# Implementation of STDR in python

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2011-11-08

# Simulated Tempering Distributed Replica (STDR)

Key functions:

Func1 $$p(T_i \rightarrow T_j) = min \begin{cases} 1 \\ e^{-(\beta_j - \beta_i)E + (\alpha_i - \alpha_j) - (DRPE_j - DRPE_i)} \end{cases}$$

Func2 $$DRPE = c_1 \sum_{m=1}^{M} \sum_{n=1}^{M} [\lambda_{m,linear} - \lambda_{n,linear} - \omega(m-n)]^2$$

$$+ c_2 \left[ \sum_{m=1}^{M} \lambda_{m,linear} - \omega \sum_{m=1}^{M} m \right]^2$$

Sarah, et al 2009

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- β: *the inverse temperature*
- *E: potential energy*
- λ: *depends on the current global temperature.*
- *DRPE: distributed replica potential energy*

Sarah, et al 2009

t1

t2

t3

t4

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| | |
| | |
| | |
| | |
| | |
| | |

time

t1

t2

t3

EX1

t3'

t4

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3',t4 |
| | |
| | |
| | |
| | |
| | |

time

t1

EX2

t1′

t2

t3

EX1

t3′

t4

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′,t4 |
| 2 | t1′,t2,t3′,t4 |
| | |
| | |
| | |
| | |

time

t1

EX2

t1′

t2

EX3

t2′

t3

EX1

t3′

t4

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′,t4 |
| 2 | t1′,t2,t3′,t4 |
| 3 | t1′,t2′,t3′,t4 |
| | |
| | |
| | |

