PSE module TP11 / TKP8100 Advanced simulation

Heinz Preisig, 2009-08-28 2010-08-24, 2012-08-23, 2013-08-30, 2014-08-20, 2015-08-21, 2016-09-09, 2017-08-23

Project themes:

9999	**Subject**	**Domain**	**Goals**
2017-00			
2017-01	Subject in molecular modelling Continuation of last years Problems - sugar in water – application in bio-fuel - ionic liquids		
2017-02	Ontology for particulate systems – molecular level		
2017-03	Docker – build a stand-alone simulation Docker is a tool designed to make it easier to create, deploy, and run applications by using containers. Containers allows you to package up an application with all of the parts it needs, such as libraries and other dependencies, and ship it all out as one package. By doing so you can be sure that the application can run on any machine and across operating systems. The user does not have to install any software on his/hers computer. The user only have to download the docker container and then run the software within that container. A possible application of a docker container is to pack a simple dynamic simulator into the container and be able to run the simulation in the container without having to install any software on the computer.		

2017-04	CFD – Distributed systems / multi-physics : two domains to couple possibly two physical phenomena and multiple solution methods to compare		
2017-05	Ontology-- approximation of operators		
2017-06	LUA – build a parser and implement for plant simulation		
2017-07	Ortogonal collocation on spectral elements – analysis of chromatographic data - separation process such as butyrate		
2017-08	Population balance models in dispersed systems		
2017-09	Optimisation – surface response techniques, Sandia lib's packages		
2017-10	CFD – Gridding		
2017-11	Block coupled systems Multi-physics problems involve requires the solution of multiple equations that are coupled, for example the Navier-Stokes equations (continuum, momentum and energy conservation). The traditional methodology involves solving the equations separately and resolve the coupling through iteration. However, instead of solving a matrix for one-variable at a time, which leads to explicit coupling between variables, it is possible to facilitate allowing for implicit dependencies between the variables and solve multiple matrix systems that describes the solutions of all the variables through all the equations at once.		
2017-12	Design of component based graphcial design environment for exeriment control as we use it in the felles lab		
2017-13	TensorFlow project – can we put the automatically produced models into TensorFlow ?		
2017-14	Make an app for a mobile - to control a felles lab process - to get physical property data		

2016-0	**Models / Methods / Approaches**		
2016-1	CFD simulating a fix-bed mixer where the mixer consists of a set of identical elements. Objective is to simulate one element and then derive the input/output behaviour for a multi-element unit.		
2016-2	CFD for a vortex with a fluid and a solid that is heavier than water and sits on the bottom → rotating the liquid results in a pile of the solid agglomerating in the centre of the bottom.		
2016-3	Molecular to continuous, a simple molecular simulation for which we can simulate the behaviour with reasonable computing times.		
2016-4	Different type of empirical model to fit to another, complex model. Emphasis on the workflow development		
2016-5	Something around Porto ?		
2014-0	**Models / Methods / Approaches**		
2014-1	More on Krylov space methods Coupling of simulators. We simulate one part of the process in one simulator and the second in another, for example a domain of heat transfer coupled with a domain of flow. A simple system in geometry shall be chosen. The two domains are interacting. Orange		
2014-2	Multi-grid methods – combine with complex differentiation Use different meshes in parallel Straw berry + nutty **Adriaen**	Mild multi-scale	
2014-3	Implicit / explicit integration methods combined in one solver in go or python or matlab or Julia or … **Kjetil**	Numerics	Learn more about numerical techniques and possible alternatives

2014-4	Drift flux model (lumped momentum but separate mass balances, energy ignored) coco **Fahad**	Numerics	
2014-5	Automatic differentiation simple flow problem – thermo with derivatives apple	Model utilisation in numerical schemes	Learn about advanced numerical schemes that utilise analytical derivative methods
2014-6	Application of Julia – pvm type of parallel virtual machines using several machines to solve a problem Mango **Kjetil**	Languages	An new development using on-need compilation. Fast but as descriptive as Python
2014-7	Application of Modelica – extend with generic interface for thermo alternative to CAPE-Open **Daniel**	Languages / simulation systems	Learn about Modelica and explore the possibilities of using alternative phys property interface
2014-8	Comsol multi-physics	Multi-physics	
2014-9	Data base – alternative to SQL **Cansu**		
2014-10	Lua application as interpreter for models Peach	Model portability	Improve model portability through standardisation. Here in terms of language being used.
2014-11	Decoupling fast and slow processes in distributed systems **Kasper**	Model approximations enhanced numerical schemes	Learn about time-scale separation and their utilisation in numerical schemes
2014-12	Complex step differentiation nutty	Algorithms	An interesting alternative for generating first-order derivative information at high accuracy
2014-13	Ontology technology - Data mining	High-level information	Learn about a technology that is increasingly used

