A Python extension for the massively parallel framework waLBerla

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Outline

- waLBerla Framework
  - Data Structures
  - Communication patterns
  - Application
- Python interface:
  - Motivation: Simulation Setup
  - Data structure export for simulation evaluation/control
  - Challenges of writing a C++/Python interface

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waLBerla Framework

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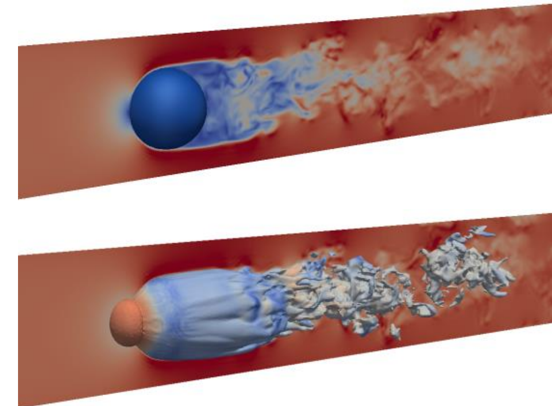
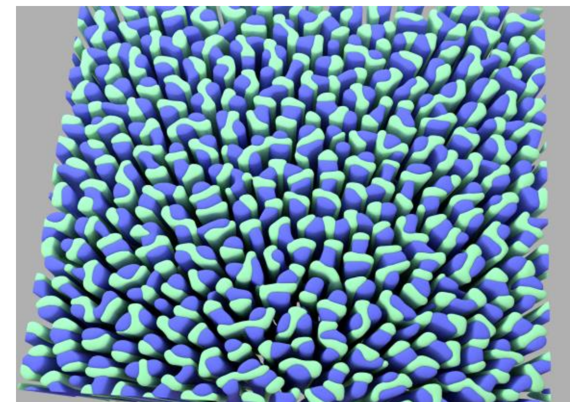
- widely applicable Lattice-Boltzmann from Erlangen
- general HPC software framework, originally developed for CFD simulations with Lattice Boltzmann Method (LBM)
- but other algorithms working on structured grid also possible: phase field models, molecular dynamics with linked cell algorithm
- coupling with in-house rigid body physics engine pe



Turbulent flow (Re=11000) around a sphere



Microstructure simulation of ternary, eutectic solidification process (phase field method)

waLBerla Framework

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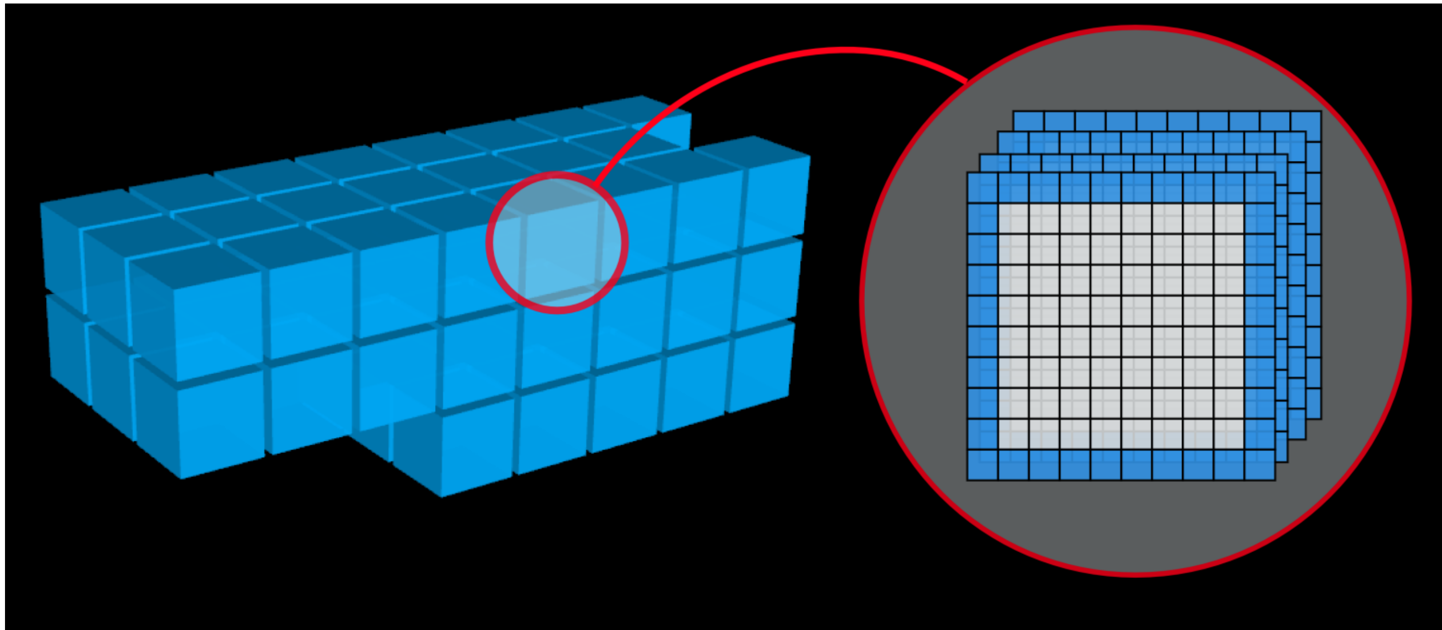
- Written in C++ with Python extensions
- Hybridly parallelized (MPI + OpenMP)
- No data structures growing with number of processes involved
- Scales from laptop to recent petascale machines
- Parallel I/O
- Portable (Compiler/OS)
- Automated tests / CI servers
- Open Source release planned

llvm/clang

Block Structured Grids



- structured grid
- domain is decomposed into blocks
- blocks are the container data structure for simulation data (lattice)
- blocks are the basic unit of load balancing