time

t1

EX2

t1′

t2

EX3

t2′

t3

EX1

t3′

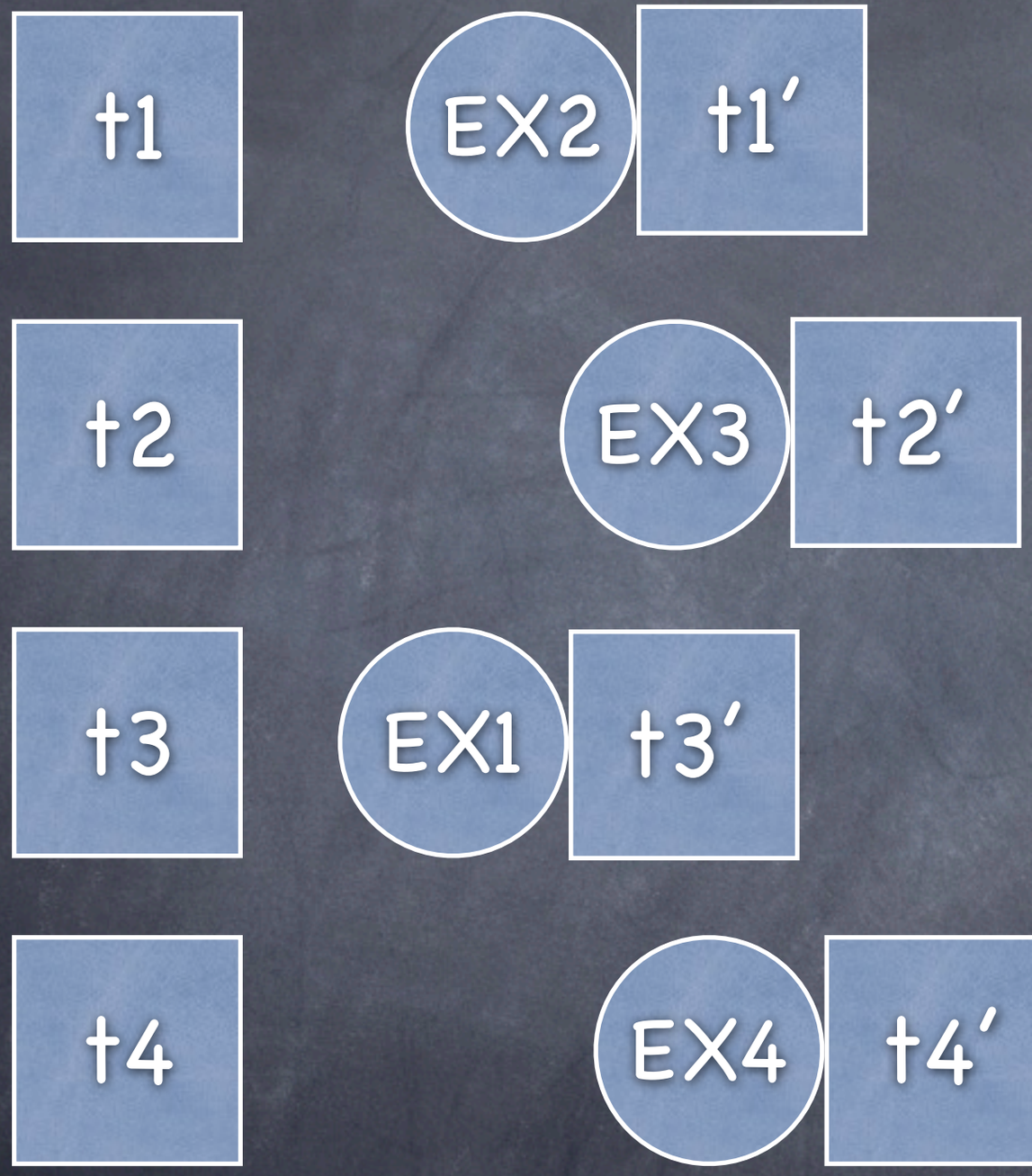
t4

EX4

t4′

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′,t4 |
| 2 | t1′,t2,t3′,t4 |
| 3 | t1′,t2′,t3′,t4 |
| 4 | t1′,t2′,t3′,t4′ |
| | |
| | |

time




| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3',t4 |
| 2 | t1',t2,t3',t4 |
| 3 | t1',t2',t3',t4 |
| 4 | t1',t2',t3',t4' |
| 5 | t1',t2',t3'',t4' |
| | |

