Chapter 7 Scientific Computing in Urban Water Management

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Abstract Urban water management is concerned with the supply of drinking water to households and industry and the discharge of stormwater and waste water from the urban environment. The system is highly dynamic and driven by meteorology, urban development, change in land use and technological innovations. Key mechanisms in urban water systems are on the one hand the transport of water and substances in the environment and the pipe network and on the other hand the conversion of substances due to physical and biochemical processes. Urban water management thus requires computer simulations in time (ranging typically from hours to years) and space (one to three dimensions). With the models becoming more and more complex by simulation at detailed spatio-temporal scale and by simulating whole urban environments, the limits of traditional numerical methods have been reached. In this chapter three emerging topics in scientific computing in urban water management are discussed and the need for advanced software methods is exemplified.

7.1 Introduction

Urban water management is concerned with the supply of drinking water to households and industry and the discharge of stormwater and waste water from the urban environment. Key mechanisms in urban water systems are on the one hand the transport of water and substances in the environment and the pipe network and on the other hand the conversion of substances due to physical and biochemical

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processes. Urban water management thus requires computer simulations in time (ranging typically from hours to years) and space (one to three dimensions).

The requirements for urban water management like hygiene, economics, environment protection, etc. resulted in traditional engineering design (centralized network systems based on pipes and nodes). The evolvement of such a system is highly dynamic and driven by meteorology, urban development, change in land use and technological innovations [\[62\]](#page-20-0) or climate change [\[24\]](#page-18-0).

Traditionally, in the design process and assessment of water networks, different parts of the networks were regarded separately and frequently even by analytical equations and/or empirical relations. But in the last decades and assisted with increasing computer power, the assessment of water networks is proceeding from investigations on different, separate parts (e.g. a single catchment with a combined sewer overflow (CSO) structure or waste water treatment plant (WWTP)) to a numerical, model-based view on the entire network system [\[48\]](#page-19-0). Going one step further, in the 1990s, integrated models were developed and applied. In these models different sub-systems/models (i.e. sewer, CSO, WWTP and receiving water) are combined to integrated approaches in order to assess water pollution in the receiving water (e.g. [\[20\]](#page-18-1)).

Usually, in such approaches, the engineering system (i.e. network structure) and its boundary conditions (e.g. dry weather flow, drained area, etc.) are kept static. Therefore, the spatial dynamic drivers of urban water systems (i.e. cities) are not considered explicitly, but only as multipliers for expected future conditions (e.g. prospective demand, population growth, etc.)

New developments in data management and increasing availability of digital data enabled engineers to use GIS-software and raster-based spatial distributed data for their investigations. Among others, raster-based GIS-data can be used to obtain input parameters for numerical network simulations (e.g. topography, impervious area from processing ortho-photos, land-use and population densities). For example, Sitzenfrei et al. [\[60\]](#page-20-1) presented a procedure for automatic generation of water distribution networks based on GIS data topography and population densities. Also, simulation engines are integrated in GIS-software environment to use the capabilities of GIS-software for visualization, data processing and data modification combined with different hydraulic simulation models. This even enables to investigate different infrastructure systems in a comprehensive approach (multi-utility, e.g. Mike Urban, [\[7,](#page-17-0) [59\]](#page-20-2)). Only an interlinked digital description of a city enables new comprehensive investigations and the identification of coherences. With such an integrated "Digital City" [\[53\]](#page-19-1) interlinked infrastructure systems can be investigated (e.g. water supply under consideration of water saving strategies or water reuse and the impact on the sewer system [\[55\]](#page-19-2)). Further, this helps not only to test plausibility of data (intersection and alignment of different data, etc.) but also to complement insufficient data sets with e.g. stochastic approaches [\[31\]](#page-18-2) or inverse modelling. But taking this approach one step further, the question arises: are the network-based descriptions and models still necessary respectively advantageous for up-coming modelling tasks? To face challenges of climate change and future developments, decentralized solution for on-site water reuse strategies are increasingly developed,

investigated and implemented [\[33\]](#page-18-3). Especially for simulation and analysis of the spatial dimensions of decentralized solutions (rain-water infiltration, water and rain-water reuse, etc.), the network-based models are not effective.