Block Structured Grids

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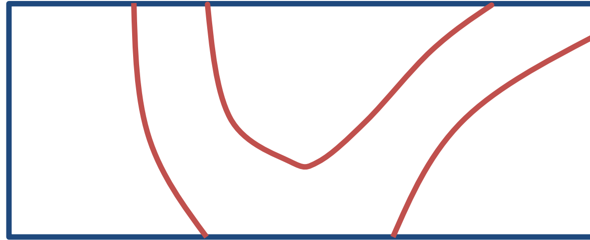
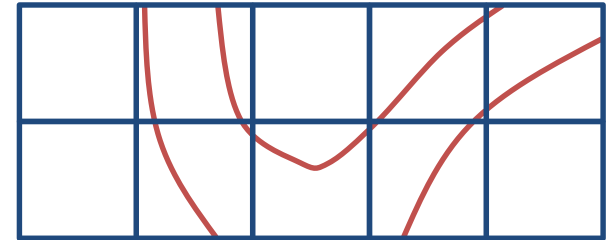
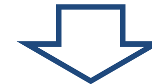
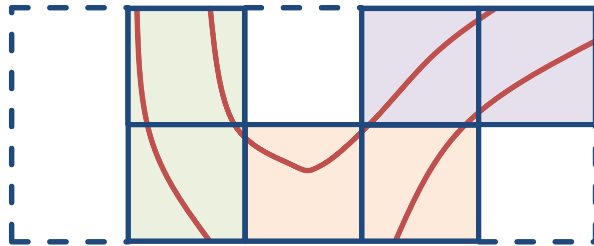
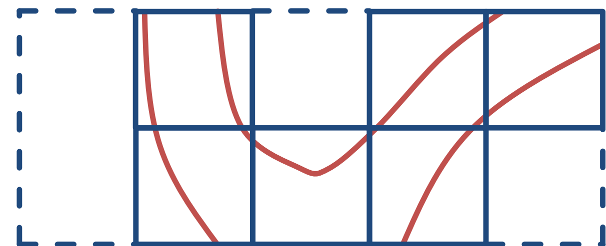
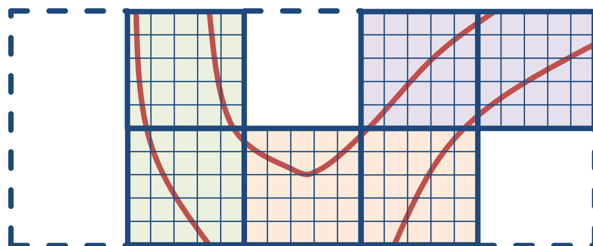

Complex geometry given by surface


Add regular block partitioning




Load balancing


Discard empty blocks


Allocate block data

Block Structured Grids

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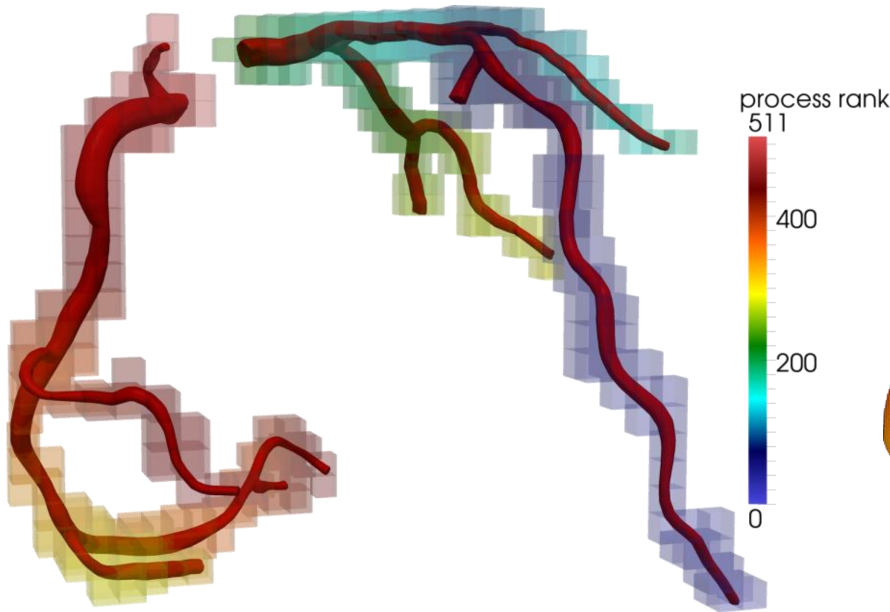
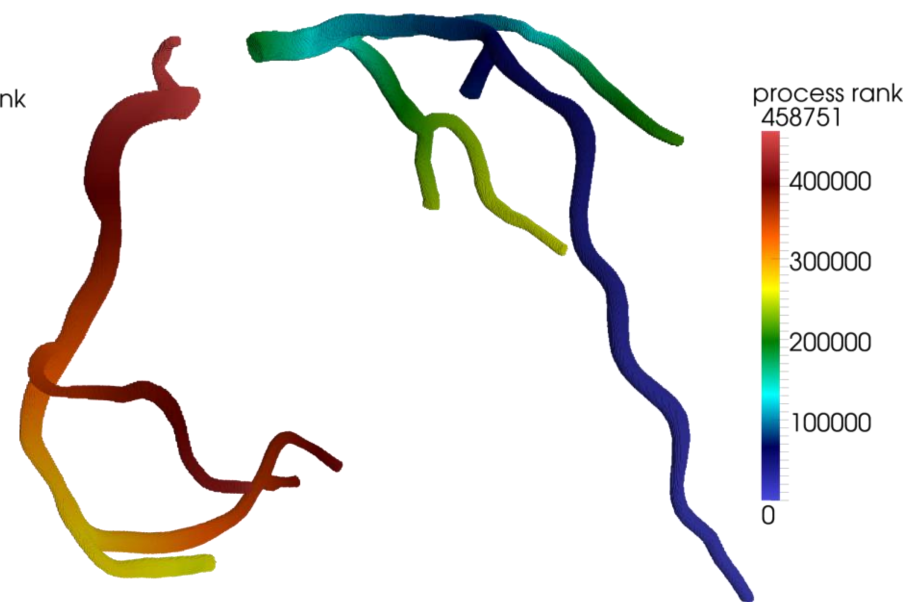
Domain partitioning of coronary tree dataset
One block per process



