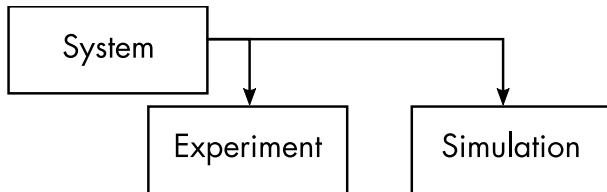
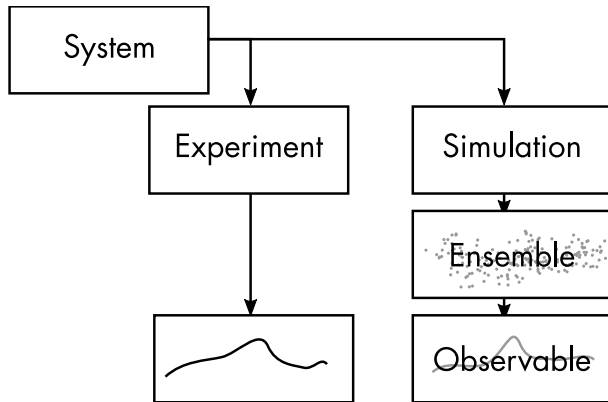


External Potentials from Experimental Data.

Christian Blau

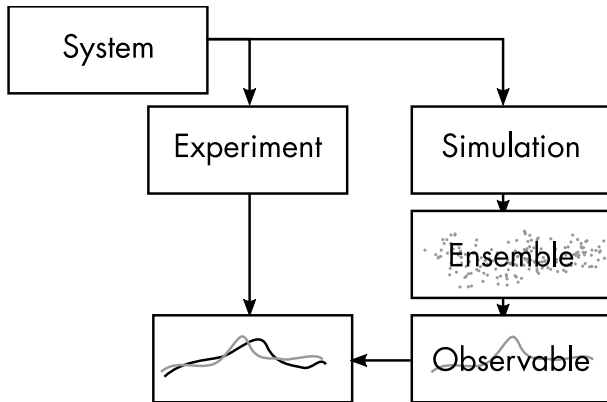
2016-05-20





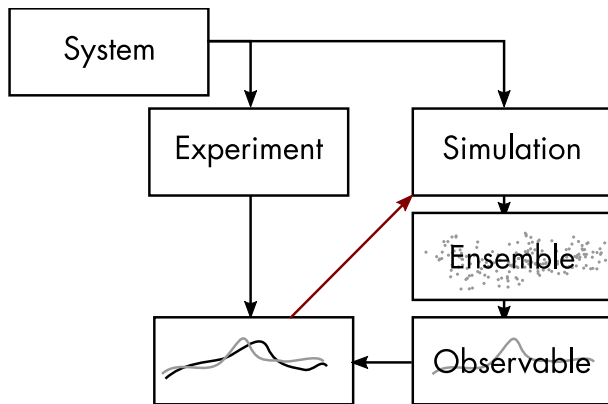
Adding Information from Experiment

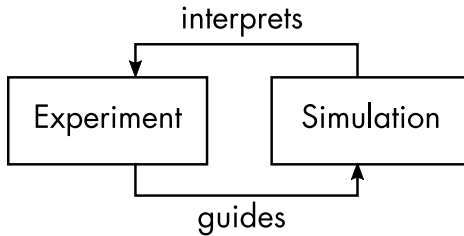
Christian Blau.SciLifeLab.TCB



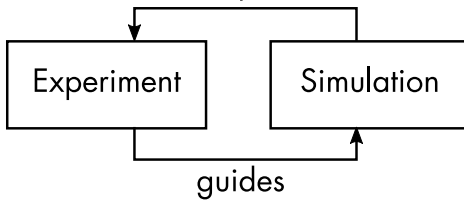
Adding Information from Experiment

Christian Blau.SciLifeLab.TCB

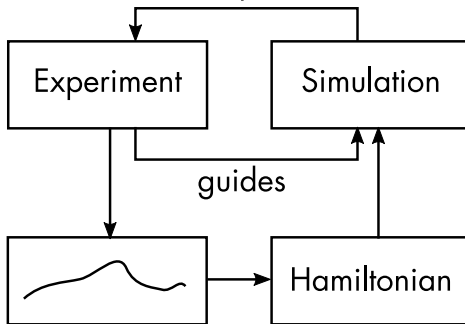




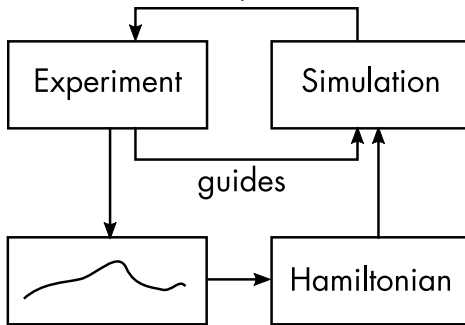
What is the ensemble behind the observable?
interprets



