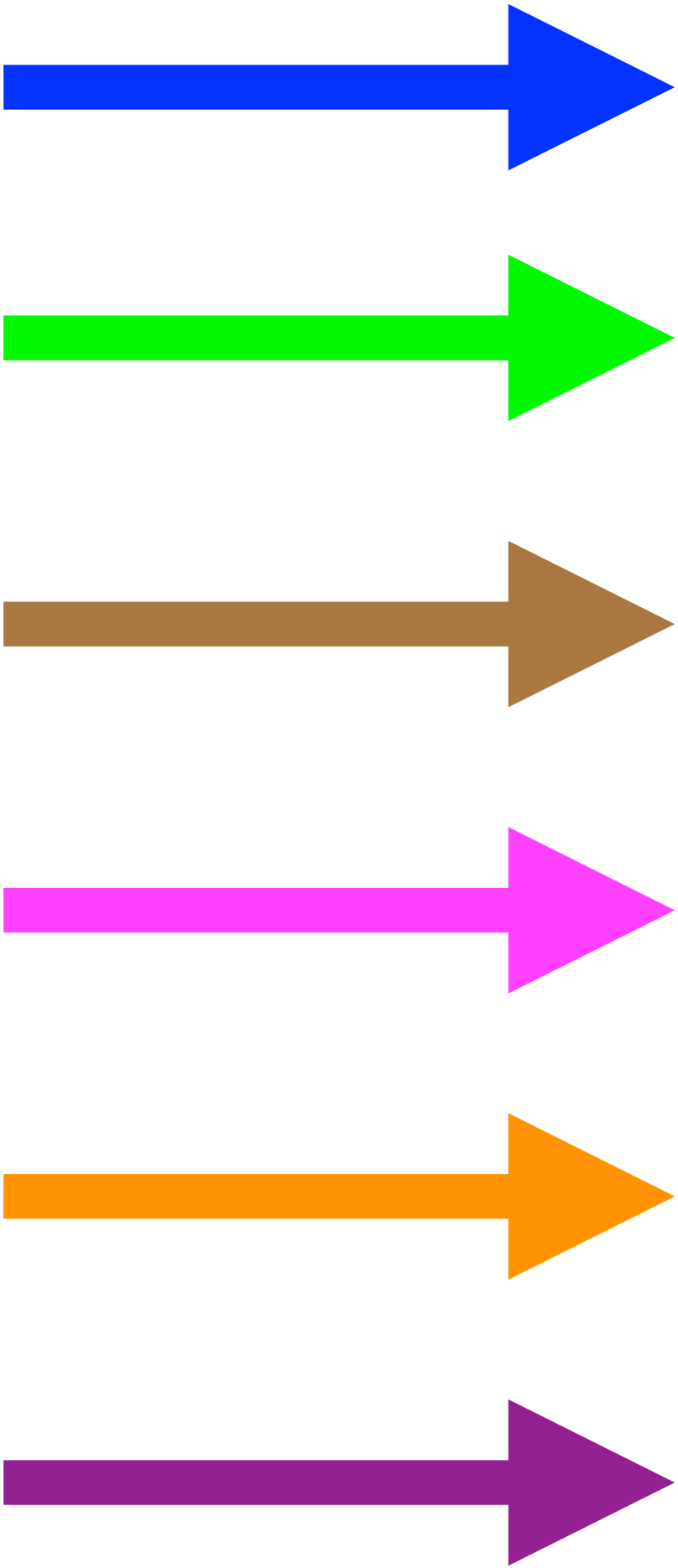
=

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