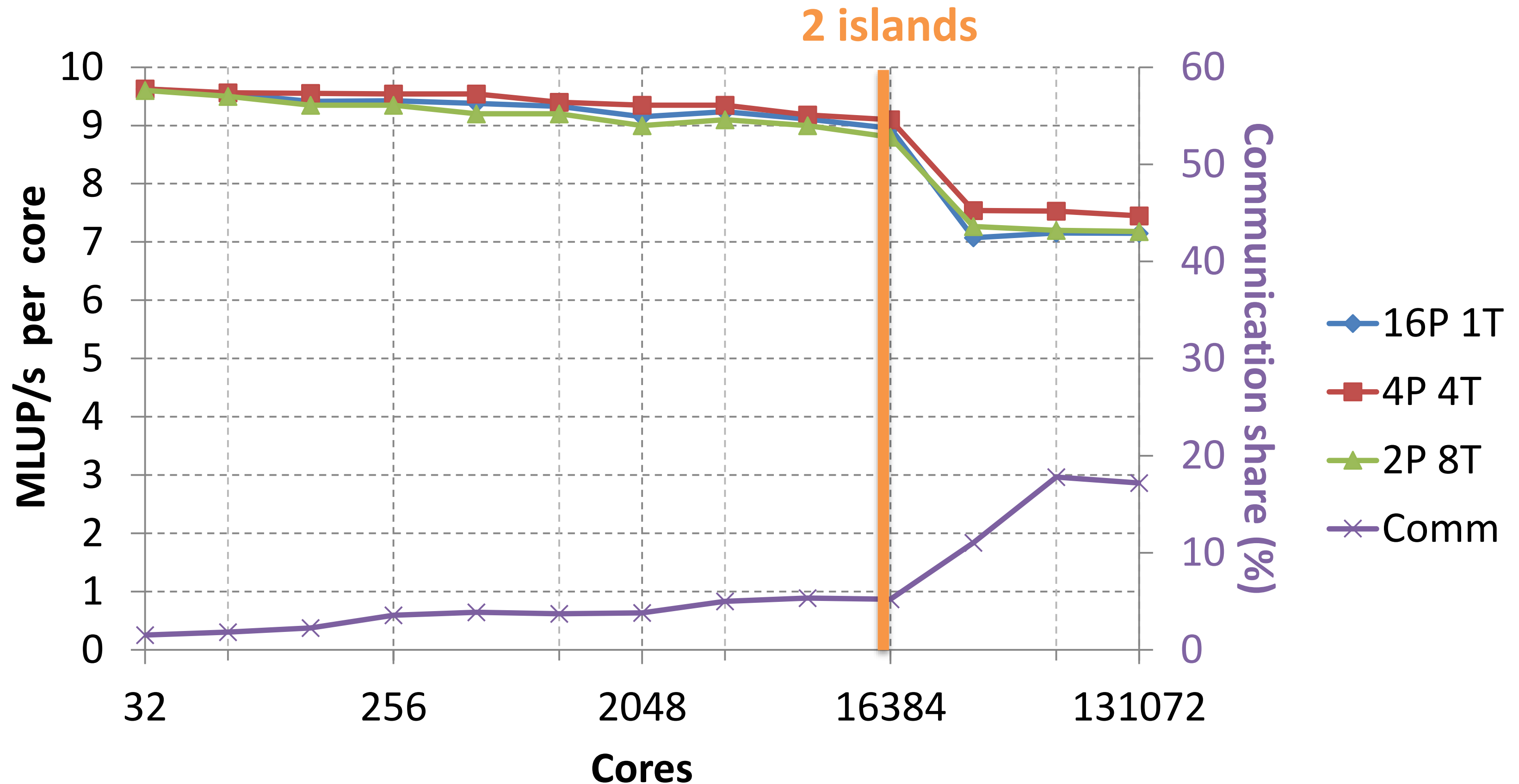


512 processes

458,752 processes

Weak scaling

- Weak scaling - TRT kernel (3.34 million cells per core)



Modular Software Design

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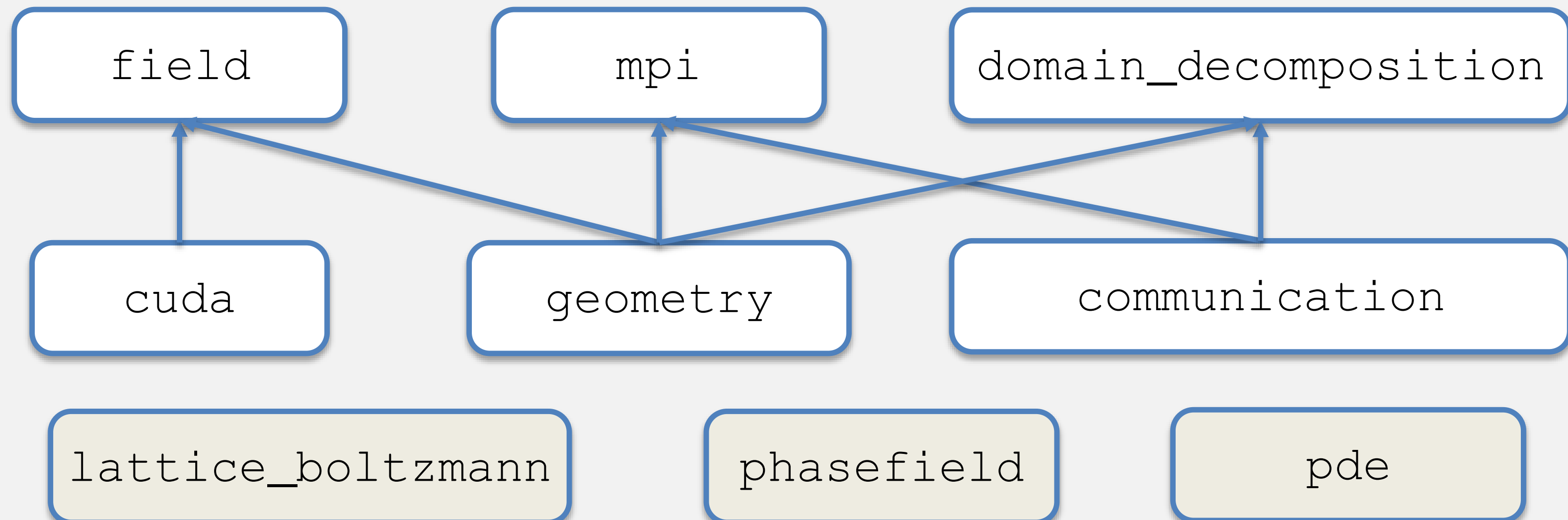

