TECHNISCHE UNIVERSITÄT DRESDEN

Fakulty of Architecture Institute of Building Climatology, Chair of Building Physics

Towards a Semi-Generic Simulation Framework for Mass and Energy Transport in Porous Media

Andreas Nicolai & John Grunewald
TU Dresden, Germany

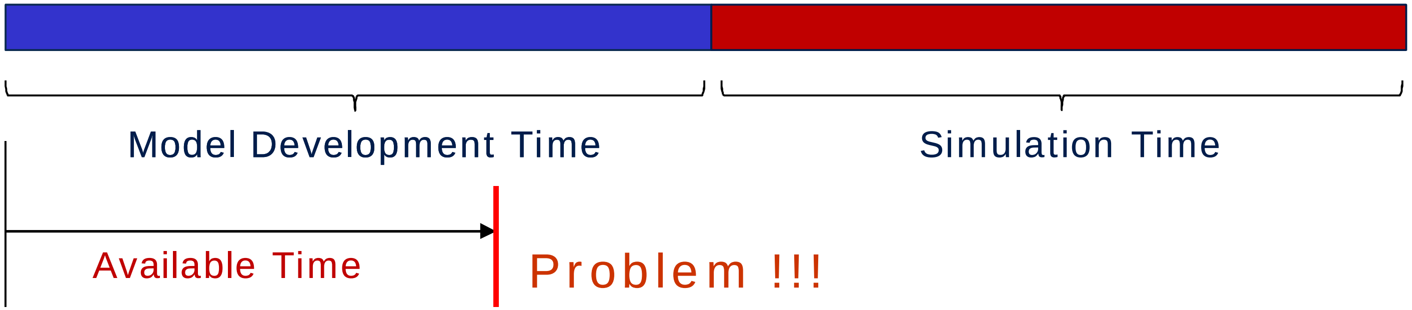
andreas.nicolai@tu-dresden.de

Tampere, 29th May – 3rd June

Motivation

#1 Reduction of Overall Project Time

A typical simulation model development project



Approach #1 (... *I'm a math software user* ...)

Approach #2 (... *I'm a coder and numerics guru* ...)

Approach #3 (... *I'm still writing code but I use a <u>suitable</u> framework*

Problem Solved ☺

Implies additional learning curve for using the framework

Motivation

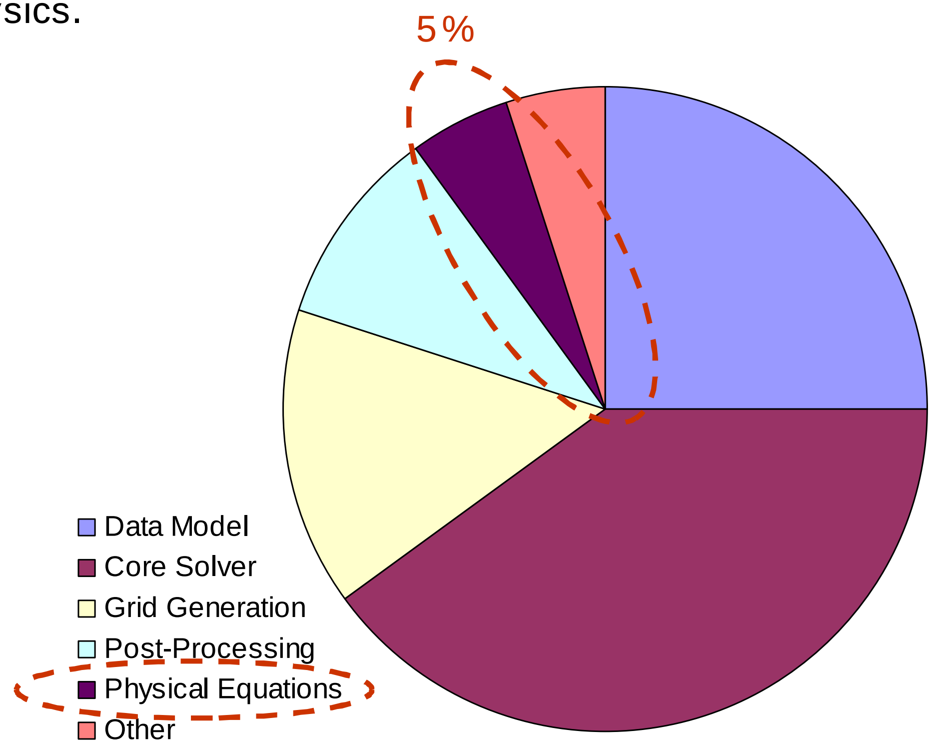
#2 Out-sourcing time-consuming tasks

Analysis of Development Time

We want to spent most of our research and development time with the actual physics.

