Documentation

ContaminationFlow on Linux and Windows

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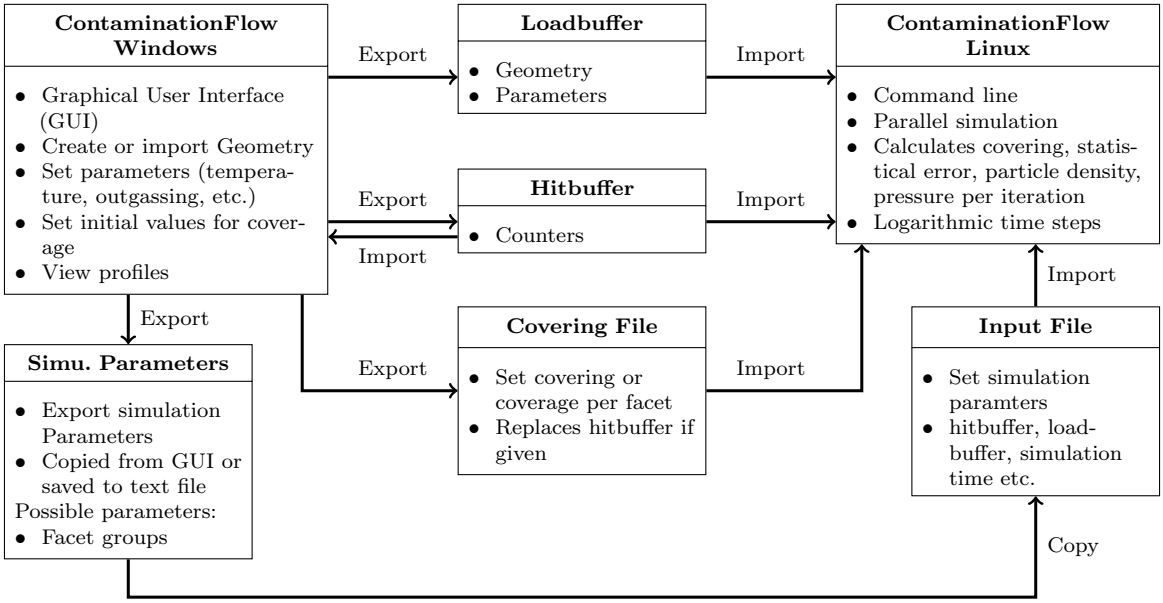
Contents

1. General Structure



General structure for ContaminationFlow simulation

- Code adapted from Molflow
- The Windows executable of ContaminationFlow is used to create Geometry, define the initial value problem and export it via two files (Loadbuffer & Hitbuffer). It cannot simulate the contamination transfer.
- The Linux version of ContaminationFlow is used for simulation.
- Loadbuffer contains information of geometry.
- Hitbuffer contains information such as hit counters, profiles, etc.
- Import and export of buffer files are used for communication between ContaminationFlow on Windows and ContaminationFlow on Linux. The import function of the loadbuffer does not work properly yet.
- Optional: export/import of covering text file that replaces covering in hitbuffer

2. ContaminationFlow Linux

- Parallel simulation on several subprocesses
- Control and of data processing in main process

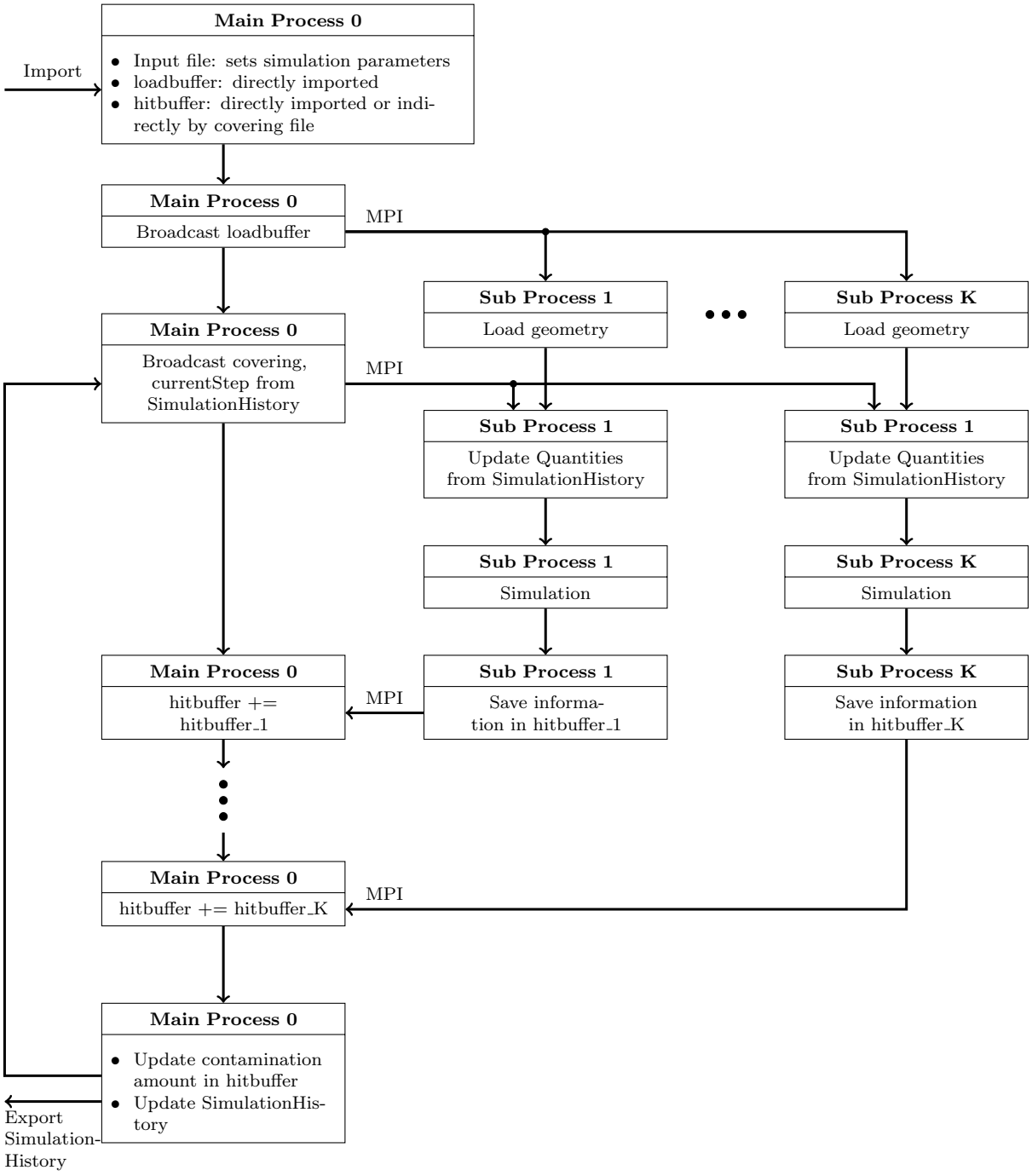


Figure 2.1.: Processing of data in main and sub processes

2.1. Call of Application from Command line

New class ProblemDef

- Defines parameters used for simulation
- Possible adaptation of default paramaters through input file
- Creates result folder for simulation if desired:
  - Final covering, error, pressure, particle density as text files
  - Input file and console output as text files

