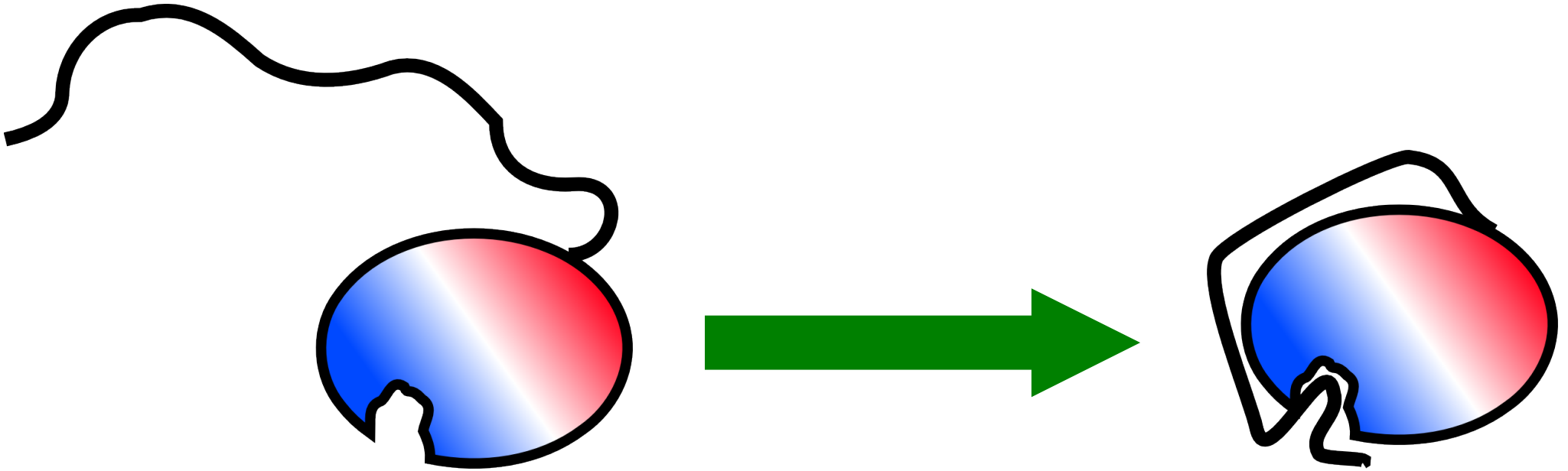
FloppyTail as a case study

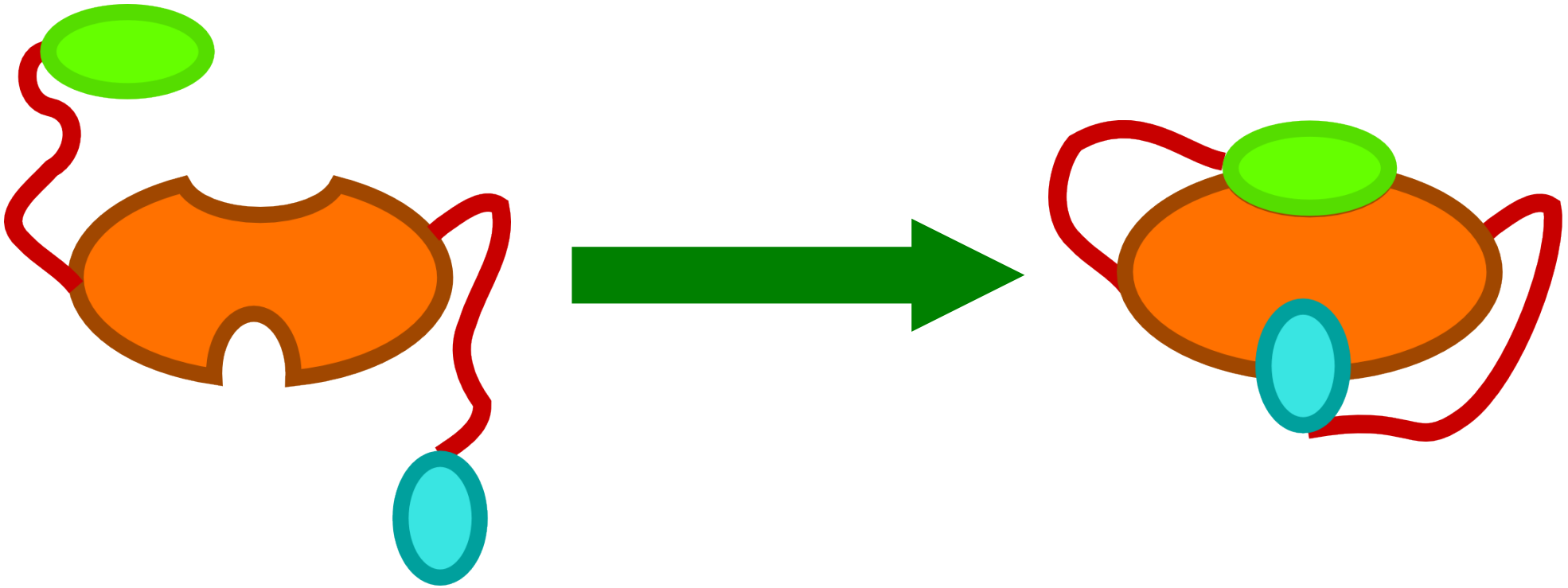
(There is some “dirty laundry” here, code that predates or fails to comply with our official standards...so pretend you don't see that!)