time

t1

EX2

t1′

t2

EX3

t2′

t3

EX1

t3′

EX5

t3″

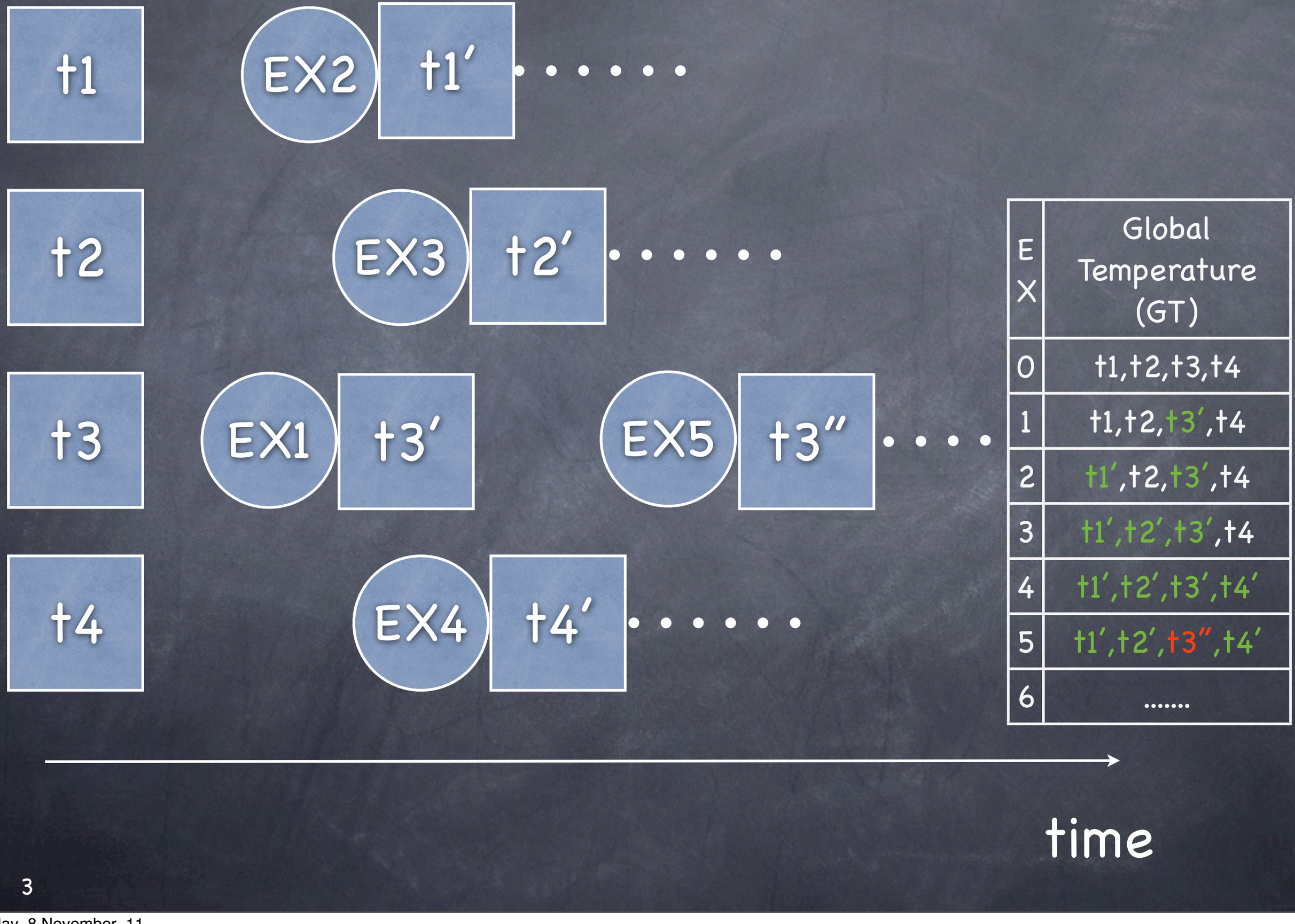
t4

EX4

t4′

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′,t4 |
| 2 | t1′,t2,t3′,t4 |
| 3 | t1′,t2′,t3′,t4 |
| 4 | t1′,t2′,t3′,t4′ |
| 5 | t1′,t2′,t3″,t4′ |
| | |

time




| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3',t4 |
| 2 | t1',t2,t3',t4 |
| 3 | t1',t2',t3',t4 |
| 4 | t1',t2',t3',t4' |
| 5 | t1',t2',t3",t4' |
| 6 | ..... |

t1

EX2

t1′

what happened in EXi ?