Application with custom parameters using input file

Requirements: Input and buffer files readable, N $\geq$ 2, zero moments in loadbuffer;

Call of ContaminationFlow Linux application in the command line:

```
$ module load mpi
$ mpirun -n N --options  MolflowLinux inputfile save
```

With the following MPI `--options`:

- (No option): use processor cores (recommended if possible)
- `--use-hwthread-cpus`: use hardware threads instead processor cores (recommended if N > number cores)
- `--oversubscribe`: ignore available slots, for any number of MPI processes

And command line parameters:

- `N`: desired number of worker processes; simulation on K=N-1 worker processes
- `MolflowLinux`: path to application, e.g. `~/MolflowLinux/Debug/MolflowLinux`
- `inputfile`: path to file that defines simulation parameters
- `save`: determines whether result directory is created (1: true, 0: false); default: `1`

For convenience use the tcshell script:

- `source StartContaminationFlow N inputfile`: MPI is loaded and `MolflowLinux` is executed.

and the input file defining the following parameters:

- $loadbufferPath$: Path to loadbuffer file, contains geometry, e.g. `~/loadbuffer`
- $hitbufferPath$: Path to hitbuffer file, contains counters, etc., e.g. `~/hitbuffer`
- $coveringPath$: Path to covering file, contains either covering or coverage per facet, file can be exported from the Windows version of ContaminationFlow, e.g. `~/covering.txt`; default: `""`
- $simulationTime$: Simulation time resolution. After each $simulationTime$ the error and particle number will be checked; default: `10.0`
- $unit$: Simulation time unit; default: `s`
- $maxTime$: Maximum simulated time; default: `10.0`
- $maxUnit$: Maximum simulated time unit; default: `y`
- $iterationNumber$: Number of iterations; default: `100`
- $usePCMethod$: Use predictor-corrector method "1" or simulate without predictor-corrector method "0"; default: `0`
- E_{de}: Binding energy of a particle on pure substrate; default: `1.6E-19`
- H_{vap}: Vaporization enthalpy of a particle if multilayer contamination; default: `0.8E-19`
- $errorMode$: Type of error monitored, "covering" or "event"; default: `covering`

- *targetParticles* : Minimum number of desorbed test-particles per iteration; default: `1000`
- *targetError* : Avg. statistical uncertainty (error) to be achieved for each iteration, calculated as the (by the facets area weighted) average of the normalized standard deviation of events per facet; default: `0.001`
- *noupdateError* : Error value above which the covering will not be updated; default: `0.1`
- *t_min* : Min. time for step size; default: `1E-4`
- *t_max* : Max. time for step size; default: `max`
- *maxTimePerIt* : Max. simulation time [s] per iteration; default: `max`
- *coveringMinThresh* : Min. covering (through multiplication); default: `1000000`
- *histSize* : Size of history lists; default: `max`
- *vipFacets* : Very important facets: facets with own target error. Alternating sequence of facet numbers and respective target errors separated via blanks; default: `[]`
- *outgassingTimeWindow* : Duration [s] of outgassing impulse; default: `0.0`
- *counterWindowPercent* : Percentage of step size (posterior fraction of the step size) at which pressure and density is sampled; default: `0.1`
- *rollingWindowSize* : Number of iterations for average statistics; default: `10`
- *convergenceTarget* : Target for average statistics to indicate convergence; default: `1`
- *stopConverged* : Stop simulation if average statistics indicate convergence; default: `1`
- *convergenceTime* : Minimum simulated time to stop simulation if converged; default: `0`
- *facetGroups* : Indices of facets belonging to a group, groups divided by -; default: `[]`
- *focusGroup* : Indices of facet groups to be monitored; default: `[]`
- *doFocusGroupOnly* : Determines if only focusGroup facets are monitored facets; default: `1`
- *saveResults* : Determines if results are saved; default: `1`
- *saveConsole* : Determines if console output is additionally saved; default: `0`

Optional covering file to replace covering values form hitbuffer. Hitbuffer's covering values will not be imported if covering file is given. There are two options (that can both be exported from ContaminationFlow Windows):

- set covering: `covering` followed by covering values per facet, seperated via blanks
- set coverage: `coverage` followed by coverage values per facet, seperated via blanks

Terminology

- Simulation time: desired computation time until check if target is reached for iteration
- Simulated time: physical time in the simulated system, e.g. flight time of particle
- Maximum simulated time: desired total simulated time
- Step size: desired simulated time per particle for iteration

2.2. Communication

Import and export of buffer files

- New Databuff struct that replaces Dataport struct from MolFlow+ Windows

```
typedef unsigned char BYTE;
typedef struct {
  signed int size;
  BYTE *buff;
```

```
} Databuff;
```

- New function `initBuffSize(·)` to initialize buffer size
- New functions `importBuff(·)` / `exportBuff(·)` to import buffer file/export Databuff struct
- New functions `checkReadable(·)` / `checkWriteable(·)` to check if file is readable/writeable

Communication between worker processes via MPI

- Main process 0 sends Databuff structs containing loadbuffer/hitbuffer and required SimulationHistory values to sub processes using `MPI_Bcast(·)`
- Subprocesses send updated Databuff struct containing hitbuffer and required SimulationHistory values to main process 0 using `MPI_Send(·)` and `MPI_Recv(·)`

2.3. Usage of *boost* Library

Multiprecision

- Increase precision for variables if required (float128, uint_128t)
- Avoid overflow for integer and underflow for floating point numbers

2.4. New Quantities

New counter `covering`

- Number of particles on facet
- Increases with adsorption, decreases with desorption
- Extracted from new FacetHitBuffer counter in `getCovering(·)` (`SimulationCalc.cpp`)

Coverage

- Number of layers of adsorbed particles
- Calculated from covering, particle diameter and facet area
- Coverage computed in `calcCoverage(·)` (`SimulationCalc.cpp`)

Binding energy

- Either E_{de} or H_{vap}, depending on the coverage
- If coverage is smaller than a monolayer, it will be decided at random.
- Used in `StartFromSource(·)` & `PerformBounce(·)` (`SimulationMC.cpp`) and `calcDesorption(·)` & `calcStartTime(·)` (`SimulationCalc.cpp`)

Desorption

- Number of desorbing particles
- Calculated from binding energy, coverage, facet area, temperature and step size
- Desorption computed in `calcDesorption(·)` (`SimulationCalc.cpp`)

Outgassing

- Number of particles outgassing from the bulk of the material, whose surface is represented by a facet
- Calculated from facet's (time-dependent) outgassing
- Outgassing computed in `CalcTotalOutgassingWorker()` (`Worker.cpp`)