- Main Goal: Modularity
- Decoupling: heavy use of template concepts

Motivation: Simulation Setup

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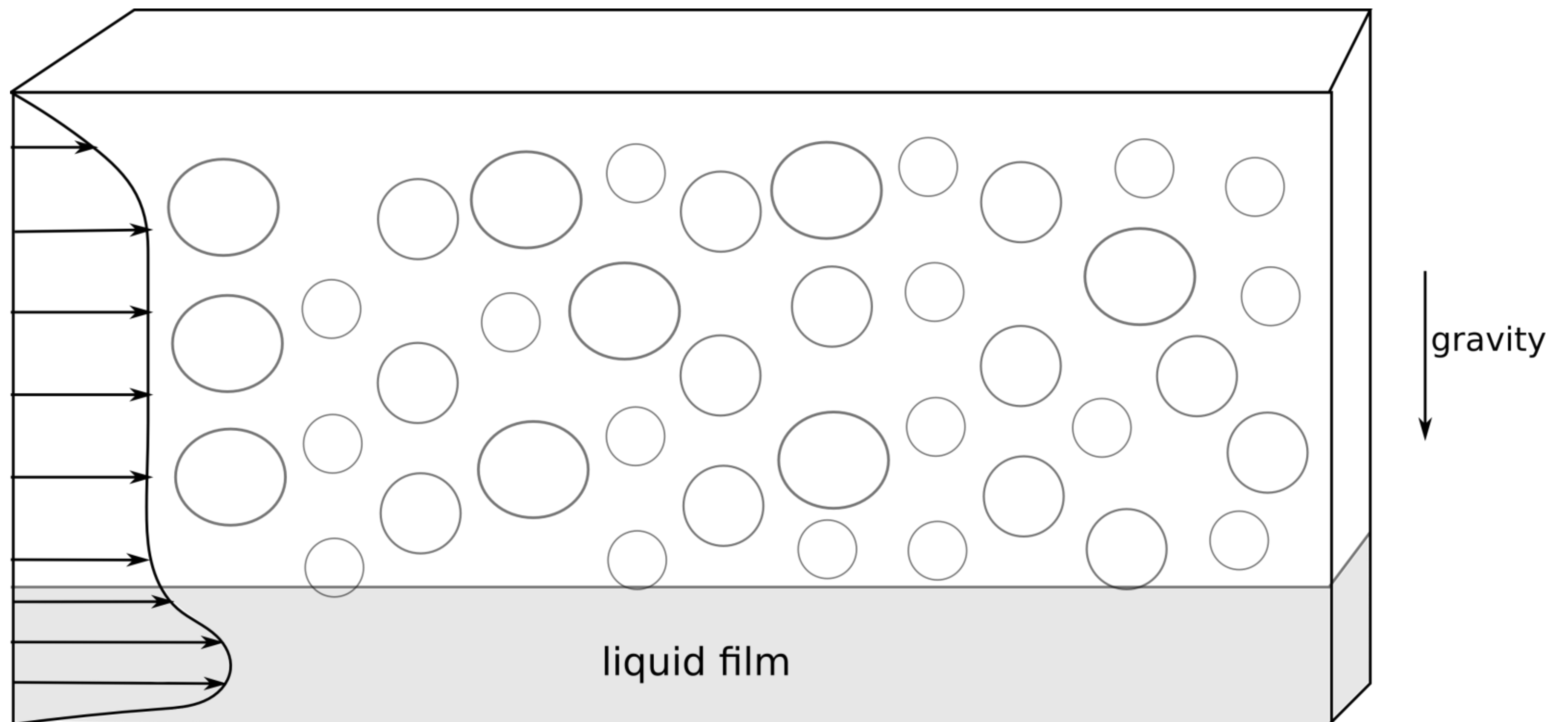
Simulation Setup