t2

EX3

t2′

t3

EX1

t3′

EX5

t3″

t4

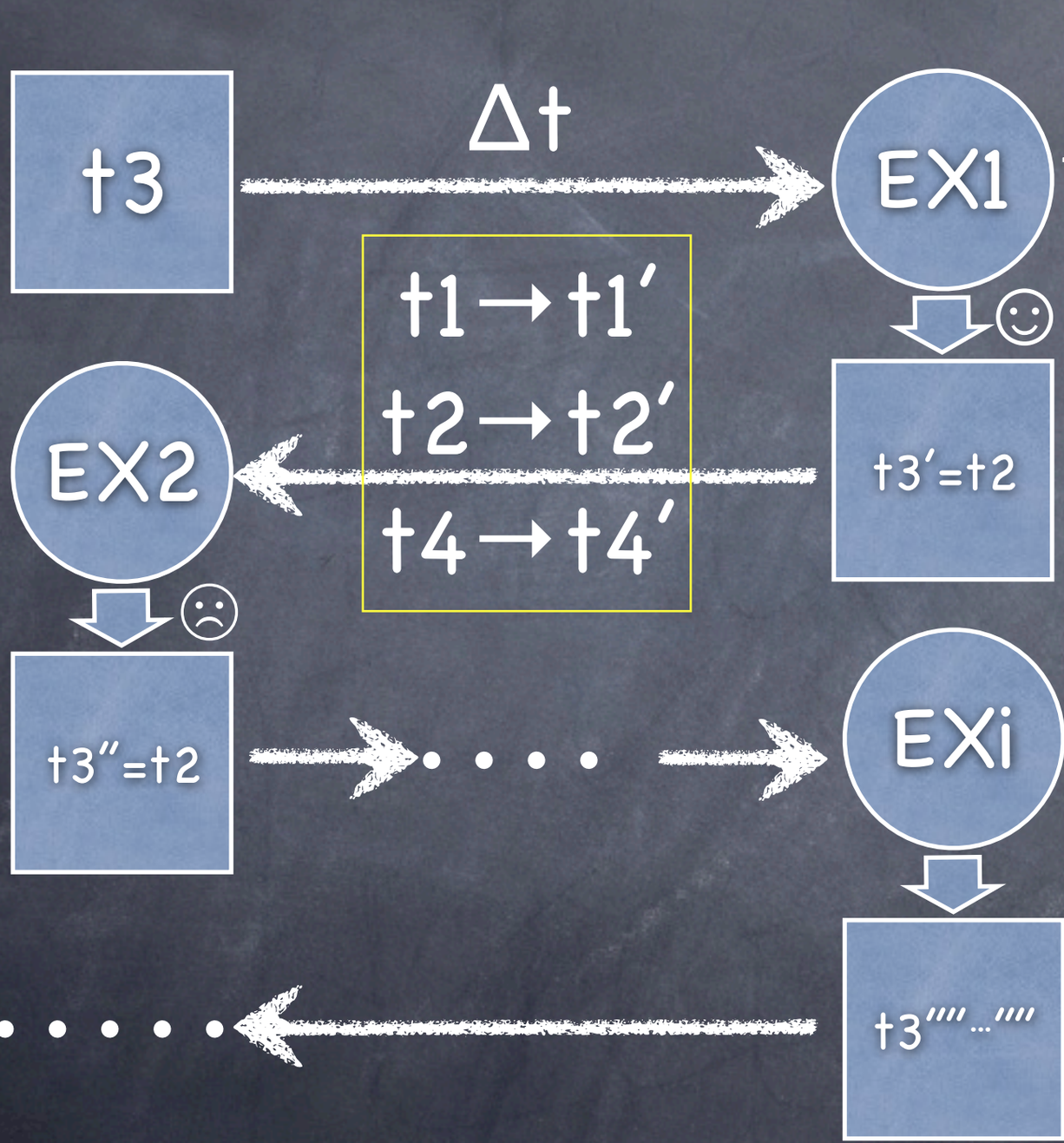
EX4

t4′

| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′,t4 |
| 2 | t1′,t2,t3′,t4 |
| 3 | t1′,t2′,t3′,t4 |
| 4 | t1′,t2′,t3′,t4′ |
| 5 | t1′,t2′,t3″,t4′ |
| 6 | ..... |

time

# Take t3 as an example




| EX | Global Temperature (GT) |
|---|---|
| 0 | t1,t2,t3,t4 |
| 1 | t1,t2,t3′(t2),t4 |
| 2 | t1′,t2,t2,t4 |
| 3 | t1′,t2′,t3′,t4 |
| 4 | t1′,t2′,t3′,t4′ |
| 5 | t1′,t2′,t3″(t2),t4′ |
| 6 | ..... |

# Objectives

1. Automate the whole process

   - overhead: pre-equilibrate all replicas at different temperatures; given necessary files (gro, top, itp, mdp), configuration files (e.g. pydr.cfg), template files of mdrun code & postprocessing code (mdrun.tmp)
   - everything else should be fine till the end of the whole STDR is done, then you could start analyzing trajectories right away.