$K_{\text{real/virtual}}$

- Number of real, physical particles represented by Monte-Carlo test-particles
- Calculated from desorption & outgassing as well as the number of desorbed & outgassed test-particles
- $K_{\text{real/virtual}}$ computed in `GetMoleculesPerTP(·)` (`SimulationCalc.cpp`)

Statistical uncertainty ("error")

- Statistical uncertainty based on all particle-wall interaction events ('event'): calculated from the number of 'hits', desorbed and outgassed test-particles (of every facet and the entire surface)
- Statistical uncertainty based on all particle-wall interaction events, which change the 'covering' value ('covering'): calculated from adsorbed and desorbed test-particles (of every facet and the entire surface)
- Used to determine significance of simulation results of iteration
- Error calculated in `UpdateErrorList(·)` for facet error & in `UpdateErrorAll(·)` for the average error weighted by the facets' areas (`UpdateSubProcess.cpp`)

Step size

- Step size computed in `getStepSize()` (`UpdateMainProcess.cpp`)

Particle density

- Calculated from sum of the reciprocal, orthogonal velocity portions, facet area and $K_{\text{real/virtual}}$
- Particle density computed in `calcParticleDensity(·)` (`SimulationCalc.cpp`)

Pressure

- Calculated from sum of orthogonal velocity portions, facet area, gas mass and $K_{\text{real/virtual}}$
- Pressure computed in `calcPressure(·)` (`SimulationCalc.cpp`)

Start time

- Determines time of desorption/outgassing for particle based on the distribution
- Start time computed in `calcStartTime(·)` (`SimulationCalc.cpp`)

2.5. Iterative Algorithm

2.5.1. Initialization of simulation

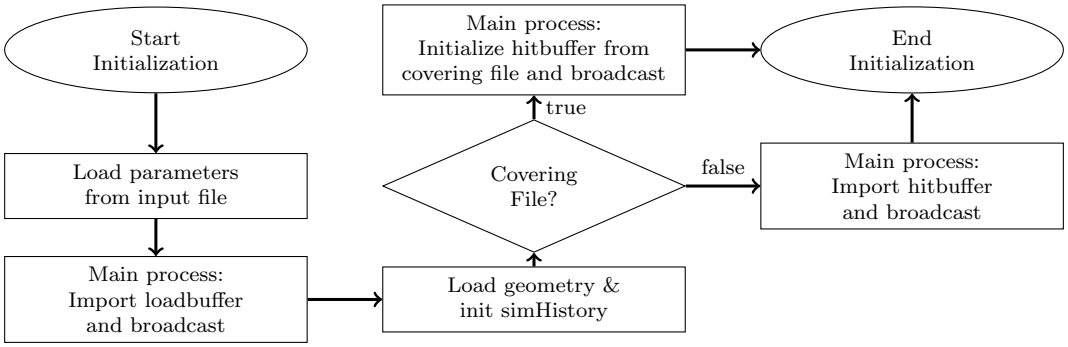


Figure 2.2.: Overview: Initialize simulation

New class to store Simulation History

- HistoryList and SimulationHistory class in `SimulationLinux.h` and `SimulationLinux.cpp` file

```
template <typename T> class HistoryList {
public:
 HistoryList();
 pair<vector<double>,vector<vector<T>>> historyList;//(vec(time), vec(facets))
 vector<pair<float128,float128>> statisticsList;//vec(mean, std)
 vector<T> currentList;//facets
 vector<T> predictList;//used for predictor-corrector method };
```

```
class SimulationHistory {
public:
 SimulationHistory();
 SimulationHistory(Databuff *hitbuffer);

 HistoryList<uint_128t> coveringList;//covering
 HistoryList<double> hitList;//MC hits
 HistoryList<llong> desorbedList;//Number of desorbed particles
 HistoryList<llong> adsorbedList;//Number of adsorbed particles
 HistoryList<double> errorList_event;//error event:  hits & desorbed particles
 HistoryList<double> errorList_covering;//error covering:  desorbed & adsorbed
 HistoryList<double> particleDensityList;
 HistoryList<double> pressureList;

 double lastTime;
 int currentStep;
 int pcStep;//Loop variable for predictor-corrector method
};
```

- Updated at the end of each iteration in `UpdateParticleDensityAndPressure(·)`, `UpdateCovering(·)`, `UpdateErrorMain(·)` (`UpdateMainProcess.cpp`)
- Recorded quantities: covering, error (event and covering), particle density and pressure for each facet and iteration, total hits, desorbed and outgassed test-particles for each facet
- lastTime: simulated time (accumulated time steps) instead of computation time

2.5.2. Simulation on subprocesses

Calculate step size

- Calculation from `simHistory→currentStep` in `getStepSize()` (`UpdateMainProcess.cpp`)

Calculate covering threshold

- Set lower threshold for covering for each facet to prevent covering getting negative
- Stop simulation once threshold is reached
- Threshold set in `setCoveringThreshold(·)` (`Iteration.cpp`)

Multiply small covering

- Multiply covering counter so that smallest covering $\geq$ `ProblemDef::coveringThreshMin`
- Multiply covering threshold with same factor
- Calculation in `checkSmallCovering(·)` (`SimulationLinux.cpp`)

Calculate desorption and outgassing

- Desorption in `UpdateDesorption(·)` (`UpdateSubProcess.cpp`)
- Outgassing in `CalcTotalOutgassingWorker()` (`Worker.cpp`)

Create particle and calculate start time

- Facet randomly selected based on total desorption and outgassing
- Desorption or outgassing randomly selected based on ratio on facet
- Start time randomly generated based on temporal distribution of desorption or outgassing