Steven Lewis
Part of the RosettaCON 2013 tutorial

Original case

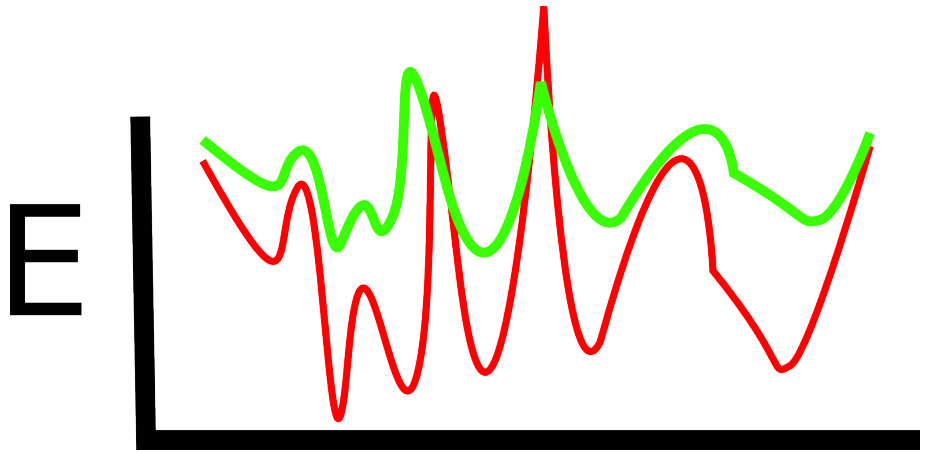


Current status



How does the protocol run?

- Traditionally, centroid/fullatom
  - Centroid
    - reduced sidechains
    - fast
    - less rugged energy function
    - wider sampling
  - Fullatom opposite



Centroid/Fullatom

- `ResidueTypeSet`
- `ScoreFunction`
  terms non-obviously must match

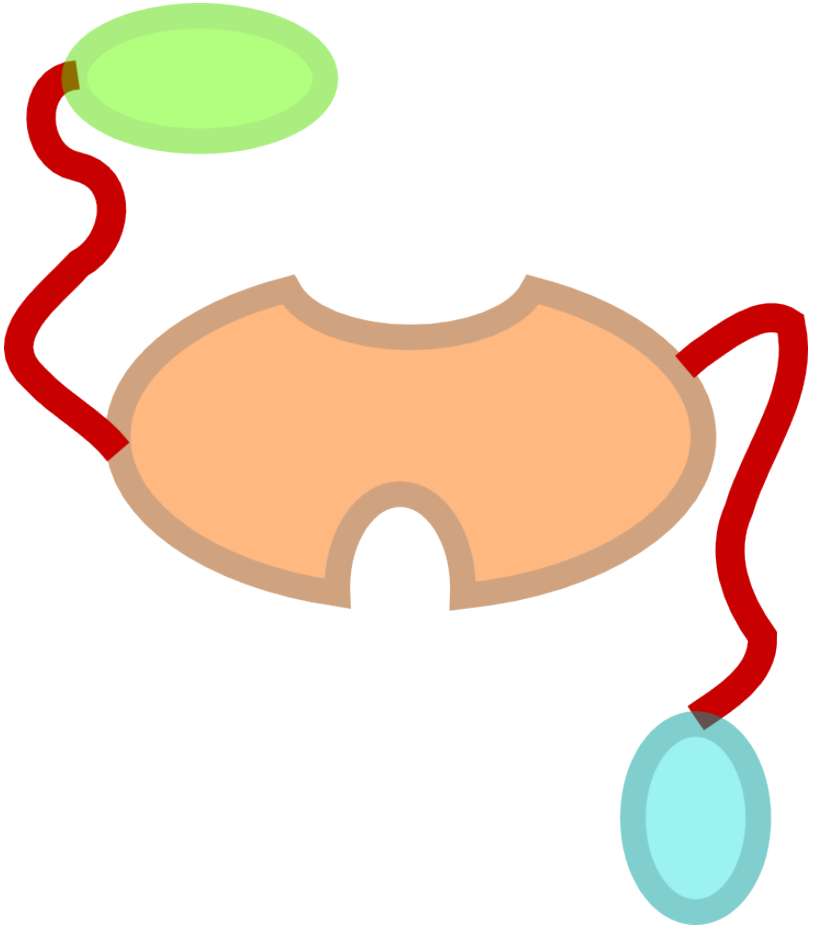
- `SwitchToResidueTypeSetMover`
  - Generally TO centroid
- `ReturnSidechainsMover`
  - Pipes sidechains around centroid phase