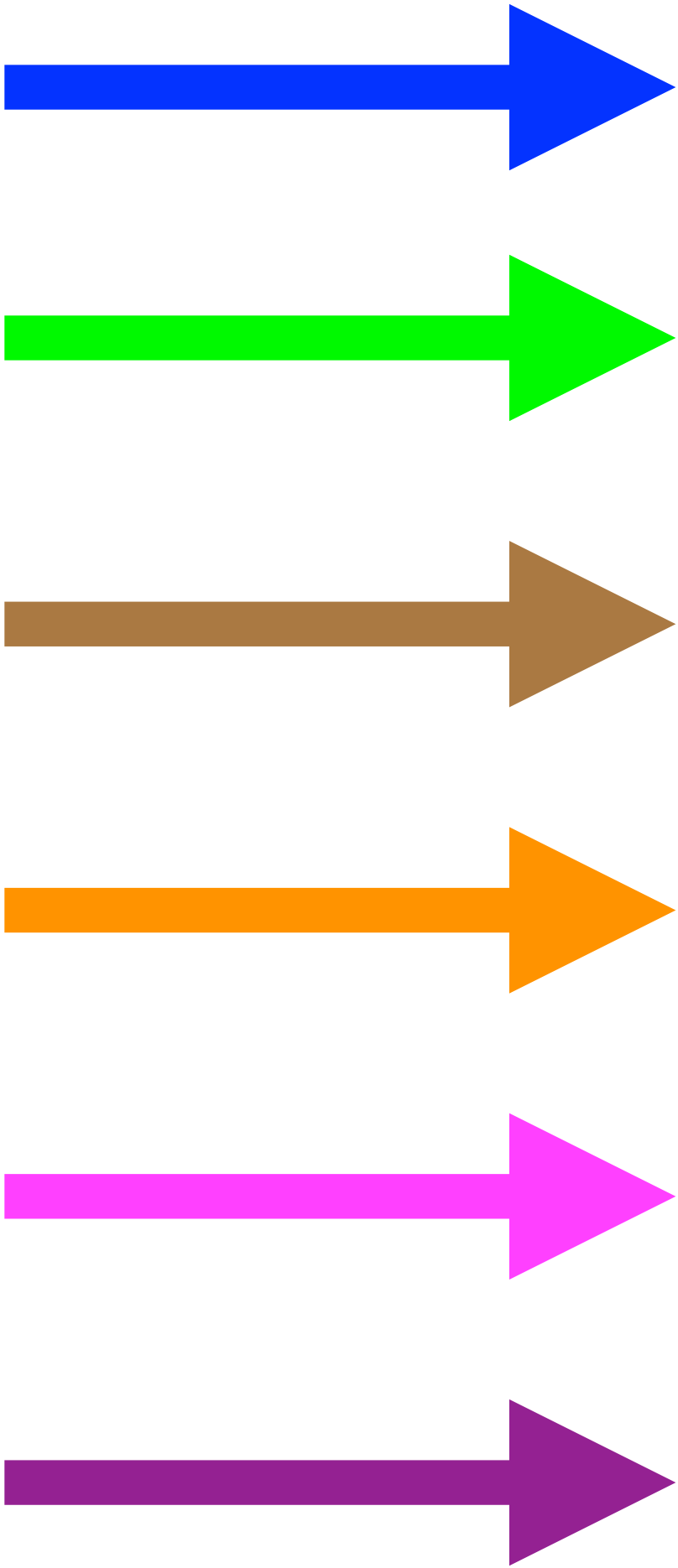
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8