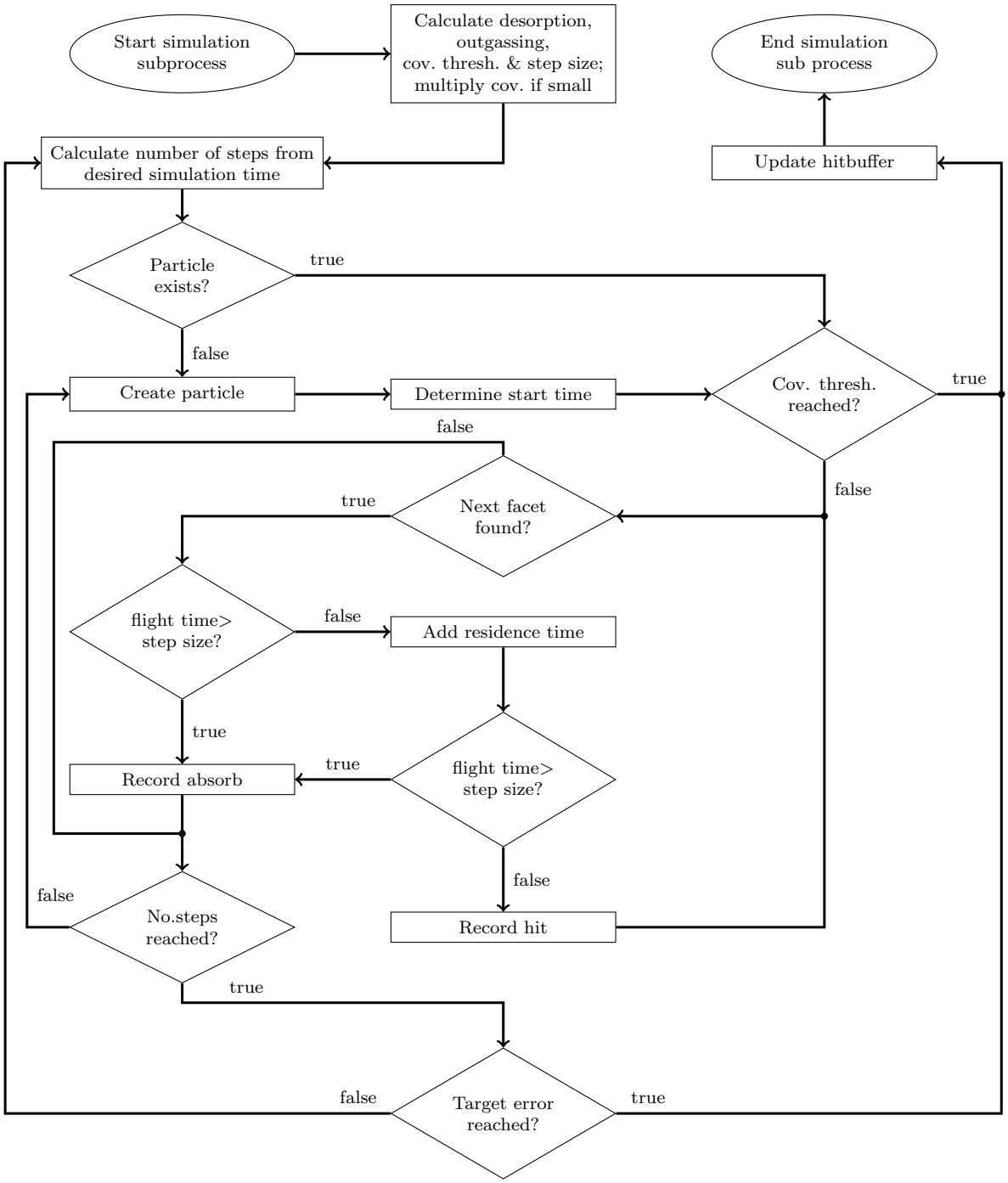


Figure 2.3.: Overview: simulation on subprocesses

- Calculation in `StartFromSource(·)` (`SimulationMC.cpp`)

Calculate residence time

- Residence time randomly calculated from binding energy, facet temperature and oscialltion frequency in `PerformBounce(·)` (`SimulationMC.cpp`)

Increase facet counters in case of desorb, absorb or hit

- Increase hit, desorb, outgassed or absorb counter according to event

- Increase velocity counters only if event within `p→counterWindowPercent`
- Facet counters increased in `IncreaseFacetCounter(·)` (`SimulationMC.cpp`)

Target error reached?

- Calculate statistical uncertainty 'error' in `UpdateError()` from `UpdateSubProcess.cpp` file
- Average error calculated from summing up the facets' errors corrected by the number of facets
- Error to check can be either covering or event error
  - Additional check, if VIP facets reached their own target error
  - Check, if average error reached target error
- Facets with error=inf are not considered
  - Facets with no events or no change of covering (no desorb and no absorb)
- Check in `checkErrorSub(·)` (`UpdateSubProcess.cpp`)

2.5.3. Update main process

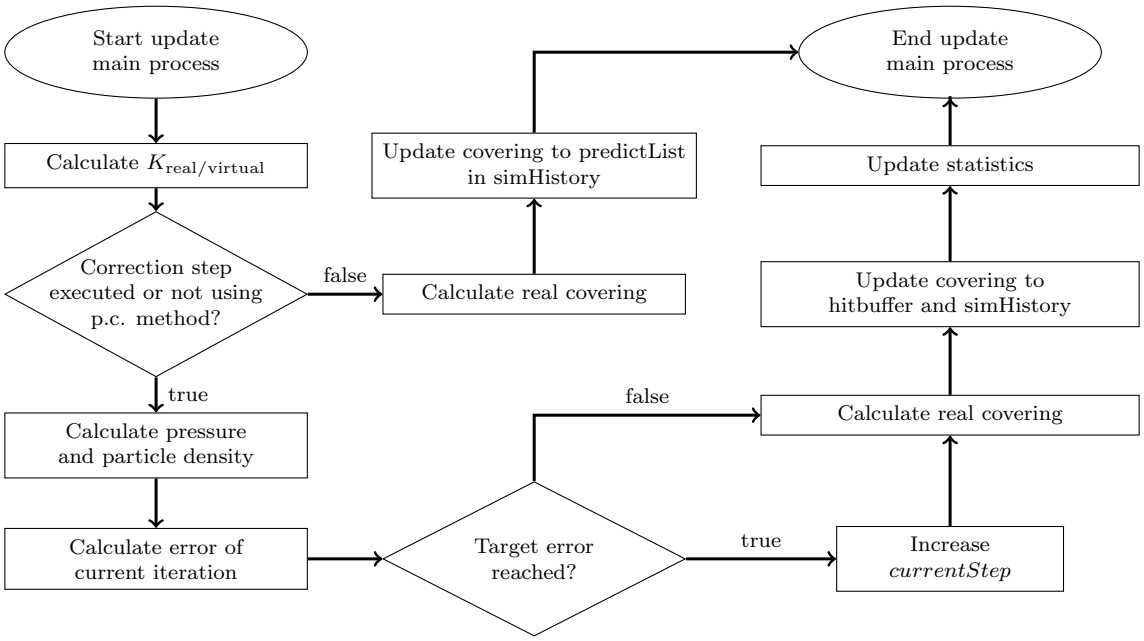


Figure 2.4.: Overview: update of covering in hitbuffer and simHistory

Predictor-corrector method

- Analogous to Heun's method for solving ordinary differential equations numerically
- In the prediction step, the iteration for the current time step is executed and the resulting covering values are saved in `simHistory→coveringList.predictList`
- In the correction step, the iteration for the current time step is repeated. In `PerformBounce(·)` (`SimulationMC.cpp`), the covering values from `currentList` will be read, if `sHandle→currentParticle.flightTime <= 1/2*simHistory→stepSize`. Otherwise covering values from `predictList` will be read.
- At the end of the correction step, the main process is updated as usual and continuing with the next iteration

- Used only, if `p->usePCMethod` is set to `1` (as opposed to `0`) explicitly via the input file
- If `usePCMethod` is set to `0`: not using the p.c. method; `1`: using the p.c. method;