Spatially enhanced integrated modelling approaches (including infrastructure, land use and population models) allow novel insights how dynamic urban systems work and to identify system coherences [\[42\]](#page-19-3). Recent research focuses on the integration of urban simulation models in the assessments of water infrastructure systems to integrated urban simulation approaches (e.g. $[8,56,58]$ $[8,56,58]$ $[8,56,58]$ or $[45]$). Therein, the infrastructure models (e.g. water distribution system or combined sewer system and WWTP) are coupled with urban simulation tools for dynamic simulation of population development under consideration of socio-economic issues. For these investigations and for an interactive consideration of time dynamics in the submodels, spatially distributed information on parameters is required. Therefore, raster-based models (e.g. based on local water balances with regional interactions) are in this context more capable to model especially decentralized systems and to enable spatially distributed, time dynamic interactions. The transition from centralized systems to decentralized systems is an important part, respectively, and the coexistence and functionality of both systems has to be investigated (e.g. rainwater harvesting and water distribution system).

In this chapter we will focus on three issues that have been in the centre of scientific attendance for the last decade. The first topic, the estimation of possible solutions for water management in megacities requires the spatially distributed, dynamic and grid-based simulation of the evolution of public water infrastructure under consideration of changes (e.g. climate, global, environment, economy, land use). Currently, these simulations can be realized with the help of frameworks for integrated modelling like, e.g. "DynaMind"—a workflow engine especially designed for urban water management simulations.

Second topic is the utilization of multicore facilities in software for simulating the dynamics in water networks. The basic features of parallel coded network simulations are discussed for standard public domain software tools in the field that is SWMM for drainage systems and EPANET for water supply networks.

Third, smoothed particle hydrodynamics (SPH) is presented as an alternative numerical method to explore fluid flow phenomena in urban water management based on the simulation of particle movement that can easily be extended towards multiphase flow phenomena, solids transport and bioconversion processes. Thus SPH could potentially be the core numerical engine to simulate fluxes and processes in the complete water infrastructure on a very detailed level.

7.2 From Water Networks to an Integrated Assessment of Urban Water Systems

To identify different steps of model complexity and also to evaluate the according model requirements a literature review is used. Based on this, different levels of modelling approaches are outlined/defined and their advantages and disadvantages are pointed out, respectively.

7.2.1 State-of-the-Art Modelling Approaches

Traditionally individual parts of the drainage systems were calculated by engineers independently with simplified or empirical equations (empirical Manning equation for open channel flows, time area method, etc.). Among others, the software tool SWMM enabled modelling of the entire sewage system and the tool is increasingly developed (starting from 1973 to the current version SWMM5 [\[51\]](#page-19-6)). With increasing computer power but also with progressing understanding of the relevant mechanism in the different sub-parts of wastewater systems, integrated models are developed which couple different sub-systems of the urban (waste)water cycle (e.g. [\[20\]](#page-18-1)). In the last few years, the requirement of integrated water management approaches increased and new modelling approaches were developed and applied. Hardy et al. [\[19\]](#page-18-4) developed an integrated water management approach (UrbanCycle) to investigate urbanization in the context of efficiency of the implemented technical systems. Especially, for regions with high climatic variability, changes in boundary conditions can possibly produce highly inefficient technical solutions of the urban water management systems. Traditionally, investigations are performed with top– down approaches, but for interacting systems new approaches are required [\[19\]](#page-18-4). UrbanCycle is a modelling framework for an integrated view on water supply, wastewater and stormwater solutions which aims to model interacting systems from bottom up. Therefore, clusters for allotments represent the water cycle/reuse at that scale. For a performance assessment, these clusters are connected to headwork systems (e.g. main trunks, etc.). Doglioni et al. [\[8\]](#page-17-1) developed another integrated framework to model interactions of the urban water systems with urban expansion. The developed integrated framework dynamically couples a land use change model, a sewer simulation model and a wastewater treatment plant (WWTP) model to an integrated approach. For the infrastructure (sewage system and WWTP) no dynamic update (redesign over time) was regarded. Therewith, the impact of urban expansion on the existing sewage system (node-based) and the WWTP were investigated. A multi-agent model combined with a cellular automata-based model was used to model the (raster-based) urban expansion and population dynamics. But for coupling of the raster-based information of the urban development model the spatially distributed information was abstracted to the node based representation of the sewage network and no information feedback and therefore no infrastructure adaptation was regarded.

All these integrated approaches couple different models with data generalization from raster-based to node-based information and vice versa, respectively and work on different modelling scale (i.e. allotment cluster, head network level). In general, such approaches bring up the problem of data abstraction and generalization. Especially for integrated models with population and land-use dynamics, information feedback through the coupled models is crucial. There is also an increasing requirement of new modelling approaches from another research field. Brown et al. [\[3\]](#page-17-2) formulated a transitions framework for urban water systems to describe the historical and future scenarios of water management in Australian cities. Therein, different steps of the transition from traditional urban water systems (centralized water supply and sewage) to integrated urban water cycles (fit for purpose water sources, i.e. water sources with different qualities are appropriately used) and sustainable water management are defined. The framework encompasses six transition steps to an adaptive, water sensitive city. For the transition to such water sensitive cities, integrated modelling approaches including dynamic socioeconomic issues and decentralized solutions are required.

