

mapFoam solver and library class structure

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1. INTRODUCTION

To simulate a system that involves reactive crystallisation (precipitation) a new solver has to be developed. In order to capture necessary physics a set of necessary model elements have to be included in the solver:

- Standard hydrodynamics solution loop;
- Energy transport and reaction heat model;
- Species transport and reaction model;
- Solid product species transport and size evolution model.

Each of the elements need to be properly addressed so that the methodology was correct.

1.1. PU COUPLING

1.2. ENERGY EQUATION

1.3. SPECIES EQUATION

1.4. POPULATION BALANCE EQUATION

2. LIBRARIES STRUCTURE

Keeping to the OpenFOAM® class structure, different parts of the model are split into it's separate class. Main abstract class is called *precipitationSystem* which then has to main subClasses: *liquidSolutionReactiveSystem* and *populationBalance*. The former class is taken from www.openqbmm.org which has been released as an open source code under GNU General Public License. New functionality to the *OpenQBMM* code will be added to suit the purposes of our project.

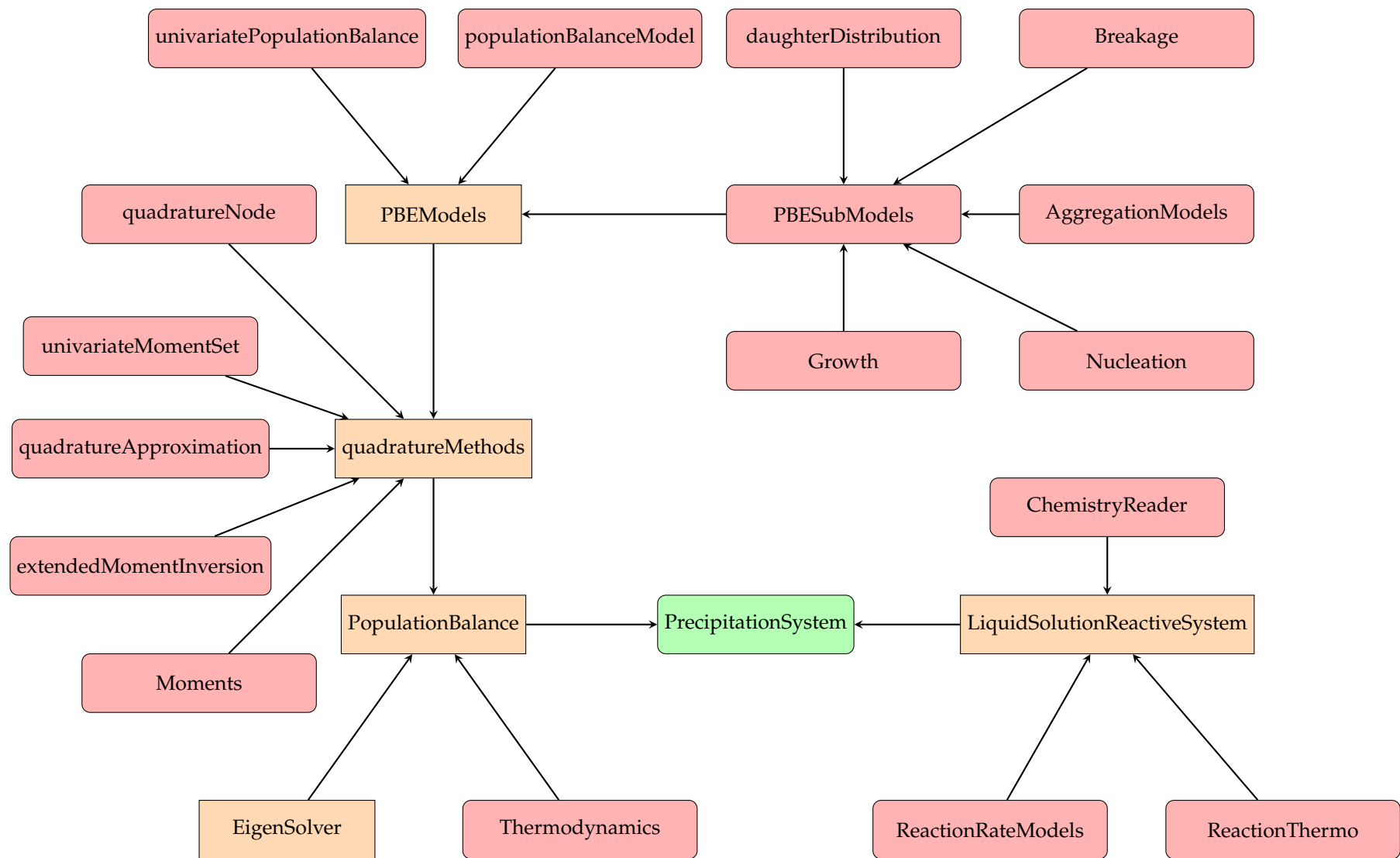


Figure 1: mapFoam libraries structure.