Calculate pressure and particle density

- Calculation in `UpdateParticleDensityAndPressure(·)` `(UpdateMainProcess.cpp)`
- Values per facet saved in `simHistory→pressureList` / `simHistory→particleDensityList`

Calculate error

- Calculation analogous to sub processes in `UpdateErrorMain(·)` (`UpdateMainProcess.cpp`)
- Save error per facet in `simHistory→errorList_event` / `simHistory→errorList_covering`
  ⇒ Increase `simHistory→currentStep` if target errors reached

Calculate & update covering

- $K_{\text{real/virtual}}$ computed in `GetMoleculesPerTP(·)` (`Simulationcalc.cpp`)
- Divide covering in `hitbuffer` if previously multiplied (in case of 'smallcovering')
- Use $K_{\text{real/virtual}}$ to calculate new covering
- Save new covering in `currentList` in `simHistory→coveringList` and `hitbuffer`
- Calculation in `UpdateCovering(·)` from `UpdateMainProcess.cpp` file
- Update buffers in `UpdateCoveringPhys(·)` (`UpdateMainProcess.cpp`)

Calculate & update statistics (with respect to the points in time) of coverage values

- Calculate mean and standard deviation of covering over the last `p→rollingWindowSize` iterations
- Update statistics in `HistoryList::updateStatistics(·)` (`SimulationLinux.h`)
- End simulation if `p→convergenceTarget` is reached by average statistics weighted with area. This is evaluated in `HistoryList::getAverageStatistics(·)` (`SimulationLinux.h`)

2.6. Summary

General Pipeline

- Initialize MPI, `ProblemDef p` and `SimulationHistory simHistory`
- Check, if all simulation parameters are valid
- Load geometry into `Simulation sHandle` and check if values are valid using `loadAndCheckSHandle()`
  - Load geometry using `LoadSimulation`
  - Hitbuffer: import using `importBuff(·)` or initialize size using `initBuffSize(·)`
  - Check for correct hitbuffer size
  - Check for zero moments
  - Check for no two-sided facets with finite opacity
  - Check for valid covering file and import covering values
- Iteration of simulation steps until `p→maxTimeS` or `p→convergenceTarget` (`p→convergenceTime` , `p→stopConverged`) is reached. If `p→usePCMethod` is not set to `0` , repeat same iteration twice:
  - Reset hitbuffer counters using `initbufftozero(·)`
  - Broadcast `simHistory→coveringList` using `MPI_Bcast(·)`
  - Set covering threshold `covthresh` using `setCoveringThreshold(·)`
  - Update relevant simulation values using `simHistory→updateStepSize(·)` , `UpdateSticking(·)` , `CalcTotalOutgassingWorker(·)` , `UpdateDesorption(·)` . If using p.c. method: done only for the prediction step. The remain set in the correction step.
  - Multiply covering and `covthresh` with `simHistory→smallCoveringFactor` , if covering is small
  - Simulation in subprocesses:
    - Simulate until `targetParticles` and `targetError` or `covthresh` reached
    - Update hitbuffers of subprocesses from `sHandle` using `UpdateMCSubHits(·)` (`UpdateSubProcess.cpp`)
  - Update main process:
    - Send hitbuffer to main process using `MPI_Send(·)` and `MPI_Recv(·)`
    - Update of hitbuffer in `UpdateMCMainHits(·)` (`UpdateMainProcess.cpp`)
  - If using p.c. method and while in prediction step:
    - Calculate real, physical covering in main process using $K_{\text{real/virtual}}$ in `UpdateCovering(·)` (`UpdateMainProcess.cpp`), save in `simHistory` : `predictList`
  - If not using p.c. method or otherwise while in correction step:
    - Update pressure and particle density using `UpdateParticleDensityAndPressure(·)` `(UpdateMainProcess.cpp)` , save in `simHistory`
    - Update error of iteration using `UpdateErrorMain(·)` (`UpdateMainProcess.cpp`), save in `simHistory`
    - Calculate real covering in main process using $K_{\text{real/virtual}}$ in `UpdateCovering(·)` (`UpdateMainProcess.cpp`), save in `simHistory` : `historyList` and `currentList`
    - Update real covering in hitbuffer of main process in `UpdateCoveringphys(·)` (`UpdateMainProcess.cpp`)
    - Update statistics using `simHistory→coveringList.updateStatistics(·)`
- Export final results (`simHistory` lists) to results folder
- Close MPI