For environmental processes [\[44\]](#page-19-7) described the need for integrated assessment and modelling of such systems. Interdisciplinarity is described to be the key to address environmental problems of the twenty-first century [\[43\]](#page-19-8). Modelling the water cycle with taking into account socio-economic processes is a challenging task. Especially, investigations based on agent based modelling techniques have the potential to manage such spatially distributed and dynamic systems [\[36\]](#page-18-5). Also, investigations on the impact of climate change have to be done on a large temporal scale. To estimate, e.g. the impact of climate change on our environment requires therefore the inclusion of the temporal change of demography and infrastructure in the investigations. For example, Barth et al. [\[2\]](#page-17-3) investigated these aspects on the rural Upper Danube Catchment with a multi-actor simulation framework denoted DANUBIA including agent-based approaches. To assess the impact on the entire water cycle in that approach, scenario analyses were performed with this modelling framework. Therein a raster-based modelling concept (proxel concept) was used for a description of interdisciplinary interactions. Each raster cell (i.e. each proxel) is connected to other proxels through fluxes [\[29\]](#page-18-6). In the approach a 1 km proxel size is used for (mesoscale) modelling of land surface and socio-economic processes.

The European FP7 project "PREPARED enabling change" aims to develop a software tool for modelling an integrated urban water management cycle. This includes the technical water systems as well as socio-technical dynamics (urban development, socio-economic transition, etc.). The project aims to model interactions of water infrastructure including decentralized solutions, (multi-utility assessment) including urban development, dynamic adaptation of technical urban water systems under consideration of socio-economic transitions.

7.2.2 Raster-Based and Node-Based Models

With raster-based models, the available spatial information can be directly used (see Fig. [7.1\)](#page-5-0). There is no need of data generalization or abstraction (abstraction for node-based models). This helps to cut down calculation time in terms of feedback loops (computation time of data conversion) but also assists to evaluate decentralized systems (e.g. rain-water harvesting).

Fig. 7.1 Node-based and raster-based models in context with a "Digital City" description

Fig. 7.2 Different modelling approaches for urban water systems

7.2.3 Definition of a Framework for Modelling Approaches

In the following, different steps of model complexity to evaluate urban water systems are identified. Therewith, the shift in approaches to assess water systems is described and discussed. Further, the theoretical framework of an integrated "Digital City" [\[53\]](#page-19-1) to comprehensively assess urban water systems on a raster-based description of the investigation areas is characterized (see Fig. [7.2\)](#page-5-1).

1. *Single structures* of systems are investigated (traditionally with "paper and pencil" based methods). Detailed information on a specific structure is required and therefore very case specific, local results are obtained. With these approaches no holistic view can be obtained. Traditionally, such investigations are performed due to either limited computer power or because of very specific questions (e.g. specific design issues). In regulatory guidelines (e.g. in Austrian guideline for design of CSOs) there has already been a shift in the requirements for assessment of such systems. While the former guideline focuses on design of specific CSO structures [\[40\]](#page-19-9), the new version aims already on an assessment of the entire combined sewer system performance [\[23,](#page-18-7) [41\]](#page-19-10).