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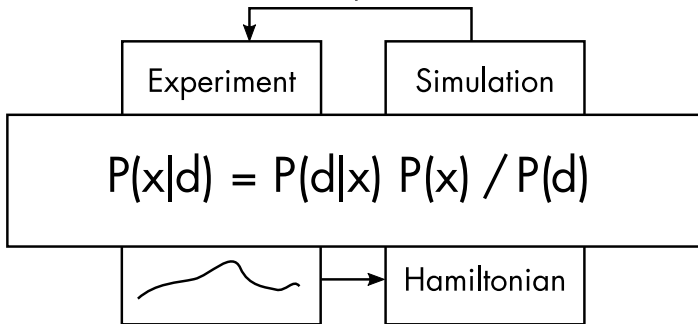


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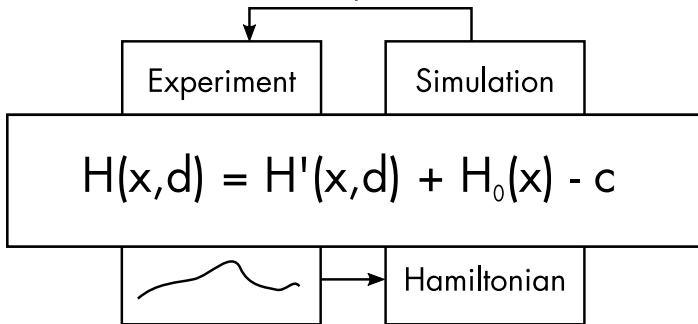
How does the observable (re)shape phase space density?

What is the ensemble behind the observable?
interprets



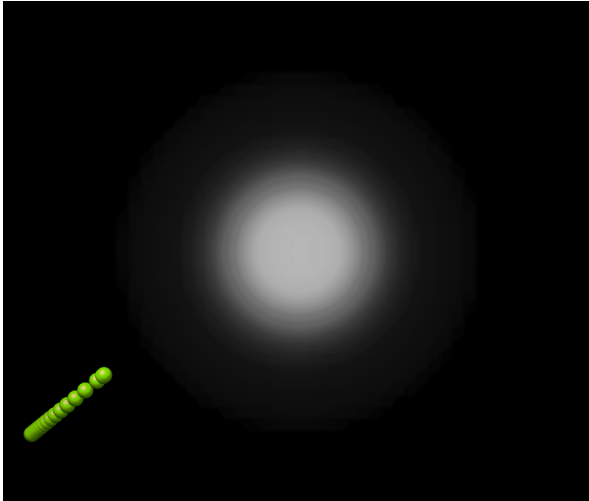
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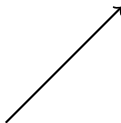
How does the observable (re)shape phase space density?





density → simulation

parameters

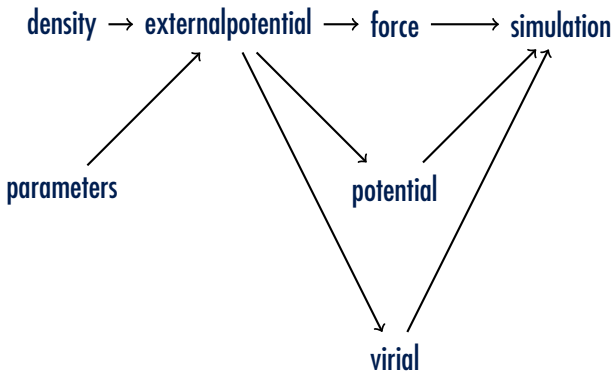


$$V_{\text{fit}} = -k_b T \sum_v \rho_v^e \log \rho^s$$

$$\mathbf{F}_{\text{fit}}^i = k_b T \frac{f_i}{u_i^2} \sum_v \frac{\rho^e(\mathbf{x}_v - \mathbf{r}_i) G_{u_i}(\mathbf{r}_i - \mathbf{x}_v)}{\rho^s}$$