What is happening in those phases?

- Movers Movers Movers
- Build Movers, run movers along with `MonteCarlo`
- Aggressive moves in centroid
- Minimizing moves in fullatom

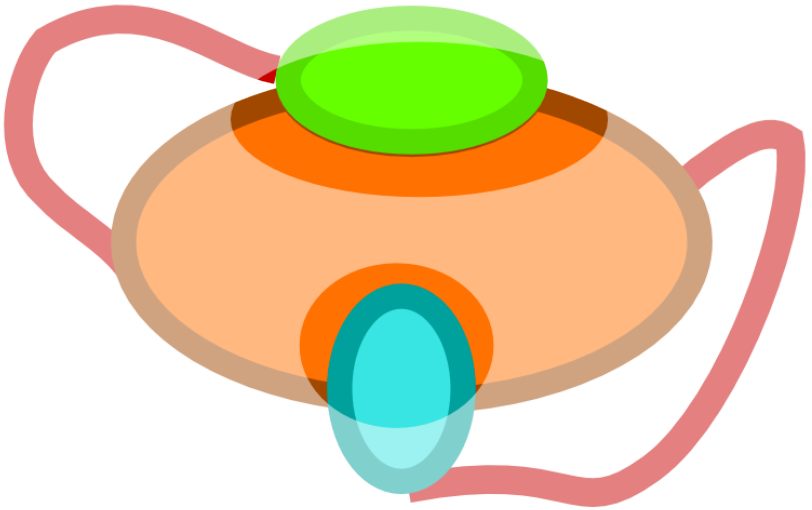
What determines flexibility?

- `MoveMap`
- `FoldTree`



What determines packability?

- Packing:
  - `TaskFactory`
  - `TaskOperations`
  - `PackerTask`
  - Interface detectors



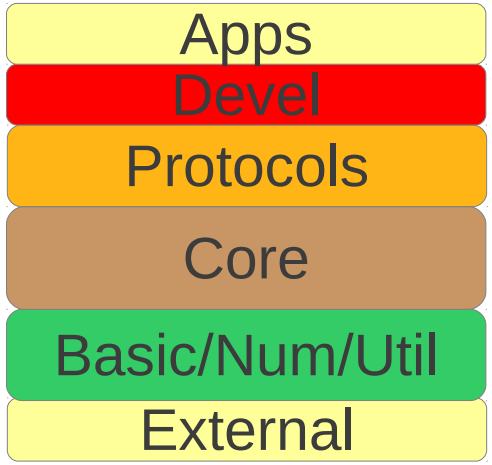
Using the cluster?

- `JD2`
- Simple app-level wrapper

Getting it to compile?

- Scons settings
- Init if using load-time factory registration systems

What does a Mover need?



- `virtual void apply( Pose & )`
  - Strictly necessary
- Getters and setters for all options
  - Option use restricted to one setup function
- RosettaScripts hookups
  - `virtual void parse_my_tag(...)`
- Operator>> for PyRosetta
- Miscellaneous JD2 hookups

Collections of useful classes

- src/core/scoring/constraints
  - Useful for incorporating experimental data and biasing trajectories
- src/core/pack/task/operation
  - TaskOperations for controlling packing
  - Also src/protocols/toolbox/task_operations
- src/protocols/toolbox/pose_metric_calculators
  - General system for calculating “things”

Load-time factory registration

- Side effect of good organization: low code can't see high code
- System allows high-level code to route into low-level code
  - Your new EnergyMethod in protocols works with ScoreFunction in core