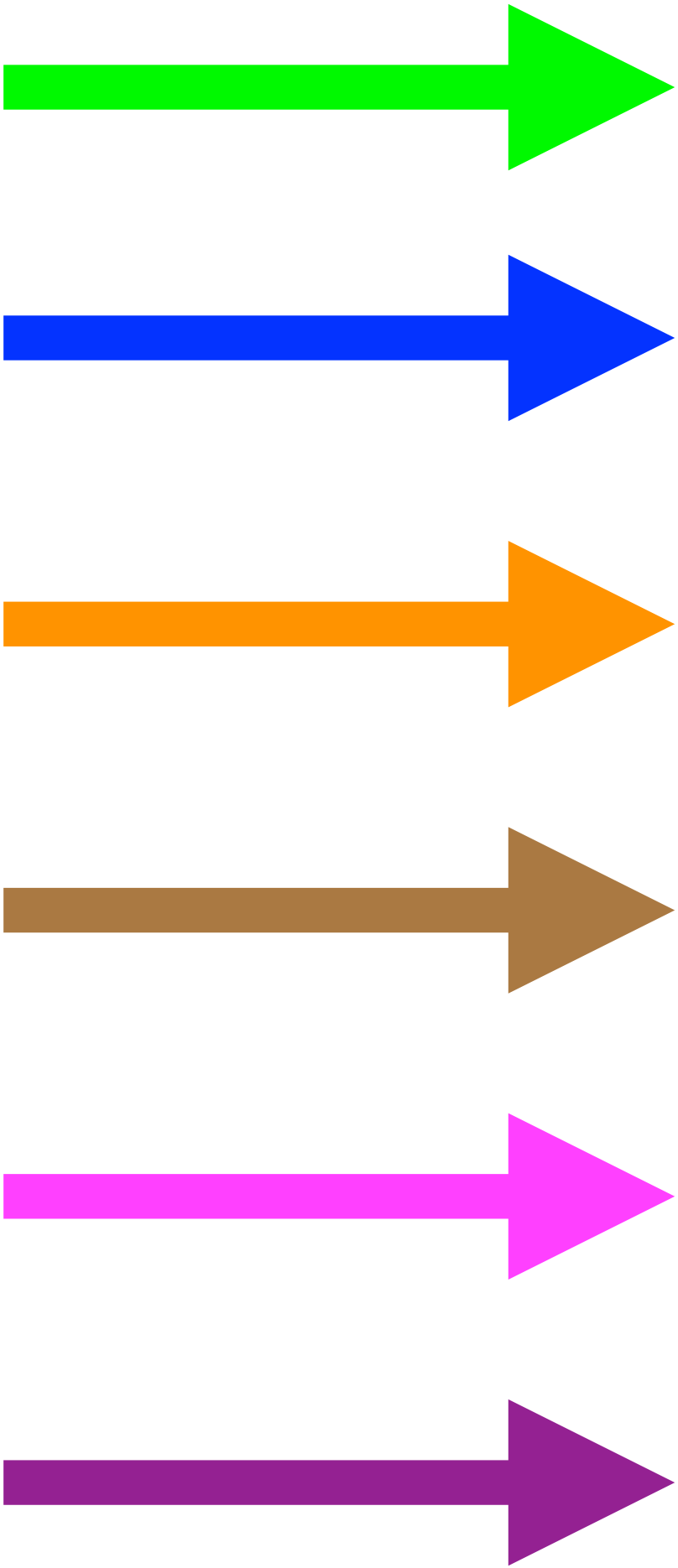




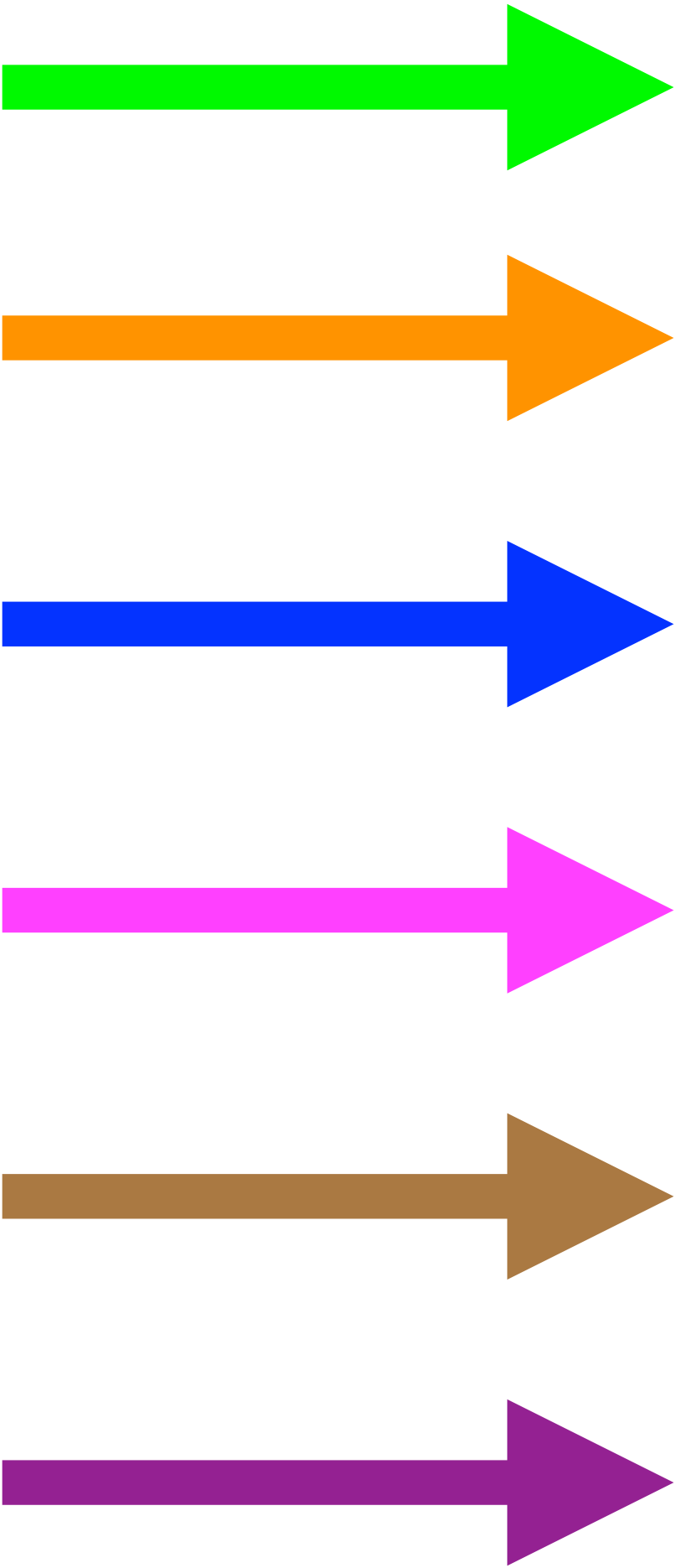




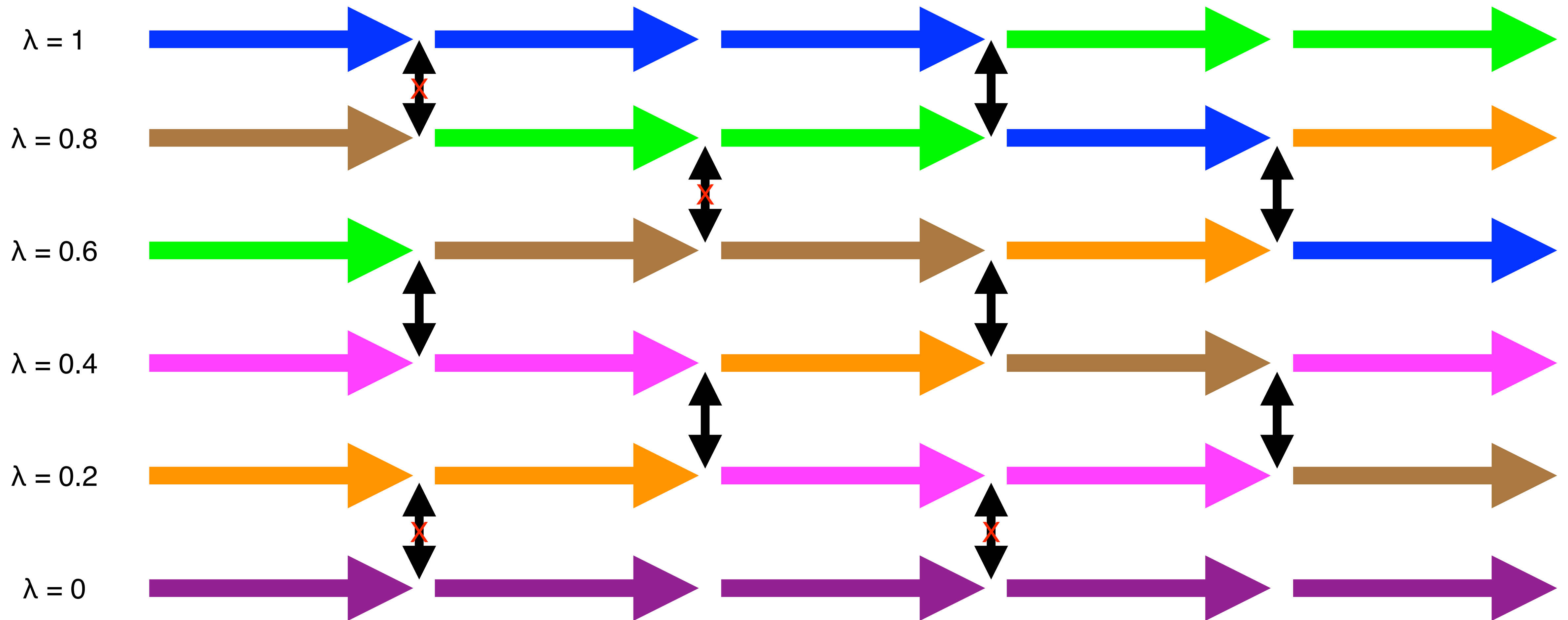








Replica exchange



Analysis with YANK

- See <http://getyank.org/latest/analysis.html#analysis-usage>
- You can perform automatic analysis with
 - `yank analyze --yaml={Some YAML file which ran with ``yank script``}`

```
ccb:[~/YANK]: yank analyze --store=/home/bxie4/restraint_simulation/YANK/TEST_SYSTEMS/bromodomain/3mxf/40flat_output_repeat1/experiments
/home/bxie4/local/miniconda3/lib/python3.6/site-packages/openmmtools/multistate/__init__.py:75: UserWarning: Warning: openmmtools.multistate API is experimental
  warnings.warn('Warning: openmmtools.multistate API is experimental')
/home/bxie4/local/miniconda3/lib/python3.6/site-packages/yank/multistate/utils.py:253: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted as an array index, `arr[np.array(seq)]`, which will result either in an error or a different result.
  equilibrated_data = cast_data[slc]
Free energy          :    99.786 +- 0.005 kT (59.489 +- 0.003 kcal/mol)
DeltaG solvent       :    99.786 +- 0.005 kT
Enthalpy             :   100.720 +- 0.034 kT (60.045 +- 0.020 kcal/mol)
```