2. Easy to restart & continue simulations of all/certain replicas after SciNet/certain nodes are down

3. log information about every exchange.

# Server Client Model

- Server: permission to read & write exchange information to an database (e.g. pydr.db)
- Client: in charge of running mdrun.sh (not necessarily bash script) for each replica
- Server & client coexist on each node, but only one server is active at a time with others all idling.

Server Client(00)

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
./sq1e
    ./replicas
            ./00
            ./01
            ./02
            ./03
./parametersets
            ./300.mdp
            ./310.mdp
            ./320.mdp
            ./330.mdp
./miscellaneous
            ./eth.itp
            ./sq1.itp
            ./sq1e.top
./mdrun.tmp
./pydr.cfg
./hostfile
./pydr.db
```

in each replica directory, there is a equilibrated gro file and pydr.py

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

Server

Client(00)

ready to go

```
./sq1e
    ./replicas
            ./00
            ./01
            ./02
            ./03
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            ./300.mdp
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| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

Server

Client(00)

ready to go

This is 00, haven't done anything, Give me the mdp

```
./sq1e
    ./replicas
            ./00
            ./01
            ./02
            ./03
./parametersets
            ./300.mdp
            ./310.mdp
            ./320.mdp
            ./330.mdp
./miscellaneous
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            ./sq1.itp
            ./sq1e.top
./mdrun.tmp
./pydr.cfg
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```

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            ./300.mdp
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            ./sq1.itp
            ./sq1e.top
./mdrun.tmp
./pydr.cfg
./hostfile
./pydr.db
```

in each replica directory, there is a equilibrated gro file and pydr.py

Server

Client(00)

ready to go

This is 00, haven't done anything, Give me the mdp

first time asking, here is your mdp, 300.mdp

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
./sq1e
    ./replicas
            ./00
            ./01
            ./02
            ./03
./parametersets
            ./300.mdp
            ./310.mdp
            ./320.mdp
            ./330.mdp
./miscellaneous
            ./eth.itp
            ./sq1.itp
            ./sq1e.top
./mdrun.tmp
./pydr.cfg
./hostfile
./pydr.db
```

in each replica directory, there is a equilibrated gro file and pydr.py

Server

Client(00)

ready to go

This is 00, haven't done anything, Give me the mdp

first time asking, here is your mdp, 300.mdp

grompp, mdrun, calc pot_energy, new_t

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
./sq1e
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ready to go

This is 00, haven't done anything, Give me the mdp

first time asking, here is your mdp, 300.mdp

grompp, mdrun, calc pot_energy, new_t

this is 00, mdrun done, attempting to change to new_t, here are my current t & pot_enregy, can I exchange?

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
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```
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new_t, t, pot_energy received, not first time asking anymore, let me see

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
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new_t, t, pot_energy received, not first time asking anymore, let me see

query the database, get global temperature, calc DRPE, probability, write to database, target new mdp assign to 00

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
./sq1e
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            ./03
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    ./mdrun.tmp
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    ./hostfile
    ./pydr.db
```

in each replica directory, there is a equilibrated gro file and pydr.py

Server Client(00)

ready to go

This is 00, haven't done anything, Give me the mdp

first time asking, here is your mdp, 300.mdp

grompp, mdrun, calc pot_energy, new_t

this is 00, mdrun done, attempting to change to new_t, here are my current t & pot_enregy, can I exchange?

new_t, t, pot_energy received, not first time asking anymore, let me see

query the database, get global temperature, calc DRPE, probability, write to database, target new mdp assign to 00