- Example Application: free surface LBM simulation
- Bubbly Flow through channel



Simulation Setup

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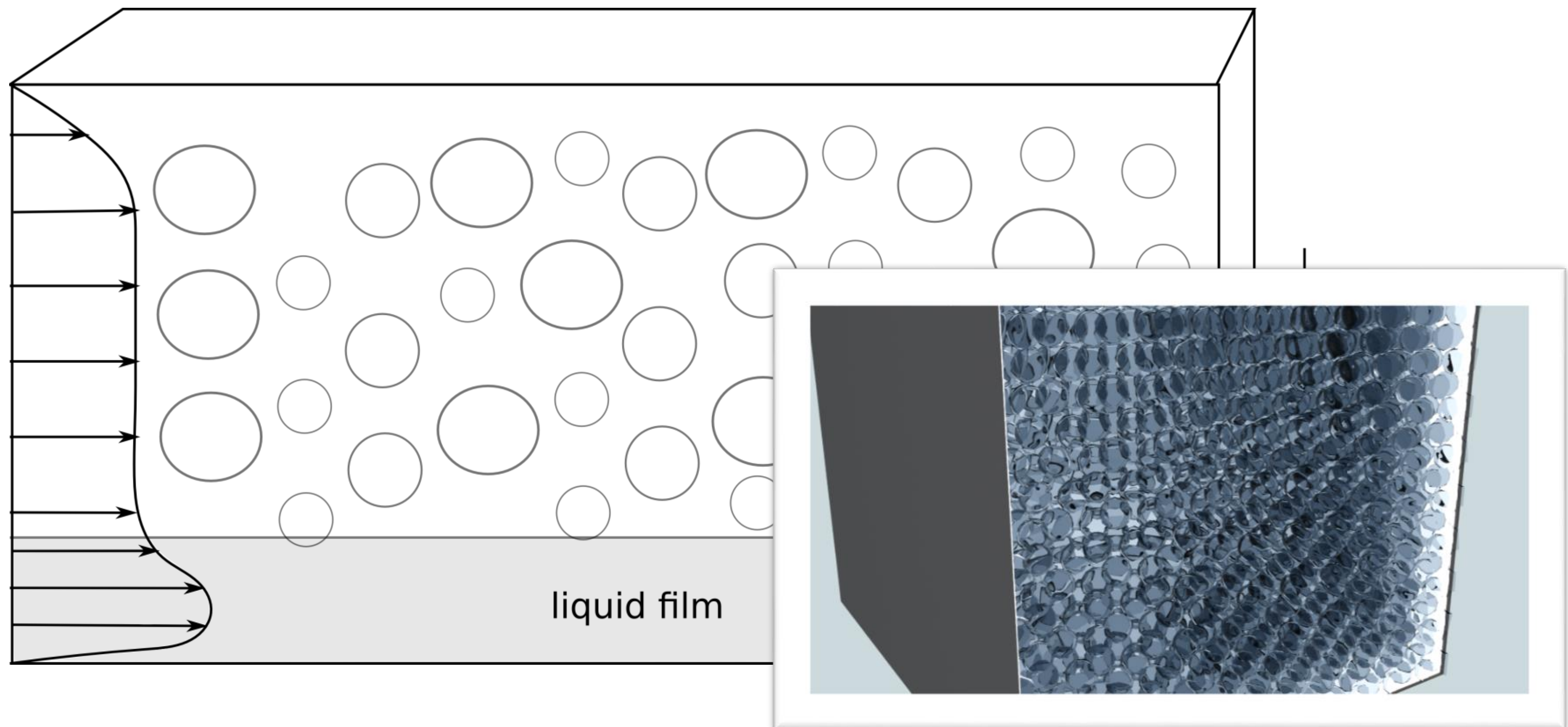
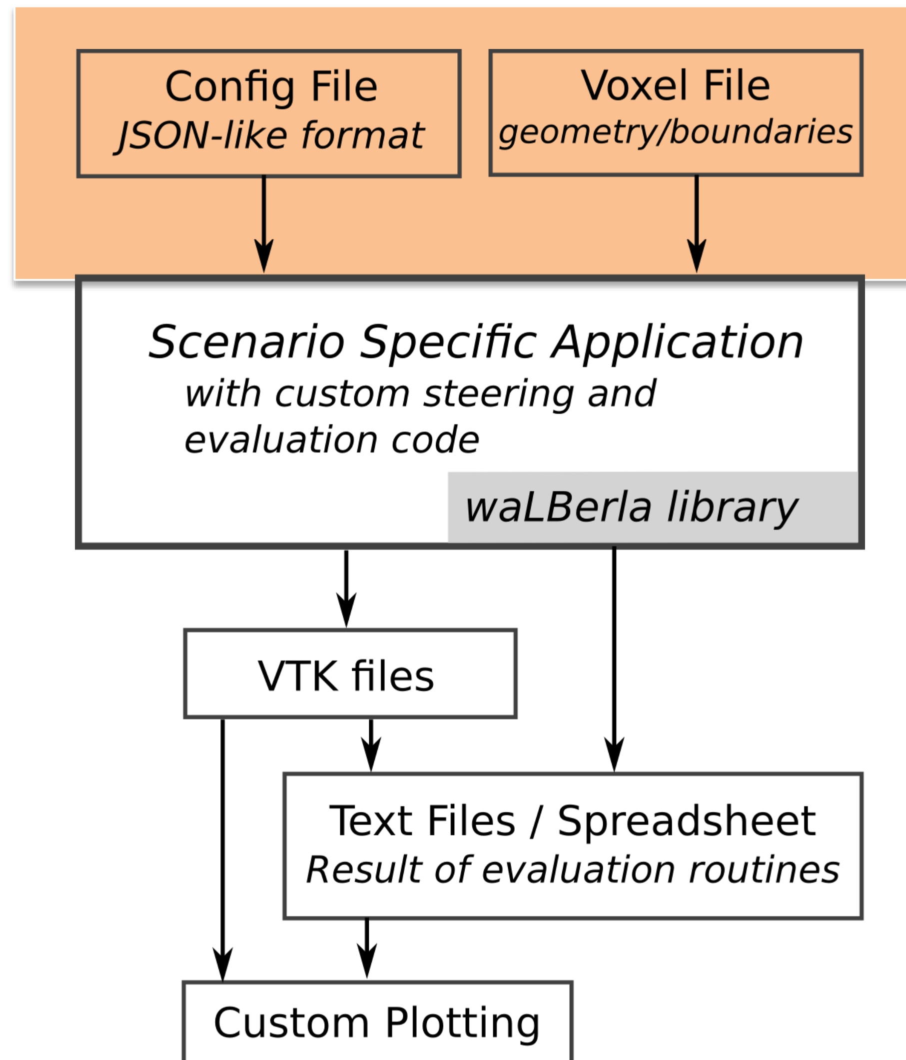


Simulation Workflow



Motivation: Configuration files

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- waLBerla provides a hierarchic key-value pair configuration
- specified in a JSON-like syntax

```
DomainSetup {
    dx  0.01;
    cells < 200,200,1000>;
}

Physics {
    LBM_Model {
         type SRT;
         relaxation_time 1.9;
    }
}

Geometry {
     free_surface {
           sphere { position < 100,100,500>;  radius 10; } //…
     }
     at_boundary { position west;  type inflow; vel 0.01; }
}
```

Compute from dx,dt,viscosity?

Use previous values? cells/2”

Check valid range? Physical Units?

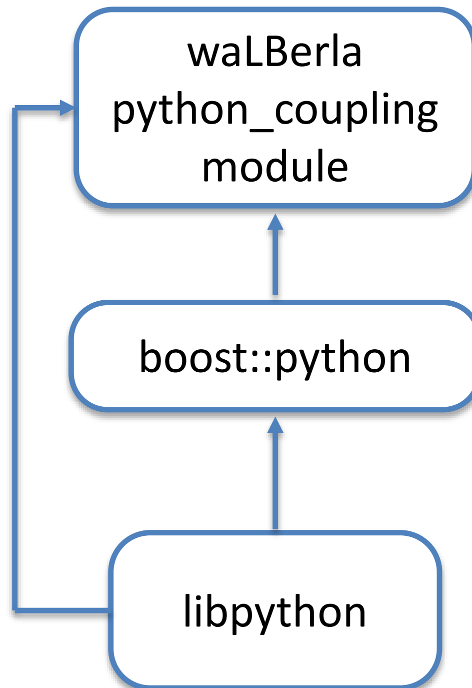
Motivation: Configuration files

- Special C++ modules were developed to enhance the config file
  - unit conversion
  - automatic calculation of missing parameters
  - check for valid parameter combinations and ranges
  - support for functions/macros?
- essentially we started to develop a custom scripting language

Python was chosen because:

- popular in scientific community
- easy to use together with C/C++
- *boost::python*

Library Stack



- interface to expose waLBerla datatypes and call Python functions
- C++ Interface
- C Interface

Callbacks

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- Simulation (still) driven by C++ code,
- Callbacks to Python functions
- configuration provided in a Python dict

```
import waLBerla

@waLBerla.callback( "config" )
def make_config( **kwargs ):
   return { 'DomainSetup' : { 'cells' : (200,200,1000), }
            'Geometry'    : { } }
```

```
python_coupling::Callback cb ( "config" );
cb(); // run python function
auto config = convertDictToConfig ( cb.returnValue() )
```