- 2. *Entire systems*/processes are investigated (e.g. sewer network, water distribution system or WWTP, etc.). But still, each system is assessed separately and only the performance of the specific system (network, etc.) is simulated. But there is no holistic view, and no broader assessment of the entire water systems (no system interconnections).
- 3. *Integrated* urban water methods couple models of different sub-processes to an integrated approach. By coupling different sub-systems to such an integrated assessment helps to understand and identify holistic system coherences like real time control for combined sewers and oxygen depletion in the receiving water. Also coupled water supply and urban drainage models can be used to assess low flow conditions $[54]$.
- 4. *GIS-assisted integrated* infrastructure systems (different infrastructure models, are embedded in a GIS environment as, e.g. provided in the software Mike Urban or Hystem-Extran). The rising amount of available digital data enables engineers to use GIS-software and raster-based spatially distributed data for their investigations. Especially for data intersection, multi-utility interactions, data verification, plausibility tests these new approaches have comprehensive potential. Going one step further, population models are integrated in holistic modelling approaches to investigate dynamic interactions. For raster-based population models, this requires extensive calculation time for data conversions and dynamic feedback loops.
- 5. The *Digital City* approach denotes integrated urban systems (interlinked infrastructure and urban simulation models for population dynamics with socioeconomics, etc.) combined with raster-based models and data management. This allows both the consideration of decentralized systems and spatiotemporal interactions and the dynamic feedback of population models to water infrastructure. The spatial resolution requirements to model such systems node-based are (especially for larger systems) at least a significant computational burden and sometimes even prohibitive for available computer power. Approaches including urban dynamics with data conversion (raster to node-based data conversion and vice versa) represent a pre-stage of such a "Digital City". Fully raster-based models respectively also fully vector based descriptions on the other hand enable comprehensive and extensive investigations of the urban system. For consideration of socio-economic processes in a detailed spatio-temporal model (e.g. impact of general conditions/constraints on the choice of technical solutions) such approaches are a prerequisite. For traditional network based system description such an assessment is only feasible with transfer functions/data conversion. One of the main advantages of the "Digital City" are the interfaces and linkage with GIS approaches that can be implemented with ease. Since there is a direct interface, neither data

Fig. 7.3 Workflow of an integrated urban environment used in DAnCE4Water

conversion nor generalization (loss of spatial information) is required. The software implementation of concepts can be realized with fewer efforts which offer more opportunities to model interactions. The "Digital City" represents an easier way to model spatial correlations of different technical systems. Primarily in the context of decentralized solutions there are strong linkages between the drainage efficiency, groundwater recharge and high water impacts. The "Digital City" meets requirements of upcoming modelling tasks such as efficient integration of population models, but has yet not been applied.

7.2.4 Assessment Tools and Applications

As discussed by [\[6\]](#page-17-4) traditional GIS systems are unsuited to model dynamic urban systems due to their limitations to represent time. Therefore, to model the evolution of a city spatially explicitly, new software tools are required. The open source software tool DynaMind [\[63\]](#page-20-4) provides such a modelling environment to create dynamic urban simulations. Like in GIS the urban system is represented with simple geometric objects (nodes, edges, faces) and raster data. Linking of these data enables the representation of complex objects like buildings or combined drainage networks. These objects are altered by means of data encapsulated modules. To create a module, DynaMind provides easy to use interfaces $(C++$ and Python) to accessed/modified spatial data during the run time. DynaMind comes already with a set of modules for data import/export and basic GIS functionality (spatial joining, etc.) as well as more complex modules that enable the procedural generation of parcels, buildings or sewer and drainage systems [\[64\]](#page-20-5). It also provides interfaces to external hydraulic solvers like SWMM [\[51\]](#page-19-6) and CityDrain3 [\[4\]](#page-17-5). These modules can be linked together to describe a complex workflow in the urban environment. Figure [7.3](#page-7-0) conceptually shows the workflow of an application [\[49\]](#page-19-12) to describe the evolution of the urban environment and its water infrastructure.

DynaMind enables the procedural evolution of cities and their water infrastructure under numerous future scenarios to identify possible development strategies.

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Fig. 7.4 Procedural evolution of Innsbruck, Austria with DynaMind

This can be used to test, e.g. the robustness of a climate change adaptation strategy. Figure [7.4](#page-8-0) exemplarily shows one out of 1,200 realizations for the City of Innsbruck, Austria.

7.3 Utilization of Multicore Facilities in Software for Simulating Complexity and Dynamics in Urban Water Management

In the following section different strategies to improve the computational performance of urban water models are presented. This is required to take advantage of recent developments in information technologies as the development of multicore processors to deal with upcoming challenges for urban water systems.

7.3.1 Requirements for Simulations in Urban Water Management

Urban water management requires computer simulations in time (timeframe ranging typically from hours to years) and space (one to three dimensions). The models typically include both physical/biochemical process descriptions as socio-economy considerations of water infrastructure planning and operation. Urban water models have to be calibrated and validated on measurement data and parameter values have to be determined during model calibration. This process is a mathematical optimization problem aiming to minimize the deviations between measured data and model output [\[26\]](#page-18-8). This means that multiple model runs are required before a model can be used in any planning process. With models and their applications becoming more and more complex by either tackling processes at a detailed spatial scale, simulating whole urban environments or performing numerous model runs for scenario or uncertainty studies, boundaries of traditional numerical solutions are reached.