	- Diagnostics - Lanuage analysis - Biology Flavour of AI – knowledge-based systems - materials hub - Philosophy of time-space **Alexander** **Huang**	structuring	
2013-0	**MULTI PHYSICS as main theme**		
2013-1	Use of Lua to represent models The Lua model is to be used in another appropriate environment such as Pyhton, for example. Use a language widely used as plug-in in games for the representation of models	Model portability	Improve model portability through standardisation. Here in terms of language being used.
2013-2	Coupling of simulators. We simulate one part of the process in one simulator and the second in another, for example a domain of heat transfer coupled with a domain of flow. A simple system in geometry shall be chosen. The two domains are interacting.	Multi-domain simulation	Learn about coupling issues, data exchange and multi-processing.
2013-3	OpenFoam simulation of two coupled phenomena. Examples : Heat transfer & flow or flow & concentration & conductivity	Multi-domain simulation	Ditto
2013-4	Use of Julia as orchestrator. Example can be a simple version of one of the above.	Multi-domain simulation	Ditto
2013-5	Implicit integrators vs explicit solvers	Numerics	Learn more about numerical techniques and possible alternatives
2013-6	Dynamic vs static: we look at a plant characterised by two time scales one part of the process is fast and the other is slow – relative to each other. What is faster simulating a fast and the slow process as dynamic process in a stiff differential equation system or using a pseudo-steady	Behaviour of numerical schemes	Ditto

	state assumption for the fast part		
2013-7	Simulation of a fast stochastic process coupled to a slow larger-scale process, which is deterministic. For example simulate the behaviour of a gas as a stochastic system and couple a slow system such as a piston moving on the other domain	Coupled domains	Simulation of connected systems
2013-8	Coupled physical system in which the interface is given in different co-ordinates or with a different resolution / mesh	Coupled domains	Ditto
2012	**Move towards integrated multi-language/programming systems**		
2012-x	Physical property calculations: Use of higher derivative through the utilisation of symbolic differentiation in a package like Maple. Or more general: can we construct a simple environment in which we enter the DAE, compute the required higher derivatives of the RHS and generate automatically code for Matlab. Possible approach: - use Python/Qt to generate an interface for the equation input and editing. - feed into Maple either directly or indirectly using a script - generate MatLab code in Maple using the existing facilities - assemble the integration task (script) - execute (script)	Simulation systems Advanced integrators / solvers	Use of higher-order derivatives in integrators. • Analytical derivatives vs numerical approximations • Analytical derivatives from computer code • Analytical derivatives from models (though also coded in one or the other form). Here the meaning is “like it would be done by hand” so the use of algebraic manipulators such as Maple.
2012-x	Cyclic processes: no good idea at the moment		
2012-x	Solvers: Numerical methods for Differential Algebraic Equations.	Simulation systems Advanced integrators / solvers	Generic discussion. Literature research for a review. Objective a bread review on problem settings and solvers.
2012-x	Hybrid system simulation and optimisation: Coupled discrete-event and continuous processes are very common in	Logistics Discrete-event	Nature of what is often called hybrid systems.

	today's manufacturing environment. Raw materials are shipped in discrete units, production is continuous and distribution is discrete again. Optimisation of the storage is one of the issues of interest.	dynamic systems / continuous systems	• What's the issue … • Simulators and their ability to represent and handle problems • optimisation ?
2012-x	Supervisory control: batch processes are an example of hybrid systems in which the high-level control actions are event driven implementing a production recipe. Petri nets is one of the technologies being used for designing controllers and simulate the behaviour.	Simulation, DEDS	
2012-x	Dynamic phenomena Several technical systems show “strange” behaviour patterns. For example limiting cycle behaviours. An example is a pipe in a steam generator as they are used in thermal power plants. Or a reactor with a system that exhibits bifurcation. Tore had an example in mind.	Simulation, dynamic behaviours	Complex systems and their behaviour in the context of simulation. • Chaotic systems • Limit cycle behaviours • Multiple attraction points
2012-01 **Stephen**	Model exchange: "Functional mock-up interface for model exchange and co-simulation" an alternative to CAPE-OPEN. Beyond others Cybernetica is implementing this interface. http://www.functional-mockup-interface.org/ The use of Modellica and Matlab is suggested here the process can be discussed, but should be reasonably simple. Main objective is to demonstrate portability issues of models.	Simulation systems	Question of model exchange on all levels. • What is a model • what is need to capture the information. • Expanding the information when expanding the use of the model (simulation, optimisation, control , etc)
2012-02 **Sohrab**	Simulation: Build your own simulator system using an advanced programming language and off-the-shelf integrators implemented in another language. Specifically the library of Buzzi-Ferraris could be targeted. The	Simulation systems, wrappers	Multi-language environments. Questions like • got an integrator in C++ want tu use Phython