Simulation Setup

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```
@waLBerla.callback( "config" )
def config():
    c = {
      'Physical' : {
       'viscosity'        : 1e-6*m*m/s,
       'surface_tension': 0.072*N/m
       'dx'              : 0.01*m,
       # ...
      }
      'Control' : {
        'timesteps' : 10000,
        'vtk_output_interval': 100,
        # ...
      }
    }
    compute_derived_parameters(c)
    c['Physical']['dt'] = find_optimal_dt(c)
    nondimensionalize(c)
    return c
```

Units Library

Computation and Optimization

Simulation Setup

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- Further callbacks, for example for boundary setup:

```
gas_bubbles = dense_sphere_packing(300,100,100)

@waLBerla.callback( "domain_init" )
def geometry_and_boundary_setup( cell ):
   p_w = c['Physics']['pressure_west']
   if is_at_border( cell, 'W'    ):
      boundary = [ 'pressure', p_w ]
   elif is_at_border( cell, 'E'    ):
      boundary = [ 'pressure', 1.0 ]
   elif is_at_border( cell, 'NSTB'):
      boundary = [ 'noslip' ]
   else:
      boundary = []

   return{'fill_level': 1-gas_bubbles.overlap(cell),
          'boundary'  : boundary }
```

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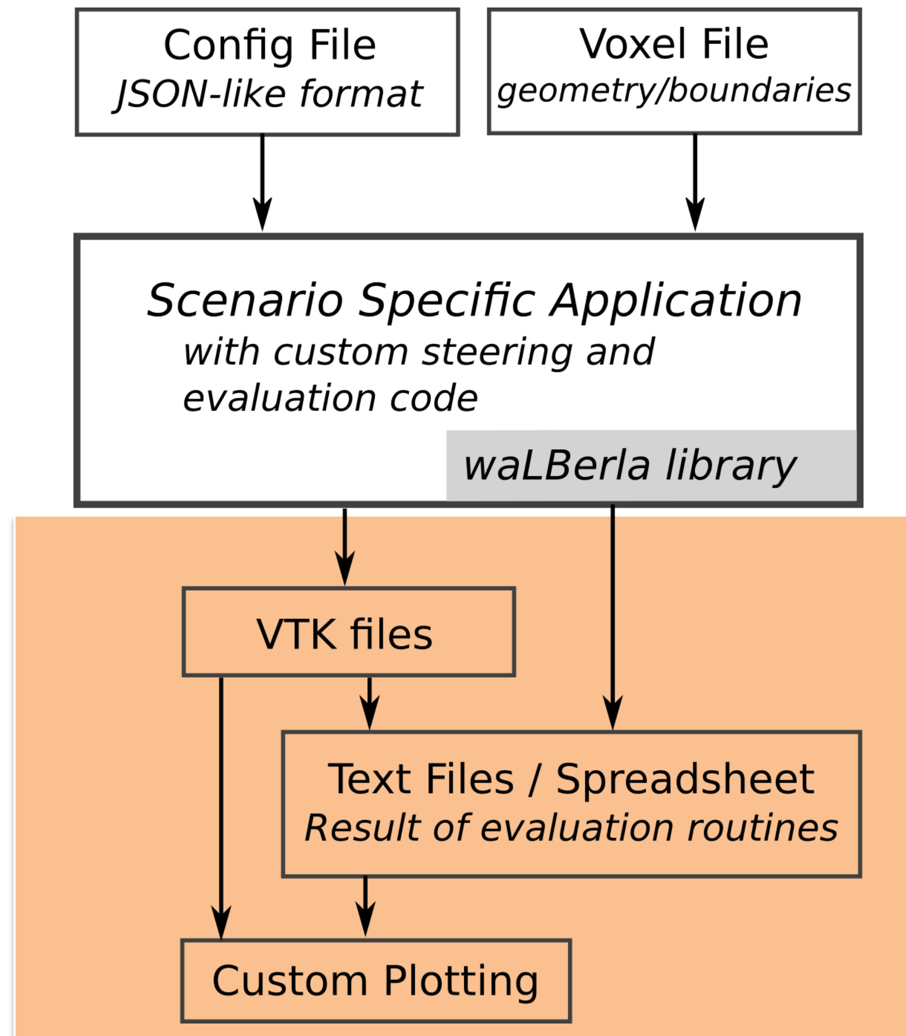
Simulation Workflow



Callbacks

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- Next step: make C++ data structures available in Python functions
- Most of them straightforward, using *boost::python* wrappers

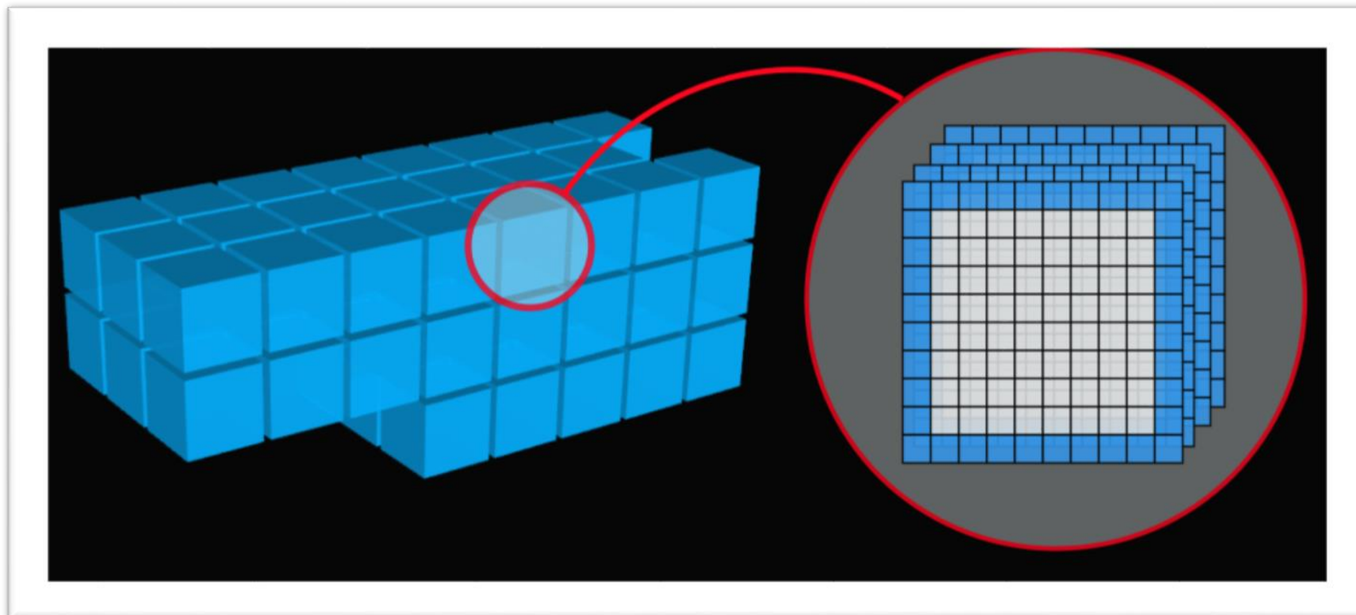
```python
import waLBerla

