# 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:

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| **9999** | **Subject** | **Domain** | **Goals** |
| **2019** |  |  |  |
| 2019- | Interoperability – semantic services |  |  |
|  | Consistant equation systems adding assumpions → model reduction |  |  |
|  | General orthogonal collocation |  |  |
|  | Molecular simulations with GROMACS |  |  |
|  | Population balance modelling – |  |  |
|  | OpenFoam gridding |  |  |
|  | Ontology related |  |  |
|  | OpenFoam user interface |  |  |
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| **2018** |  |  |  |
| 2018-01 | Population balance models in CFD simulations using OpenFoam |  |  |
| 2018-02 | User interface for OpenFoam - automata |  |  |
| 2018-03 | Equation systems – handling of assumptions |  |  |
| 2018-04 | Molecular dynamic simulations with GROMACS |  |  |
| 2018-05 | Multi-phase heat transfer in OpenFoam |  |  |
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| **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 |  |  |
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| **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 ? |  |  |
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| **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  - Diagnostics  - Lanuage analysis  - Biology  Flavour of AI – knowledge-based systems  - materials hub  - Philosophy of time-space  **Alexander**  **Huang** | High-level information structuring | Learn about a technology that is increasingly used |
| **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 state assumption for the fast part | Behaviour of numerical schemes | Ditto |
| 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 |
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| **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 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. | Logistics  Discrete-event dynamic systems / continuous systems | Nature of what is often called hybrid 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 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++ | Simulation systems,  wrappers | Multi-language environments. Questions like   * got an integrator in C++ want tu use Phython * 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 implementation using a simple plant, for example a stirred tank with a reaction. | Simulation systems |  |
| 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 |  |