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$$\mathbf{F}_{\text{fit}}^i = k_b T \frac{f_i}{u_i^2} \sum_v \frac{\rho^e(\mathbf{x}_v - \mathbf{r}_i) G_{u_i}(\mathbf{r}_i - \mathbf{x}_v)}{\rho^s}$$





```
class ExternalPotential
{
virtual void do_potential(const matrix box, const rvec x[], const gmx_int64_t step) = 0;
void add_forces(rvec f[], gmx_int64_t step, real weight);
virtual void initialize(const matrix box, const rvec x[]) = 0;
void add_virial(tensor vir, gmx_int64_t step, real weight);
void dd_make_local_groups(gmx_ga2la_t *ga2la);
void set_mpi_helper(std::shared_ptr<MpiHelper> mpi);
void add_group(std::shared_ptr<Group> group);
void set_input_output(std::shared_ptr<ExternalPotentialIO> &&input_output);
virtual void read_input() = 0;
virtual void broadcast_internal() = 0;
void set_atom_properties(t_mdatoms * mdatoms, gmx_localtop_t * topology_loc);
bool do_this_step(gmx_int64_t step);
std::shared_ptr<Group> group(const rvec x[], int group_index);
std::shared_ptr<WholeMoleculeGroup> wholemoleculegroup(const rvec x[], const matrix box, int group_index);
virtual void finish() = 0;

protected:
void set_local_potential(real potential);
void set_local_virial(tensor virial);
std::shared_ptr<MpiHelper> mpi_helper();
std::shared_ptr<ExternalPotentialIO> input_output();
virtual AtomProperties* single_atom_properties(t_mdatoms * mdatoms, gmx_localtop_t * topology_loc) =

};
```



```
void DensityFitting::do_potential( const matrix /*box*/,
const rvec x[], const gmx_int64_t /*step*/)
{
spread_density_(x);
set_local_potential(k_*
    simulated_density_->grid_cell_volume()*
    relative_kl_divergence(target_density_,
        simulated_density_));
inv_mul(simulated_density_, target_density_);
group(x, 0)->parallel_loop(
    DensityFitting::ForceKernel_KL);
};
```



```
void DensityFitting::ForceKernel_KL(GroupAtom &atom,
    const int &thread)
{
clear_rvec(atom.force);

for (int i_ZZ = 0; i_ZZ < grid_extend[ZZ]; i_ZZ++)
{
    for (int i_YY = 0; i_YY < grid_extend[YY]; i_YY++)
        {
            for (int i_XX = 0; i_XX < grid_extend[XX]; i_XX++)
                {
svmul(*force_density * *density_ratio, shift_xyz, voxel_force,
rvec_inc(atom.force, voxel_force);
                }
            }
        }
};
```



```
external-potential      = yes
external-potential-path = ../external_potential_input

density-input           = inputfile.json
density-groups          = system
density-output          =
```



```
{  
  "k" : 10000000,  
  "sigma" : 0.5,  
  "n_sigma" : 6,  
  "background_density" : 5e-4,  
  "target_density" : "../input_density/target.ccp4"  
}
```

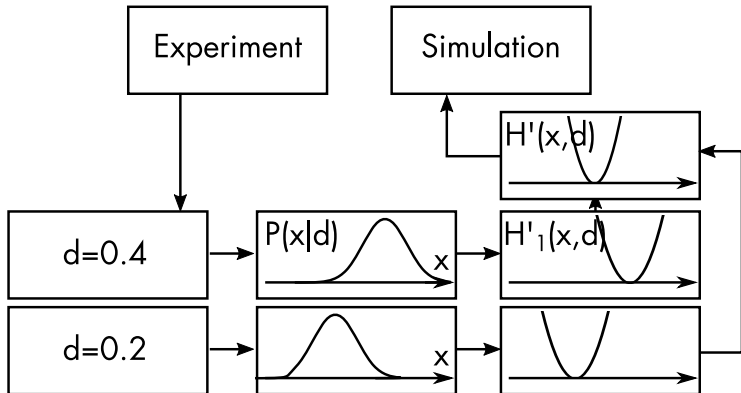


```
json::Object parsed_json(file_as_string);

k_           = strttof(parsed_json["k"].c_str(), nullptr);
sigma_       = strttof(parsed_json["sigma"].c_str(), nullptr);
n_sigma_     = strttof(parsed_json["n_sigma"].c_str(), nullptr);
target_density_name = parsed_json["target_density"];
```



- Atom-group “selection” structure
- Communication structure for external potentials
- Input file reading and parameter relay





- Atom-group "selection" structure
- Communication structure for external potentials
- Input file reading and parameter relay
- Replica communication