@waLBerla.callback( "at_end_of_timestep" )
def my_callback( blockstorage, **kwargs ):
   for block in blockstorage:
      # access and analyse simulation data
      velocity_field = block['velocity']
```

```cpp
Callback cb ( "at_end_of_timestep" );
cb.exposePtr("blockstorage", blockStorage );
cb(); // run python function
```

Field access in Python

- `Field` is the central data structure in waLBerla (stores all simulation data)
  - four dimensional array, that stores all simulation data
  - easy switching between AoS and SoA memory layout
  - distributed: field only represents the locally stored part of the lattice



Field access in Python

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  - four dimensional array, that stores all simulation data
  - easy switching between AoS and SoA memory layout
  - distributed: field only represents the locally stored part of the lattice

- user friendly and efficient access from Python is essential
  - no copying
  - should behave like a numpy.array (indexing, slicing, etc.)

Field access in Python

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Solution: *Buffer Protocol*

- raw memory is the interface: pointer to beginning together with strides for each dimension
- not wrapped in *boost::python* -> directly use C interface

```
import waLBerla

def to_numpy( f ):
    return np.asarray( f.buffer() )

@waLBerla.callback( "at_end_of_timestep" )
def my_callback( blockstorage, **kwargs ):
   for block in blockstorage:
      # access and analyse simulation data
      velocity_field = to_numpy( block['velocity'] )
```

Exporting template code

- heavy use of template code due to performance reasons
- all templates have to instantiated
- which combinations to instantiate?

```
namespace field { // field module
     template<typename T>  class Field;
     template<typename T>  class FlagField;
}
namespace lbm { // lbm module
     template<typename FieldType> class VelocityAdaptor;
}

namespace vtk { // vtk module
     template<typename FieldType>
     void write( const FieldType & f );
}
namespace postprocessing { // postprocessing module
     template<typename FieldType>
     void generateIsoSurface( const FieldType & f );
}
```

Exporting template code

waLBerla Library

```
using boost::mpl::vector;
namespace field { // field module
     template<typename T>  class;
     template<typename T>  class FFieldlagField;

     typedef vector< Field<double>,
                     Field<int>,
                      FlagField<unsigned char> > FieldTypes;
}
namespace lbm { // lbm module
     template<typename FieldType> class VelocityAdaptor;
     typedef boost::mpl::vector<VelocityAdaptor< double > FieldTypes;

}
```

Application

```
typedef boost::mpl::joint_view< field::FieldTypes,
                                lbm::FieldTypes >  MyFieldTypes;

vtk::              python::fieldFunctionExport<MyFieldTypes>;
postprocessing::python::fieldFunctionExport<MyFieldTypes>;
```

Evaluation

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- Example: determine maximal velocity in channel
- two stage process, due to distributed storage of lattice

```
import numpy as np

@waLBerla.callback( "at_end_of_timestep" )
def evaluation(blockstorage, bubbles):
    # Distributed evaluation
    x_vel_max = 0
    for block in blockstorage:
        vel_field = to_numpy(block['velocity'])
        x_vel_max = max(vel_field[:,:,:,0].max(), x_vel_max)

    x_vel_max = mpi.reduce( x_vel_max, mpi.MAX )
    if x_vel_max: #valid on root only
        log.result("Max X Vel", x_vel_max)
```

Evaluation

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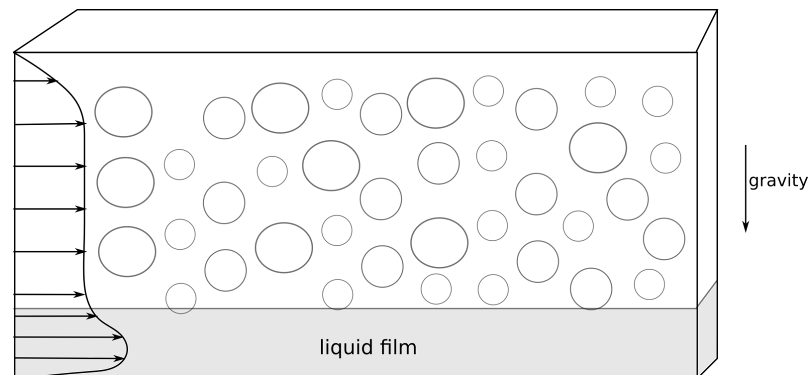
- for smaller simulations: simpler (non-distributed) version