For example, comprehensive simulation studies to determine the uncertainty bounds of model outputs (expressed as confidence intervals) require between 1,000 and 30,000 iterations [\[11\]](#page-17-6). Currently such studies are only possible for relatively simple models with a short model runtime (e.g. conceptual models with coarse spatial resolution). Uncertainties of more complex models are usually expressed in scenario uncertainties investigating only a limited number of different scenarios. Such scenarios can be future conditions as impact of climate change or urban development [\[24\]](#page-18-0), or parameter scenarios [\[30\]](#page-18-9). Therefore for each analysed scenario one model run is required.

Depending on the application, different strategies for performance improvement are possible. One possibility is to try to reduce the number of required iterations by improving the calibration/uncertainty algorithm, e.g. by reducing the parameter space which has to be investigated or by improving parameter sampling strategies [\[10\]](#page-17-7). Another possibility is to try to reduce the computational time of the iterations by different parallelization strategies ranging from batch level parallelization to model level parallelization [\[32\]](#page-18-10). In the following different methods of performance improvements are presented.

7.3.2 Model Level Parallelization

With batch level parallel strategies, a high factor of scalability and efficiency can be achieved (an overview of batch level parallelism can be found in Sect. [7.3.3\)](#page-12-0). Nevertheless, in certain scenarios batch level parallelism is not an option or cannot be used because of certain constraints. In such scenarios parallelization must be targeted at deeper levels. The parallelization level discussed in the following subsections is based on the models itself. Performance enhancements in this layer also benefit users of single model call scenarios.

Parallelization at the model level is typically more involved than batch level parallelization. This is because knowledge of the internal mathematical procedure is necessary. Changes to the source code of the model, which could potentially introduce new defects especially in the case of parallel and concurrent programming, are needed. It is often the case that the current mathematical formulation or programming model does not allow to parallelize the model. The biggest obstacle in model level parallelization is that changes to the source code are needed and therefore the source code must be available. This is different to batch level parallelization where the whole application is treated as a black box and can be called from the operating system level. In this case no changes of the model itself are needed.

The following sections show three different scenarios of model level parallelizations. Each of them shows a different approach of parallelization which makes them very interesting candidates for describing model level parallelizations. The first one is the storm water management model (SWMM) from the US-EPA for hydrodynamic sewer modelling. It is used for urban rainfall run-off simulations. The second model is EPANET, again from the US-EPA. It is used for water distribution network simulations. Models from the US-EPA are publicly funded and therefore the source code is open source. The third one is CityDrain3 for conceptual sewer modelling. With its simplified mathematical formulations of an urban drainage system it is possible to run long-term effect simulations of urban drainage systems (several decades) in a short manner of simulation run-time.

7.3.2.1 Parallel Flow Routing in SWMM 5.0

Due to its open source code and robust model implementation SWMM 5.0 is a very popular tool for engineers and scientists in the field of urban drainage modelling [\[51\]](#page-19-6). SWMM solves the 1D shallow water equations for flow routing in sewers—also known as the Saint Venant Equations (SVE) [\[52\]](#page-19-13). Parallelization of this model was imagined to be very complex. Reason for this was that the complexity of the SVE did not allow to outline a parallel algorithm implementation beforehand. The second reason was that the code was totally unknown and that it was ported from Fortran. Further it has a long history of revisions and bug fixes.

With these preconditions a very pragmatic approach for parallelization was chosen. The first step was to find the code segments that contribute the most CPU time. A profiling tool showed that the method *findConduitFlow*, responsible for calculating flow through the conduits using a finite difference scheme for solving the SVE, takes the most time. This function is called for every conduit in the system in a loop. Because the order of calculations for the conduit was not critical (the order was as taken from the input file) it seemed as if the calculations were independent and therefore a possible candidate for parallelization. After a review of the mathematical formulations it was clear that the flow was calculated based on boundary conditions upstream and downstream. These boundary conditions are calculated beforehand and therefore the loop around *findConduitFlow* could be and was parallelized.

After several iterations of finding and fixing concurrent memory accesses, introduced by the parallelization, a speedup of around ten on a twelve core machine was achieved. Contrary to initial estimates and despite the uncertain preconditions of the project very good results were achieved in the manner of weeks.

7.3.2.2 Implementation of Parallel Solvers in EPANET 2.0

The EPANET model for the calculation of water distribution systems is based on a graph of nodes with a certain demand and links (pipes) with a corresponding roughness of the represented pipe. Together with reservoirs and tanks as boundary conditions a system of non-linear equations is formulated in a Jacobian matrix and solved using the iterative Newton–Raphson method. The pressure at each node is the result of such a simulation. The pressure of the node influences the flow through the pipes and vice versa. At each iteration step the Jacobian matrix needs to be solved until pressure and pipe flow are stable [\[50\]](#page-19-14).