	process to be simulated can be discussed, but should be relatively easy to realise. One could consider using the distillation model of Dones, which used the library but was written in C++		• got the phys prop in language A but use integrator in language B
2012-03 **Petr**	CFD application issues: – How to get the geometry into the system – Adaptable grids in dynamic systems – Modelling of isotropic systems	Simulation environments, distributed systems	Distributed systems and their simulation. • Input preparation • Simulation systems • Complexity handling …?
2012-04 **Mayembe**	Complex dynamics Here a specific system was suggested, which uses an external magnetic input to a system that transfers energy in a magnetic field. Physical property estimation is the objective. (Tore)	Simulation, dynamic behaviours	Link between experiment and model: the domain of process identification
2012-05 **Matthias**	Discrete-event simulation: Faults are occurring with a certain probability in a plant, but then the plant consists of a number of units. Question arises on what the expectation of a fault in a plant are and what the consequences are. Here we have a start of simulating a gas delivery plant. Objective would be to compute the pressure distribution for the system and analyse the alarm domains in each part of the plant. This has a direct interest in industry and is one of the research subject linking to an activity at Imperial.	Simulation systems, DEDS	Fault detection is the practical background here. • Issues with detecting faults • issues with computing possible faults (HAZOP) • issues with hiding alarms
2012-06 **Ishtiak**	Multi-model simulation: conceptualise, design and realise a simulation (any language) in which simple models are used when appropriate but more complicated ones when required.	Simulation systems Advanced integrators / solvers	Model accuracy vs dynamics. • How to detect dynamics and how to control the integration error. • How to measure the model mismatch introduced by model simplification. • Integration into a

			workable framework.
2012-07 **Ishtiak**	Steady state optimization of process flowsheets. The focus here will be on comparing different formulations of the optimization problem with respect to efficiency and robustness. Three different formulations will be studied.; one feasible path and two infeasible path formulations. The comparison will be done in Matlab with existing optimization codes like fmincon.	Optimisation	
2011-x	Simulation systems tailored to bio-physical systems	Simulation systems	
2011-x	Simulation languages Different communities have generated different simulation environments using equally many ways of representing the models. The representation is done by a language, usually small, but tailored to the application. The project aims at analysing a couple of representative languages with the goal to not only demonstrate their features but also come up with a generic structure, meaning what is actually necessary for the description of a simulation problem.	Simulation systems	
2011-x	Discrete-event dynamic simulators (Petri nets or the like) The discrete systems domain is paid little attention in chemical engineering even though recently logistic problems have gotten a lot of impetus from the economical analysis side of the chemistry business and consequently is spawning research activities. Maybe even more important is the field of supervisory control and floorshop handling. Petri nets is one of the standard technologies being used in this field. We seek a discussion on the subject as a whole and some capabilities of the simulators. Different simple samples from different areas of applications would be nice.	Simulation systems	
2011-x	Implement a model as a software module in a commercial simulator Main issue of this project is to make the internal structure of the simulator visible. What is necessary in terms of interface and internal structure for this software module that represents the model of a piece of equipment, for example. The project should execute the	Simulation systems	

	implementation using a simple plant, for example a stirred tank with a reaction.		
2011-x	Interfacing an external model in a commercial simulator using CAPE Open. CAPE Open is a technology for wrapping coded models such that they can be used in different simulator environments. This project should lay open what the construction of such a CAPE open wrapper requires and entangles.	Interfacing	
2011-x	Tore's thermo Objective: make a factory for Tore's thermo so as to make it available in a user-friendly environment. Suggested approach is to wrap the C-coded software components of Tore and Bjoern-Tore into Python and then construct a simple factory in Python	Interfacing	
2011-x	Dynamic simulation in HySys	Simulation systems	
2011-x	Solvers – different integrators Integrators are a core technology in today's simulators of dynamic systems. We should like to discuss the various methods being used, their strengths and weaknesses. One of the ever-repeating discussions is if one should use implicit solvers or explicit methods. Key people are Gear and Petzold.	Simulation systems	
2011-x	Solution of two-point boundary problems	Distributed systems	
2011-x	Steady-state simulation and optimisation Optimisation is a stronghold of chemical engineering and a lot of methods and environments exist. A case study using different environments would be nice, say HySys and GAMS or TomLab.	Optimisation	
2011-x	Modelling and optimisation of biogas to liquid fuel process		
2011-x	Compartmental modelling, population balances?? This project is hanging in the air at the moment. The thought is that		

	compartmental modelling is a standard technique in bio and medical engineering for the description of how living species behave when being injected or fed with a substance. From the simulation point of view, the structure of the problem is of interest. For example if one has cycles, one has to know something about the cycle in order to extract knowledge about the operation of the cycle. For example if the cycle involves a flow one needs knowledge about the flow in order to analyse the behaviour. Here we have the need for a case.		
2011-x	Use of alternative simulation languages		
2011-x	Simulation and symbolic differentiation		
2011-x	Simulation of multi-resolution problems (micro-macro scale)		
2011-x	Solvers – wrapping a specific integrator into another environment (Python)		
2011-x	Solutions of partial differential equations		
2011-x	Stochastic process simulation, Monte Carlo methods		
2011-x	Robust data reconciliation Chemical engineering uses little to no concepts of the robust statistics literature. The idea of this project is to bring the subject up and discuss the methods in the light of data reconciliation. Key issue is handling of outliers. Key people are Huber (ETH) and a recent book is authored by R A Maronna, R D Martin and V J Yohai.		
2011-x	Optimal design of a pipe (network) – optimal geometry	Wikki Foam	
2011-x	Simulation and physical properties. How do different simulation environments handling physical properties. What are the common parts what are the differences. When using physical properties, what are the problems, what does one have to pay attention to and what are the decisions one has to take. Guidelines...	Simulation systems	