```
import numpy as np

@waLBerla.callback( "at_end_of_timestep" )
def evaluation(blockstorage, bubbles):
     # Gather and evaluate locally
    size = blockstorage.numberOfCells()
    vel_profile_z = gather_slice(x=size[0]/2, y=size[1]/2,coarsen=4)
    if vel_profile_z: #valid on root only
       eval_vel_profile(vel_profile_z)
```

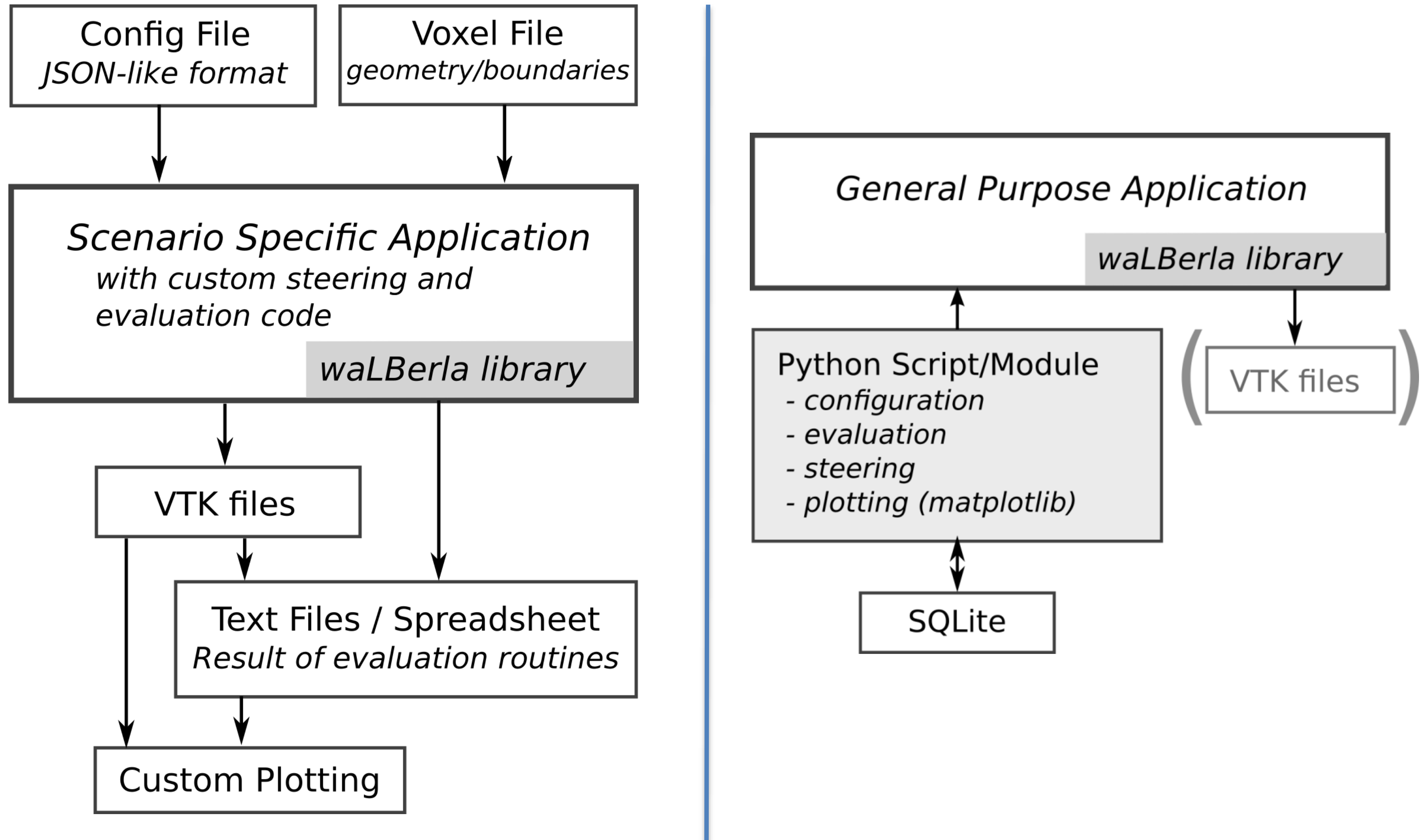
Evaluation

- Python ecosystem for evaluation
  - *scipy*: FFT to get vertex shedding frequency
  - *sqlite3:* store results of parameter studies
  - *matplotlib:* instantly plot results for singlenode, debugging runs
- Simulation Control: use results of evaluation during simulation
  - *Example*: when velocity does not change in channel a steady flow developed and simulation can be stopped
- All scenario related code (setup, analysis, control) in a single file



Summary

Summary



Summary / Outlook

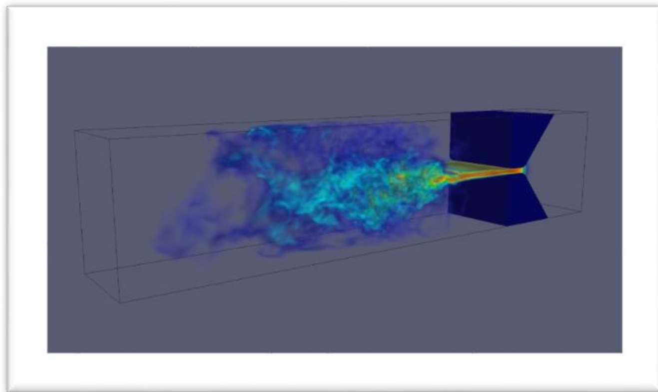
Summary

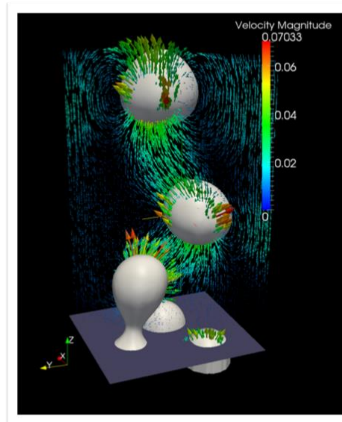
- Python simplifies all stages of the simulation workflow
  - *setup*: nondimensionalization, geometry setup
  - *evaluation*: simulation data accessible as numpy array, storage to database, plotting
  - *control*: definition of stopping criteria, output control
- all scenario dependent code in one file, no custom C++ application necessary any more

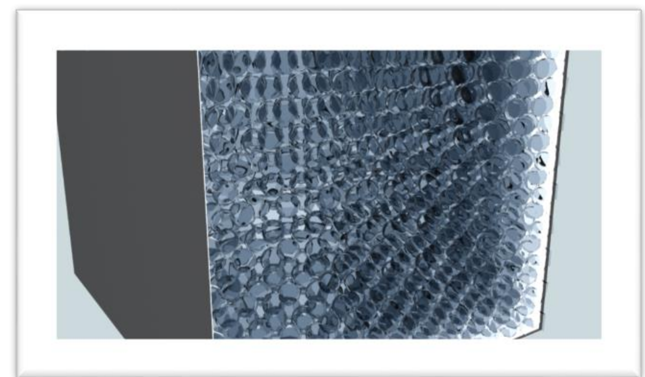
Outlook

- add possibility to drive simulation from Python (export all required data structures)

Thank you!







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