Solving of the Jacobian matrix is the most time demanding task in EPANET. Profiling assured this although the updating of the coefficients, which involves a lot of pipe flow calculations, takes more time than expected. A lot of fast and parallel solvers, even for graphical processing units (GPUs), are available for solving such symmetric positive definite systems. Speeding up EPANET was imagined to be as easy as replacing the hand crafted old solver with a call to a new parallel and highly optimized one. Because such systems are highly parallel a GPU solver was targeted.

Seven solvers, including parallel sparse direct and iterative solvers for multicore CPUs and many-core GPUs, were tested on a range of artificial and real world water distribution networks. The outcome of this research is that the solver currently implemented in EPANET, a solver that was published in a book 32 years ago [\[14\]](#page-17-8), is still the fastest one.

Linear systems from graphs are typically sparse. The algorithmic complexity of a sparse solver does not only depend on the problem size, which is the case for dense solvers. The complexity depends on the sparsity and the sparse pattern of the problem. Systems from water distribution networks, although, are very sparse. The ratio between the size of the system and the number of non-zeros is typically around two. The fact that water distribution systems are very sparse and typically very small, dimensions in the range of $10⁴$, makes them not a good target for high performance solvers which aim at systems that begin at dimensions of $10⁶$.

7.3.2.3 CityDrain3: Parallel Conceptual Sewer Modelling

CityDrain3 (CD3) is the successor of CITY DRAIN II (CD2) a very popular conceptual integrated urban drainage modelling (IUDM) toolkit. Although CD2 is, as SWMM, a simulation toolkit for urban drainage modelling (UDM), the modelling approach is very different. CD2 uses a lumped, conceptual cause–effect approach. CD2 is used for long-term simulation for which such a modelling approach is favoured due its lower computational requirements.

CD2 was implemented using Matlab/Simulink access to the internal simulation core and therefore parallelization of it was not possible. Because of this and the fact that a CD2 version free of Matlab/Simulink has additional advantages, it was rewritten into CD3 which follows the same modelling principles but uses $C++$ as its implementation base.

In CD3 the wastewater cycle is modelled as a directed acyclic graph where each node represents an element of the wastewater cycle and links represent data/flow transfer between nodes. Links have therefore no computational aspects assigned. A node can be e.g. a sewer, a catchment, a wastewater treatment plant or a river stretch. Because of the conceptual nature the precondition of a node is the outflow of its upstream connected nodes. A parallelization strategy in the same manner as in SWMM is therefore not possible.

Several strategies were implemented to exploit parallelization in such conceptual IUDM simulations. The first one exploits the fact that a wastewater system is often in the shape of a tree with lots of independent streams that eventually merge at the WWTP. At each source, typically a catchment, a thread can be started. Although this offers a way of parallelization it is very limited with regards to parallel workload. A second strategy exploits the fact that parallelization can be pipelined through the time steps. This is possible because the length of a time step is fixed and known before hand [\[4\]](#page-17-5).

The rewrite of CD2 from an interpreted general purpose simulation framework into a tailor made, native and parallelized rewrite in $C++$ made CD3 up to 40 times faster.

7.3.3 Performance Improvement by Batch-Level Parallelism

In urban water management modelling the chosen parallelization technology and especially the level of which parallelization is realized in the source code is strongly depending on the modelling aim and existing modelling software used. In the previous Sect. [7.3.2](#page-9-0) already existing and newly developed software tools and their parallelization strategy were described. Here the performance improvement according to computational efficiency and speedup on multi/many-core systems within one model simulation run was the motivation.

Another interesting research field in urban water management is to assess the sensitivity of system components according to specific performance indicators. Under the scope of this book following two different applications can be identified which are:

- Assess the sensitivity and impact of a model parameter (e.g. roughness of conduits within a hydrodynamic sewer model) on model simulation results (e.g. water level at junctions) [\[25\]](#page-18-11).
- Assess the vulnerability and consequences of existing systems according to hazardous events (e.g. pipe bursts within a water supply system due to deep temperatures [\[35\]](#page-18-12) or a sewer pipe collapse due to deterioration [\[27,](#page-18-13) [34\]](#page-18-14)). Moreover cascading effects can be assessed where the first hazardous event (e.g. failure of a source and therefore change in pressure regime) is the trigger for another hazardous event (e.g. the pipe burst) [\[57\]](#page-19-15).

From the programmers and model developers perspective this application can be realized by (1) modelling the needed adaption within an original model (e.g. pipe burst of one specific pipe), (2) simulate the model and (3) access the consequences of the adaption with global performance indicators (PI) by comparing simulation results from the adapted model with the original model. Repeating steps (1)–(3) for all components within a system, vulnerable/senstive sites according to a specific hazard can be identified.