Sorry, run with your old mdp for another 8ps/
here is your new mdp(e.g. 310.mdp)

| Preset Temperatures (ts) | t1 | t2 | t3 | t4 |
|---|---|---|---|---|
| Uniform Spacing (us) | 1 | 2 | 3 | 4 |

```
./sq1e
    ./replicas
            ./00
            ./01
            ./02
            ./03
    ./parametersets
            ./300.mdp
            ./310.mdp
            ./320.mdp
            ./330.mdp
    ./miscellaneous
            ./eth.itp
            ./sq1.itp
            ./sq1e.top
    ./mdrun.tmp
    ./pydr.cfg
    ./hostfile
    ./pydr.db
```

in each replica directory, there is a equilibrated gro file and pydr.py

Server Client(00)

ready to go

This is 00, haven't done anything, Give me the mdp

first time asking, here is your mdp, 300.mdp

grompp, mdrun, calc pot_energy, new_t

this is 00, mdrun done, attempting to change to new_t, here are my current t & pot_enregy, can I exchange?

new_t, t, pot_energy received, not first time asking anymore, let me see

query the database, get global temperature, calc DRPE, probability, write to database, target new mdp assign to 00

Sorry, run with your old mdp for another 8ps/
here is your new mdp(e.g. 310.mdp)

# Code analysis

- Protocol chosen: (Hypertext Transfer Protocol) http
- Framework used: Flask (http://flask.pocoo.org/)
- Database communication: sqlalchemy (http://www.sqlalchemy.org/)
- Classes defined: Exchange, Job, Replicas

# Exchange

- inherited from sqlalchemy.ext.declarative.Base class, used to write exchange info to the database (it's like a table)

- Headers defined: exid, rid, repcount, t1, t2, DRPE1, DRPE2, pot_ener, global_temp, date

| exid | rid | repcount | t1 | t2 | DRPE1 | DRPE2 | pot_ener | global_temp | date |
|---|---|---|---|---|---|---|---|---|---|
| 0 | -- | -- | -- | -- | -- | -- | -- | 300 310 320 330 | Sun Nov 6 16:05:31 2011 |
| 1 | 00 | 2 | 300 | 300 | 0.0 | 0.035 | -46294.7 | 300 310 320 330 | Sun Nov 6 16:05:34 2011 |
| 2 | 00 | 3 | 300 | 300 | 0.0 | 0.035 | -44503.9 | 300 310 320 330 | Sun Nov 6 16:05:37 2011 |
| 3 | 00 | 4 | 300 | 300 | 0.0 | 0.035 | -43058.8 | 300 310 320 330 | Sun Nov 6 16:05:39 2011 |
| 4 | 00 | 2 | 300 | 300 | 0.0 | 0.035 | -46526.2 | 300 310 320 330 | Sun Nov 6 16:53:13 2011 |
| 5 | 00 | 3 | 300 | 300 | 0.0 | 0.035 | -44467.8 | 300 310 320 330 | Sun Nov 6 16:53:16 2011 |
| 6 | 00 | 4 | 300 | 300 | 0.0 | 0.035 | -43039.7 | 300 310 320 330 | Sun Nov 6 16:53:19 2011 |

# Job

- a Job class represents a client, it will store PBS relevant information like PBS_JOBID, PBS_JOBNAME, etc.
- Job has the method of connecting to server (job.connect_server(uri, data)

# Replica

- Attributes include rid, old_temp, temp, directory, repcount, mdpf, deffnm
- Methods:
  - get_pot_ener
  - get_temp_to_change

# Problems to address

- How to restart & continue after SciNet/ certain nodes are Done?
- Server transferring
- make pydr.py small, modulize the other functions & classes, better configuration file.
- Maybe better schema for Exchange

code is in github, please have a look if you want

# About server transferring

- Walltime should be stored in Job class, do a self-check periodically, when it's too low, delete the hostfile. set a time in each loop, check the walltime left
- resubmitting, when a job ends, resubmit automatically.
- record the current map of rep to temperature in case of SciNet going down.

x