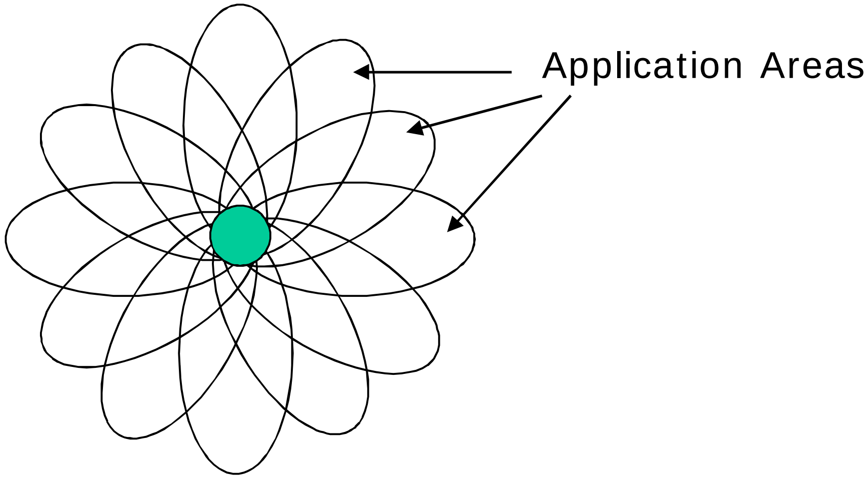
The rest is mostly overhead and COMMON to MANY projects!

Delegate overhead functionality to “others”



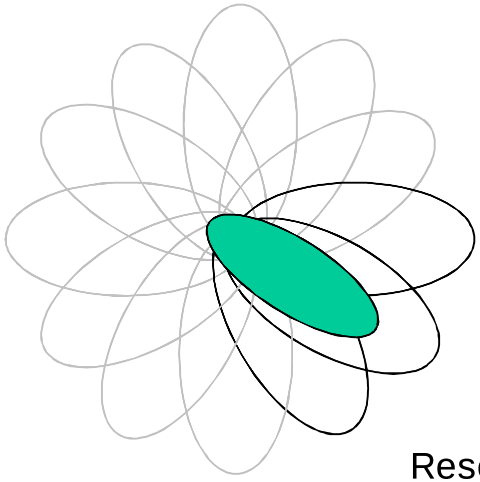
#1 What is "Semi-Generic"

A Generic Framework



Common Ground/Functionality

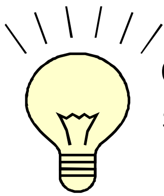
A Semi-Generic Framework



Research Areas:

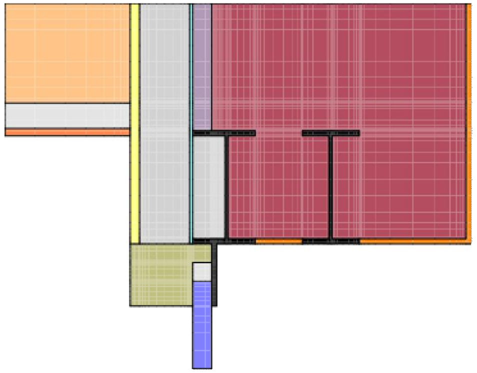
- Building Materials
- Soil Science
- Filter Technology
- ...

A suitable framework will provide most of the functionality that is necessary for the project.



Create a Framework specialized to transport modeling in porous media

Framework Introduction
#2 Scope/Limitations



Geometry

orthogonal 2D geometries (most problems can be modeled/approximated by orthogonal structures)

with arbitrary boundaries
non-adaptive grid
(user must do grid sensitivity studies manually)

Balances

coupled energy and mass balances (can be multiple energy and mass balances)

Spatial Discretization Method

Finite Volume Method, first-order upwind method for convection terms and second-order finite-difference approximation for diffusion terms
→ no equations leading to odd-even-point decoupling!!!

TECHNISCHE UNIVERSITÄT DRESDEN

Framework Details

#1 Components

Pre- and Post-Processing

- Flexible Grid generation
- Data model (very important for any non-trivial simulation model)
- User-Interface for Data Input (modeling efficiency)
- Input error checking (avoid unnecessary simulations because of input errors)
- Intelligent Post-Processing: Quick visualization of results including analysis/physical computations/unit conversion etc.