One might immediately realize that testing each component within a system against such hazardous events needs many different model runs. As each test is independent from each other all model simulations can be run in parallel moreover this parallelism is in theory embarrassingly parallel (batch-level parallelism). Many existing model software products in this field (e.g. EPANET2 and SWMM5) have grown over time and therefore often have no parallel implementation. In this kind of application one huge advantage is that the original model simulation code can be used and at the same time multicore systems can be utilized. The only limiting factor is data communication during the evaluation of all PIs which leads to a non-linear speedup.

Performance tests showed that this parallelization strategy in combination with the software presented earlier has a speedup of 12 by using twelve threads at batch-level and one thread at the model level. By using one thread at the batchlevel and 12 threads at model level a speedup of only four can be achieved. More investigations with other model simulation software products (e.g. EPANET) showed that this parallelization strategy is a good alternative to speeding up the previously described applications. Moreover if the model software comes already with a parallel implementation (e.g. parallel version of SWMM 5.0, Sect. [7.3.2.1—](#page-10-0) Model level parallelism) and at the same time parallel executing these models, investigations showed that the best CPU-load efficiency can be achieved by only applying parallelism at the batch-level [\[32\]](#page-18-10).

7.4 SPH: An Alternative Numerical Method to Explore Fluid Phenomena

7.4.1 Motivation and Aim

SPH is a computational fluid dynamics (CFD) method for solving fluid flows. In Layman's terms in SPH a fluid is represented by a myriad of small spheres which are referred to as particles. As the movement of particles is governed by the continuum equation of fluid dynamics, the overall picture resembles the true hydrodynamic phenomena. By statistically weighting the influence of each particle's neighbourhood (see Fig. [7.5\)](#page-14-0), the equations of motion reduce to a set of ordinary differential equations which are easy to understand and implement [\[37\]](#page-19-16).

Fig. 7.5 Comparison between Eulerian and Lagrangian movement (*left*) for an SPH particle with five neighbours (*right*)

SPH was introduced, at the same time, by [\[15,](#page-17-9) [28\]](#page-18-15) to solve astrophysical problems. In contrast to conventional grid based CFD methods, SPH is a fully Lagrangian meshless method such that each particle is free to move and carries physical parameters like mass, velocity and density. SPH has been applied to a wide range of problems in the fields of material science, oceanography and volcanology. However, the core application area of SPH is fluid mechanics, in particular transport phenomena $[61]$, free surface $[16, 38]$ $[16, 38]$ $[16, 38]$ and multiphase flows $[5]$.

Compared to conventional CFD methods, SPH has various advantages owing to its Lagrangian nature (see Fig. [7.5\)](#page-14-0). Namely, advection is treated exactly and conservation laws of mass, linear respectively angular momentum and energy are satisfied. In addition, SPH is a physically correct numerical scheme and can be formulated without empirical parameters such that the effort of calibration is minimized. Hence, once the SPH model is set up, it is reasonably simple to account for complex hydrodynamic phenomena like multiphase flow and transport of solid objects. However, the physical correctness of the method requires comparable large computational demand, which can be reduced by relaxing physical requirements. For example, for some practical applications it is sufficient to approximate incompressible fluids by slightly compressible analogues. Through this approach, which is referred to as weakly compressible SPH, the solution of a pressure Poisson equation is substituted by a simple equation of state and hence computational cost is significantly reduced.

Nonetheless, further reduction in simulation time is required for practical applications of SPH. This is achieved by parallelization of the method, which is simplified by the fact that the numerical scheme itself is highly parallel. SPH has already been implemented on highly parallel computing devices like graphics processing units [\[18\]](#page-18-17). In particular, an efficient parallel solution for finding neighbours, which is the process that requires most computational power, was found [\[17,](#page-18-18) [22\]](#page-18-19).

7.4.2 SPH for Sewer Modelling

Over the last three decades, urban drainage modelling evolved from simple models to high complexity [\[47\]](#page-19-18). While state of the art methods for one dimensional hydrodynamic simulations in pipe networks exist, recently more complicated CFD methods have been applied to simulate specific structures [\[12\]](#page-17-11). However, modelling of pollution transport and sewer solids is still an unresolved issue. Both deterministic and conceptual models failed to convincingly explain the underlying phenomena (see e.g. [\[9\]](#page-17-12)). In this respect there is a perspective for a novel, deterministic numerical method as represented by SPH.