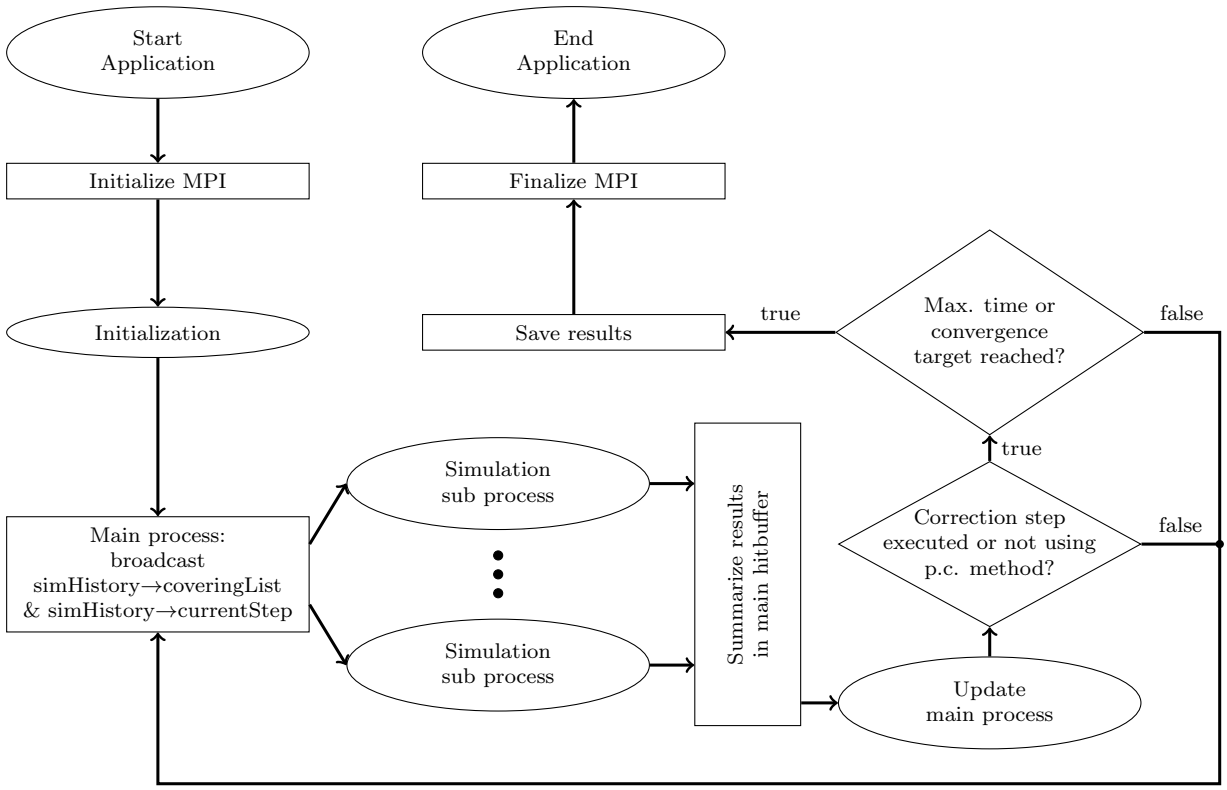
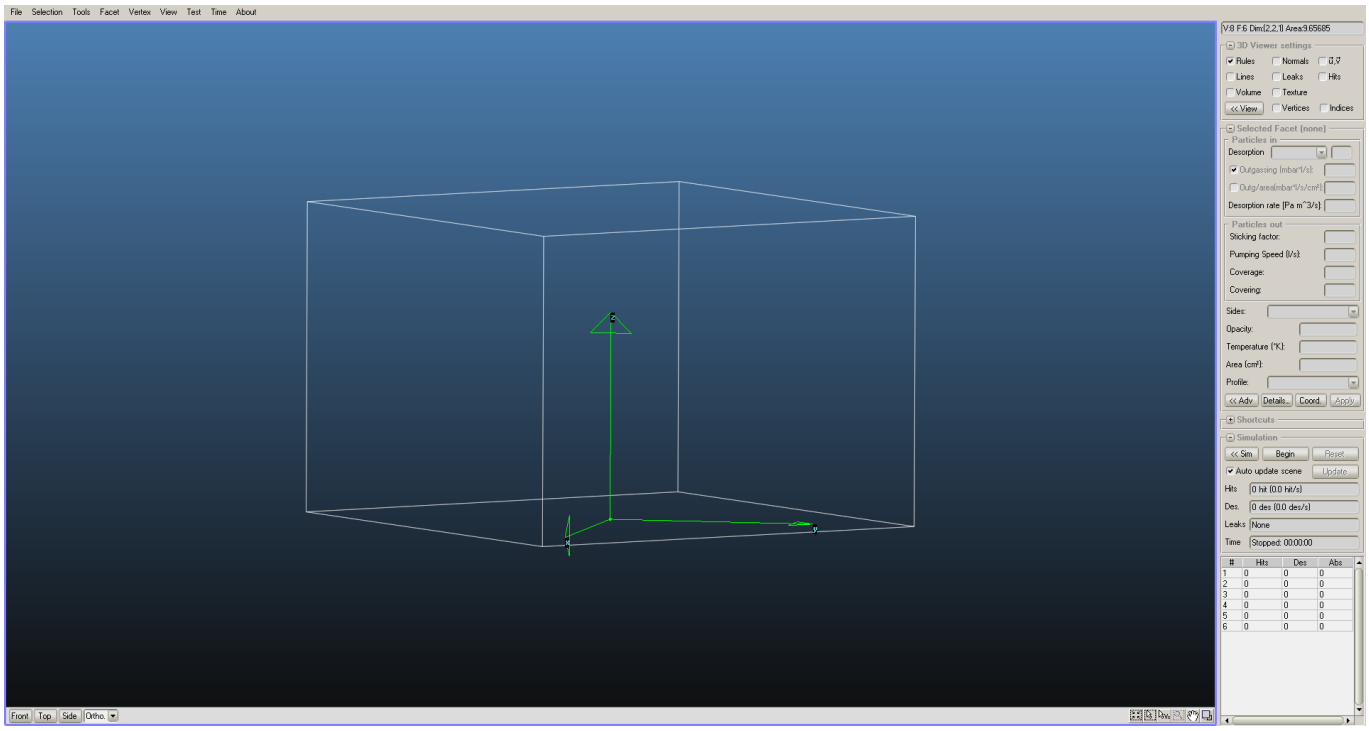


Figure 2.5.: Overview: ContaminationFlow application

3. ContaminationFlow Windows

- Extention of original Molflow+ for contamination problems
- Create Geometry and set parameters such as initial coverage and temperature
- Export of buffer files
- Export of facet groups

3.1. Graphical User Interface



New GUI elements

- "Particles out"
  - Text field for covering
  - Text field for coverage
- New menu options
  - File: Export buffer
  - Selection: Export Selections

3.2. Communication

Import and export of buffer files via GUI

- New Databuff struct

```
typedef unsigned char BYTE;
typedef struct
  signed int size;
  BYTE *buff;
Databuff;
```

- New functions `importBuff(·)` and `exportBuff(·)` for import and export of buffer files/Databuff
- New options in `File` menu: `Export buffer` and `Import buffer`

Export of Facet Groups

- New functions to output (text file or text field line) correct formating of facet groups for input file for ContaminationFlow Linux
- New options in `Selection` menu: `Export Selections`

Export of Covering/Coverage File

- Two output options: covering or coverage per facet
- New functions to output (text file or text field line) correct formating of covering/coverage file for the Linux version of ContaminationFlow

3.3. New Quantities

New counter `covering`

- Added covering counter to hitbuffer
- Added covering to GUI, can be defined through textfield
- Covering increased at adsorb

A. Formulas for (new) Quantities

Constants

$$\begin{aligned} k_B &= 1.381 \times 10^{-23}\,\mathrm{J\,K^{-1}} \\ h &= 6.626 \times 10^{-34}\,\mathrm{J\,s} \\ N_A &= 6.022 \times 10^{23}\,\mathrm{mol^{-1}} \end{aligned} \tag{A.1}$$

Variables

$$T = \text{Facet temperature} \tag{A.2}$$

Number of particles of one layer

$$N_{mono} = \frac{\text{Area of Facet}}{\text{ProblemDef::particleDia}^2} \tag{A.3}$$

Covering = Number of particles adsorbed on facet

$$N_{\text{particles on facet}} \tag{A.4}$$

Coverage θ

$$\theta = N_{\text{particles on facet}}/N_{mono} \tag{A.5}$$

Binding energy E

$$E = \begin{cases} E_{de}, & \text{if particle binds to substrate} \\ H_{vap}, & \text{if particle binds to adsorbate} \end{cases} \tag{A.6}$$

Residence time τ, average residence time $<\tau>$

$$\begin{aligned} <\tau> &= \tau_0 \exp\left(E/(k_B T)\right) \\ \tau_0 &= \frac{h}{k_B\,T} \end{aligned} \tag{A.7}$$

$$<\tau_{subst}> = \tau_0 \cdot \exp\left(\frac{E_{de}}{k_B T}\right),\ <\tau_{ads}> = \tau_0 \cdot \exp\left(\frac{H_{vap}}{k_B T}\right) \tag{A.8}$$

Small covering factor

$$\begin{aligned} mincov &= \text{Smallest covering on a single facet that desorbs} \\ \text{small covering factor} &= \begin{cases} 1, & \text{if } mincov \geq \text{ProblemDef::coveringMinThresh} \\ 1 + 1.1 \cdot (\text{ProblemDef::coveringMinThresh}/mincov), & \text{otherwise} \end{cases} \end{aligned} \tag{A.9}$$