Numerical Method

- Non-linear Newton-Raphson iteration (very important for highly non-linear equations)
- Modified Newton-Raphson (very important for larger grids)
- Difference-Quotient Jacobian Generation (only need to implement physics in one place)
- Local error control (important for inverse modeling)
- Optimized grid numbering (minimizes bandwidth and LU factorization time)

Framework Details

#2 Separation of Physics and Numerical Details

Abstraction of Physical Model and Numerical Solver

Solver for Differential-Algebraic Equations

$$\frac{d\dot{\mathbf{y}}}{dt} = \mathbf{f}\left(t, \mathbf{y}\right) \qquad 0 = \mathbf{f}\left(t, \mathbf{y}\right)$$

$$0 = \frac{d\dot{\mathbf{y}}}{dt} - \mathbf{f}\left(t, \mathbf{y}\right)$$

$$0 = F\left(t, \mathbf{y}, \dot{\mathbf{y}}\right)$$

Solved by different numerical engines:
SUNDIALS:IDA, *IBK:ImplicitEulerDAE*

User-defined Physical Equations

States, Divergences, Residuals

Compute states, potentials, material properties in all elements from vector of unknowns

Internal and Boundary Fluxes

Compute mass and energy fluxes across all element-element interfaces and boundaries

Sources and Sinks

Compute divergences/residuals of mass/energy balance equations

Tasks for Model Developers

TECHNISCHE UNIVERSITÄT DRESDEN

Framework Details

#3 Separation of Model and Parameterization

Model Equations have Exchangeable Parameter Sets

Example: 1D Heat Conduction Equation

$$c_p \rho \frac{dT}{dt} = -\frac{\partial}{\partial x}\left[-\lambda \frac{\partial T}{\partial x}\right]$$

$$c_{p,i}\rho_i \frac{dT_i}{dt} = \frac{1}{\Delta x_i}\left[\lambda_{i,L}\frac{T_{i-1}-T_i}{\Delta x_{i,L}} - \lambda_{i,R}\frac{T_i - T_{i+1}}{\Delta x_{i,R}}\right]$$

Discretized Balance Equation
(Module: BEHeat)

$$q_{bc,L,\alpha} = \alpha_L \left(T_e - T_{s,L}\right)$$

Heat Conduction Boundary Condition
(Module: BCFluxHeatConduction)

- Material Database
- Boundary Condition Parameterization
- Climate Database
- Geometry Data Model

Provided by the Framework as Part of the Object Data Model

Framework Details

#4 Implementation Structure

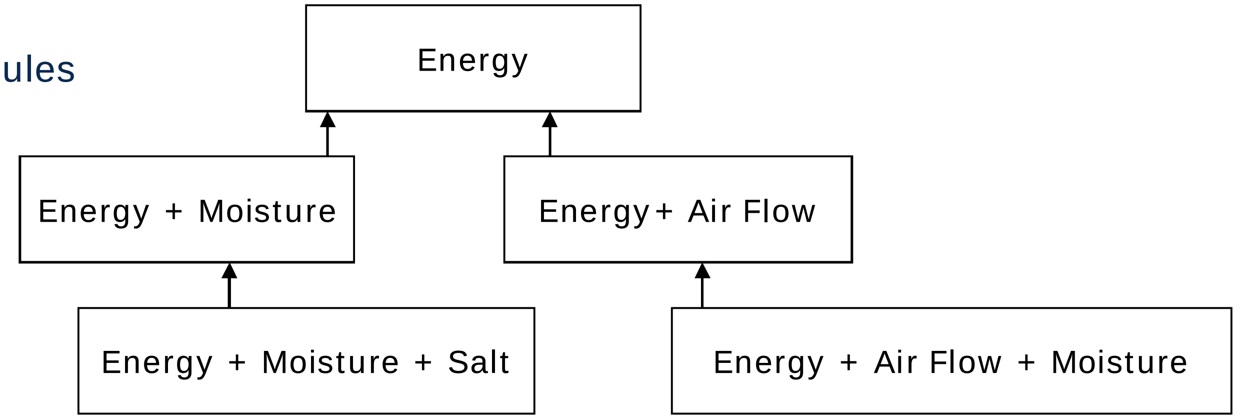
Split User-Code into Different Modules

- Balance Equations
- Material Functions
- Climatic Loads
- Flux Computation
- Source Computation

Use Object-Oriented Programming

Example:
Balance Equation Modules

Common functionality is inherited by extended modules



Work in Progress

Current State and Planned Work

Current State of Implementation

- ✔ DELPHIN 5 User Interface used as pre-processing/grid-generation tool
- ✔ DELPHIN 5 Post-Processing used for results analysis
- ✔ New extendible data model developed and implemented
- ✔ Solver framework ready with first modules (Heat and Moisture only) ported from DELPHIN 5

Work-in-Progress

- Porting existing functionality from DELPHIN 5 to new modular framework
- Extending new air flow model → *Cooperation with KU Leuven*
- VOC/Pollutant model and filter design model → *Cooperation with Syracuse University*
- Ice crystallization model
- Re-write of User Interface (→ D6) to fully support modular concept

TECHNISCHE UNIVERSITÄT DRESDEN

Fakulty of Architecture Institute of Building Climatology, Chair of Building Physics

Towards a Semi-Generic Simulation Framework for Mass and Energy Transport in Porous Media

Andreas Nicolai & John Grunewald
TU Dresden, Germany

andreas.nicolai@tu-dresden.de

Tampere, 29th May – 3rd June