SPH has several advantages which makes it a viable alternative to solving the simplified St. Venant equations, which are used in state of the art sewer hydraulic simulation models. First of all, the method is inherently three dimensional, while a reduction to two dimensions is simple but only motivated by limitations in computational power. Therefore, complex hydraulic structures can be easily modelled. Secondly, as the continuum equations of fluid mechanics can be used as governing SPH equations, it is possible to model pressure effects in pipes which are currently bypassed by the Preissman Slot [\[46\]](#page-19-19). Thirdly, extension of SPH to multiphase flow and solid transport phenomena is much simpler than the conventional Eulerian methods. Especially, the application of SPH to the latter field gives a whole new angle to tackle the problem of pollution transport in drainage systems. However, the challenge of huge computational burden for simulating SPH sewers remains. In particular, it is unclear whether the SPH method is applicable for real world pipe networks, but stringent parallel coding and use of novel technology like graphics processing units could open a pathway. Based on present results we foresee a huge potential of the method, whilst significant obstacles still need to be tackled.

7.4.3 SPH for Wastewater Treatment Simulations

As with sewer modelling, multiphase and transport phenomena are the key challenges for numerical simulations of wastewater treatment processes. Since conventional CFD methods are not particularly suitable for these problems, currently the fluid dynamics are neglected in the well-established activated sludge models (ASM) [\[21\]](#page-18-20). Even though the biological kinetics are successfully modelled with this approach, local effects are neglected. Hence, a wastewater tank is assumed to be completely mixed at all times and therefore the hydraulics are effectively uncoupled from biological processes. Whilst the development of SPH is not yet advanced enough to accurately simulate air, sludge and water phases at the same time, it is required to separate the discussion of aeration and sedimentation tanks.

Aeration processes can be modelled as two-phase air water flow, but this is challenging since huge density differences cause rapid movement at the phase interface which gives rise to instabilities in the SPH formalism. Recently, a simple two-phase SPH algorithm has been proposed to cure this problem [\[39\]](#page-19-20). In combination with adding an oxygen concentration parameter, which is evolved by an advective diffusion equation $[1]$, the local dissolved oxygen concentration is accounted for correctly. As this key parameter governs the differential equations of the ASM model, the local oxygen concentration provides a coupling interface between the local hydraulics and the biological kinetics. This approach improves the present ASM model and is the first step to advance to a full-scale three-phase model.

Similar to aeration tanks, sedimentation processes are well described by twophase SPH. In contrast to air water flow the solid phase is not modelled as a weakly compressible fluid phase, but sediments are considered as a slightly compressible pseudo-Newtonian fluid. Thereby, the Newtonian constitutive equation has to be modified [\[13\]](#page-17-14) and a yield criterion is required to correctly account for sediment-fluid scouring at the phase interface. Both the Mohr-Coulomb and the Drucker-Prager criterion yield satisfactory results, but the latter method is slightly preferred [\[13\]](#page-17-14).

7.5 Conclusions and Outlook

Scientific computing in urban water management is widespread. This chapter mainly summarizes current research activities at the Unit of Environmental Engineering within the framework of the research center "Computational Engineering" at the University of Innsbruck focusing on currently challenging issues. The first topic of the chapter reviews increasing complexity of assessing urban water systems respectively describes the shift to city scale analysis. In particular it is outlined how increasing computer power over the last decades changed the way of how system analysis in urban water management is performed. In traditional engineering approaches the complexity of the problem is reduced in order to obtain an applicable mathematical problem description. For that an in depth understanding of the that particular (sub-)system is necessary. The application of such a description but also simulation models can usually be applied in research and practice. Increasing computer power enables us to integrate and couple models with more and more complexity. Different existing models and extensive amount of data can be used for comprehensive analysis which produces an effusive amount of results data. With that the complexity of the engineering task is shifted to analysis of the result data. Such tasks are therefore usually research applications. Nonetheless, such analysis deepens the system understanding and helps also to obtain system coherences which have been usually overlooked. The second topic demonstrates the utilization of multicore facilities in software for simulating such complex systems related to urban water management. In that section it is outlined which parallelization approaches are required in order to speed up different kinds of simulation models in urban water management. This work aims to reduce computation time for existing research tasks and also practical applications. The third topic discusses alternative numerical methods SPH to explore fluid phenomena in urban water management. That approach can easily be extended towards multiphase flow phenomena, solids transport and bioconversion processes and shows therefore great potential in future. Thus SPH could potentially be the core numerical engine to simulate fluxes and processes in the complete water infrastructure on a very detailed level.

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