Statistical error

$$\text{error}(counter) = \frac{1}{N_{\text{test-particles}}} \sqrt{(counter) \text{ on facet} \cdot \left(1 - \frac{(counter) \text{ on facet}}{\text{total } (counter)}\right)} \tag{A.10}$$

counter can be the number of hits, outgassed test-particles, desorbed test-particles or adsorbed test-particles (TP). error(*counter*) is the sample mean of the (sampled) Bernoulli distribution. The overall error i.e. the sum of the contributions

$$\begin{aligned} \text{error}_{\text{event}} = & \frac{1}{N_{\text{test-particles}}} \sqrt{(hits) \text{ on facet} \cdot \left(1 - \frac{(hits) \text{ on facet}}{\text{total } (hits)}\right) + \right. \\ & \overline{(desorbed\ TP) \text{ on facet} \cdot \left(1 - \frac{(desorbed\ TP) \text{ on facet}}{\text{total } (desorbed\ TP)}\right) + } \\ & \left. \overline{(outgassed\ TP) \text{ on facet} \cdot \left(1 - \frac{(outgassed\ TP) \text{ on facet}}{\text{total } (outgassed\ TP)}\right)} \right. \end{aligned} \tag{A.11}$$

$$\begin{aligned} \text{error}_{\text{covering}} = & \frac{1}{N_{\text{test-particles}}} \sqrt{(adsorbed\ TP) \text{ on facet} \cdot \left(1 - \frac{(adsorbed\ TP) \text{ on facet}}{\text{total } (adsorbed\ TP)}\right) + } \\ & \overline{(desorbed\ TP) \text{ on facet} \cdot \left(1 - \frac{(desorbed\ TP) \text{ on facet}}{\text{total } (desorbed\ TP)}\right)} \end{aligned} \tag{A.12}$$

is smaller than 1. It has to be multiplied with the number of physical particles to yield a statistical uncertainty of the particle number.

B. Datatypes

B.1. Boost

Datatype	Alias
boost::multiprecision::uint_128t	uint_128t
boost::multiprecision::float128	float128

B.2. Class Members

Name	Datatype	Note
SimulationHistory::coveringList	uint_128t	
FacetHitBuffer::covering	llong	hitbuffer & tmpcounter
FacetProperties::desorption	float128	
Simulation::coveringThreshold	llong	

B.3. Functions

Function	Output Datatype	Relevant Input
getCovering()	float128	SimulationHistory::coveringList
getCovering()	llong	FacetHitBuffer::covering
calcCoverage()	float128	getCovering()
calcDesorption()	float128	calcCoverage()
calctotalDesorption()	float128	FacetProperties::desorption
GetMoleculesPerTP()	float128	FacetProperties::desorption

C. Overview of new Classes and Functions

C.1. New Classes

HistoryList	
historyList	list containing the complete history of a facet quantity (e.g. number of Hits, pressure, etc.) for all facets at all points in time
currentList	list containing a facet quantity at latest point in time for all facets
predictList	list containing a facet quantity after the predictor step (when using the predictor-corrector method)
statisticsList	list containing facet statistics (mean value and standard deviation) over last `rollingWindowSize` iterations; used for statistics of `covering`
currIt	current iteration number
reset()	Reset lists
initCurrent()	Initialize size of currentList
initPredict()	Initialize size of predictList
initStatistics()	Initialize size of statisticsList
initList()	Initialize size of historyList
appendCurrent()	Append currentList to historyList
appendList()	Append input list to historyList
updateStatistics()	Calculate statistics per facet (mean, std), save to statisticsList
getAverageStatistics()	Calculate average ratio (std/mean) weighted with area for all facets or focusGroup only
convertTime()	Convert time for better clarity
print()	Print historyList to terminal, optinal message
printCurrent()	Print currentList as table to terminal, optional message
printPredict()	Print predictList as table to terminal, optional message
printStatistics()	Print statisticsList as table to terminal, optional message
write()	Write historyList to file
erase()	delete desired point in historyList
empty()	Check if historyList is empty
setCurrent()	Set value of desired facet in currentList
getCurrent()	Get value of desired facet in currentList
setPredict()	Set value of desired facet in predictList
getPredict()	Get value of desired facet in predictList
setLast()	Set value of desired facet from historyList
getLast()	Get value of desired facet from historyList

SimulationHistory	
coveringList	of class HistoryList, stores covering history
errorList_event	of class HistoryList, stores error history for events
errorList_covering	of class HistoryList, stores error history for covering
hitList	of class HistoryList, stores hits for each facet
desorbedList	of class HistoryList, stores desorbed particles for each facet
adsorbedList	of class HistoryList, stores adsorbed particles for each facet
particleDensityList	of class HistoryList, stores particle density for each facet
pressureList	of class HistoryList, stores pressure for each facet
numFacet	number of facets
numSubProcess	number of subprocesses used for simulation
flightTime	lift time (start, flight, residence times) of a Monte-Carlo test-particle
nParticles	Simulated test-particles for iteration
lastTime	Total simulated time = last time in historyList
currentStep	numbe of the current 'step' affecting the time step (length of current iteration) calculation in `getStepSize()`
pcStep	current step of predictor-corrector method
stepSize	current step size
stepSize_outgassing	current step size of outgassing impulse
smallCoveringFactor	Factor used to multiply `covering` to prevent an underflow of `covering`
updateHistory()	Reset and update
updateStepSize()	Calculate stepSize and stepSize_outgassing
erase()	Erase desired point in history
print()	Print to terminal
write()	Write to file

ProblemDef	
contaminationFlowPath	Path of github directory
resultPath	Path of result folder
outFile	Path of file that contains terminal output
loadbufferPath	Path of loadbuffer file
hitbufferPath	Path of hitbuffer file
coveringPath ⇒doCoveringFile	Path of covering file, hitbuffer not imported if given
saveResults	1: save all results, 0: do not save results
simulationTime, unit ⇒simulationTimeMS	Computation time of each iteration in milliseconds
maxTime, maxUnit ⇒maxTimeS	Maximal total simulated time in seconds
iterationNumber	Number of (desired) iterations of simulation
usePCMethod	0: do not use predictor-corrector-method, 1: use predictor-corrector-method
particleDia	Diameter of particles
E_de, H_vap	Parameters to calculate binding energy, see eq. A.6
sticking	Sticking factor for all facets
targetParticles/-Error	Target values for each iteration
coveringMinThresh	Minimum covering, multiplication to this if covering low
t_min, t_max	Minimum/ Maximum step size
maxTimePerIt	Maximun simulation time [s] per iteration
histSize	Size of historyList objects (most recent values in memory)
vipFacets	Alterning: vip facet and target error, e.g. 1 0.001 3 0.002
outgassingTimeWindow	Duration of outgassing impulse
counterWindowPercent	percentage of step size (posterior) at which velocity counters are increased
rollingWindowSize	Number of iterations over which statistics are calculated
convergenceTarget	Target for average ratio (std/mean) for convergence
stopConverged	1: stop simulation at convergence, 0: continue simulation
facetGroups	Indices of facets belonging to a group, groups divided by '-' ; acting as a basis for a focus group
focusGroup	Indices of facet groups to be monitored; if focusGroup is defined, the average error is calculated involving only facets in the focusGroups; convergence of the coverage also only checked for all facets in the focusGroups;
doFocusGroupOnly	1: only monitor focus group, 0: monitor all facets

ProblemDef	
createOutput()	Create output directory and file
readInputfile()	Initialization from input file, checks if parameters are valid
printInputfile()	Print to terminal
writeInputfile()	Write to text file
SetFocusGroup()	Converts focusGroup indices to facet indices

C.2. New Functions

C.2.1. molflowlinux_main.cpp

Preprocessing	
parametercheck()	Checks validity of input parameters from input file Defines values for ProblemDef object `p`
importBuff()	Import load- and hitbuffer to main process
MPI_Bcast()	Send loadbuffer to sub processes
loadAndCheckSHandle()	Load geometry from loadbuffer and check values
initCoveringThresh()	Initialize covering threshold
UpdateSojourn()	Enable sojourn time for each facet
SimulationHistory()	Initialize SimulationHistory object

Simulation Loop	
initbufftozero()	Reset all hitbuffer counters except `covering`
MPI_Bcast()	Send `simHistory→coveringList` and `simHistory→currentStep` to sub processes
setCoveringThreshold()	Sets covering threshold for each facet
updateStepSize()	Calculate step sizes for desorption and outgassing
CalcTotalOutgassingWorker()	Calculate total outgassing for iteration
UpdateDesorption()	Set desorption for each facet
checkSmallCovering()	Multiply covering to reach threshold, if necessary
simulateSub2()	Simulation on subprocesses
MPI_Send(), MPI_Recv()	Send hitbuffer from sub- to main process
UpdateMCMainHits()	Add simulation results to main hitbuffer
UpdateParticleDensityAndPressure()	Calculate and save particle density and pressure
UpdateErrorMain()	Calculate and save error of iteration to simHistory
UpdateCovering()	Calculate and save new covering to simHistory
UpdateCoveringphys()	Save current covering to hitbuffer
`simHistory→erase()`	Erase entry in historyList; used to adapt its size to `p→histSize`
updateStatistics(), getAverageStatistics()	Statistics over `p→rollingWindowSize` iterations
End simulation if `p→maxTimeS` or `p→convergenceTarget` is reached	

Postprocessing	
simHistory→write()	Export simulation history

C.2.2. SimulationLinux.cpp

simulateSub2()	
`simHistory->updateHistory()`	Update SimulationHistory object from `sHandle`
smallCoveringFactor	If covering is small: multiplied by smallCoveringFactor to be able to have statistics without overflow of covering variable
targetParticles, targetError	Target values for simulation of all subprocesses together
SimulationRun()	Simulate for desired simulation time
UpdateError()	Calculate current error of subprocess
CheckErrorSub()	Checks, if total error reached targetError and if VIP facets reached own target
UpdateMCSubHits()	Save simulation results to hitbuffer

Small covering	
checkSmallCovering()	Find smallCoveringFactor to reach `p→coveringMinThresh` Reversion of multiplication by smallCoveringFactor is done in `UpdateCovering()`

Others	
readCovering()	Reads covering or covereage values, save to buffer
get_path()	Get path of executable
printStream()	Print input string to terminal and file
tilde_to_home(),home_to_tilde()	Exchange ∼ and home directory
convert_to/from_contflowdir()	Exchange CONTFLOWDIR and `p→contaminationFlowPath`

C.2.3. Iteration.cpp

Set Covering Threshold to avoid negative covering	
initCoveringThresh()	Initialize size of covering threshold vector
setCoveringThreshold()	Set covering threshold for each facet

Error calculations	
getErrorList()	get pointer to list corresponding to `simHistory→errorMode`
getErrorVariables()	get number hits, adsorbed, desorbed particles
UpdateErrorList()	Calculate error per facet, see eq. A.10. Save to `simHistory`
CalcErrorAll()	Sum up facet errors & weight by area for all error modes
CheckError()	Check if total error and vip facet error reached target

C.2.4. Buffer.cpp

Buffer functions	
Databuff struct()	signed int size BYTE *buff
initBuffSize()	Initialize size of buffer (without content)
checkReadable()	Check if file can be opened for reading
checkWriteable()	Check if file can be openend or created for writing
importBuff()	Import buffer file to Databuff struct
exportBuff()	Export Databuff struct to buffer file

C.2.5. Calculations in SimulationCalc.cpp etc.

SimulationCalc.cpp	
getCovering()	Get covering from hitbuffer or `simHistory`
getHits()	Get number of hits from hitbuffer
getnbDesorbed()	Get number of total desorbed molecules from hitbuffer
getnbAdsorbed()	Get number of total adsorbed molecules from hitbuffer
calcNmono()	see eq. A.3
calcCoverage()	see eq. A.5
calcDesorption()	see eq. A.8
GetMoleculesPerTP()	see eq. **??**
calctotalDesorption	Calculate desorption for `startFromSource()`
calcOutgassingFactor()	Calculate factor to determine outgassing particles
calcPressure()	see eq. **??**
calcParticleDensity()	see eq. **??**
calcStartTime()	Calculate start time of particle depending on desorption/outgassing distribution

worker.cpp	
CalcTotalOutgassingWorker()	see eq. **??**, calculate outgassing distribution for `startFromSource()`

SimulationLinux.cpp	
convertunit()	Convert simutime · unit to milliseconds

C.2.6. UpdateSubProcess.cpp

Update sHandle paramters from hitbuffer	
UpdateSticking()	Update sticking
UpdateDesorption()	Update desorption
UpdateSojourn()	Enable residence time for all facets

Error calculations	
UpdateErrorSub()	UpdateErrorList()
CalcErrorSub()	CalcErrorAll() for only one error quantity in subprocess

Update hitbuffer	
initbufftozero()	Set hitbuffer except covering to zero
UpdateMCSubHits()	Save simulation results from sHandle into hitbuffer

C.2.7. UpdateMainProcess.cpp

Update main hitbuffer from sub hitbuffer	
UpdateMCMainHits()	Add simulation results from sub hitbuffer to main hitbuffer

Update real covering in hitbuffer	
getStepSize()	Calculate step size for current step
UpdateCovering()	Use Krealvirt to calculate new covering Save to `simHistory→coveringList`
UpdateCoveringphys()	Save current real covering to hitbuffer
UpdateErrorMain()	UpdateErrorList(), adapt time entries
UpdateParticleDensityAndPressure()	Calculate pressure and particle density, see eq. **??**, **??**
CalcPerIteration()	Calculate total error (covering and event) and covering over all facets per iteration