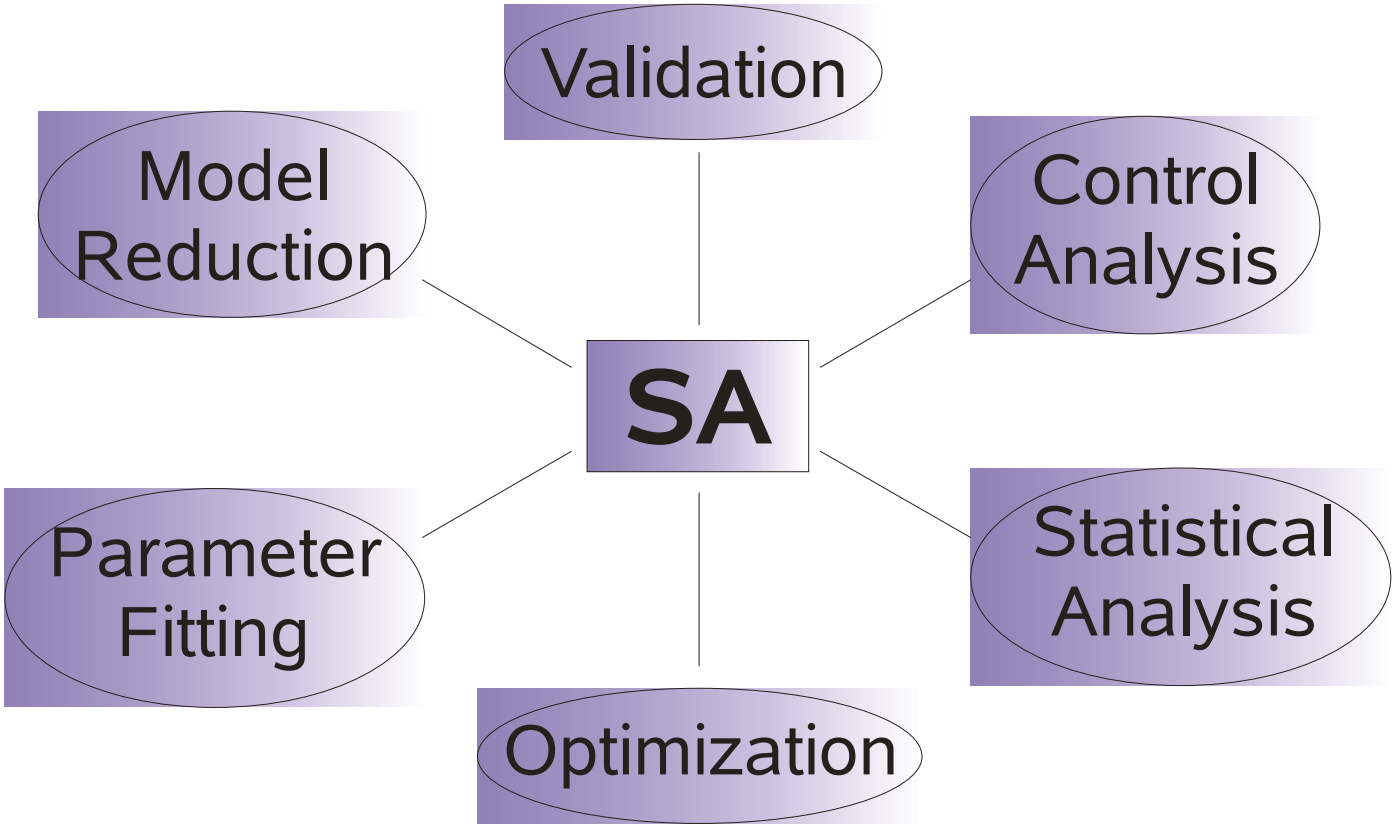
Poster-Session

- **Roland Reichardt**
  - Simulation of Mechanical Alloying
- **Thomas Haschke**
  - Numerical Simulation of the Evaporation of Solute Droplets on Polymer Polymer Substrates
- **Marc Kalkuhl**
  - Generation of synthetic SAR-rawdata - Problems and Methods
- **Frieder Hadlich**
  - Simplification of Biochemical Network Models
- **Attiya Elsheikh**
  - Automatic Differentiation of Modelica Models
- **Michael Weitzel**
  - The Topology of Metabolic Isotope Labeling Networks

Why Sensitivity Analysis?



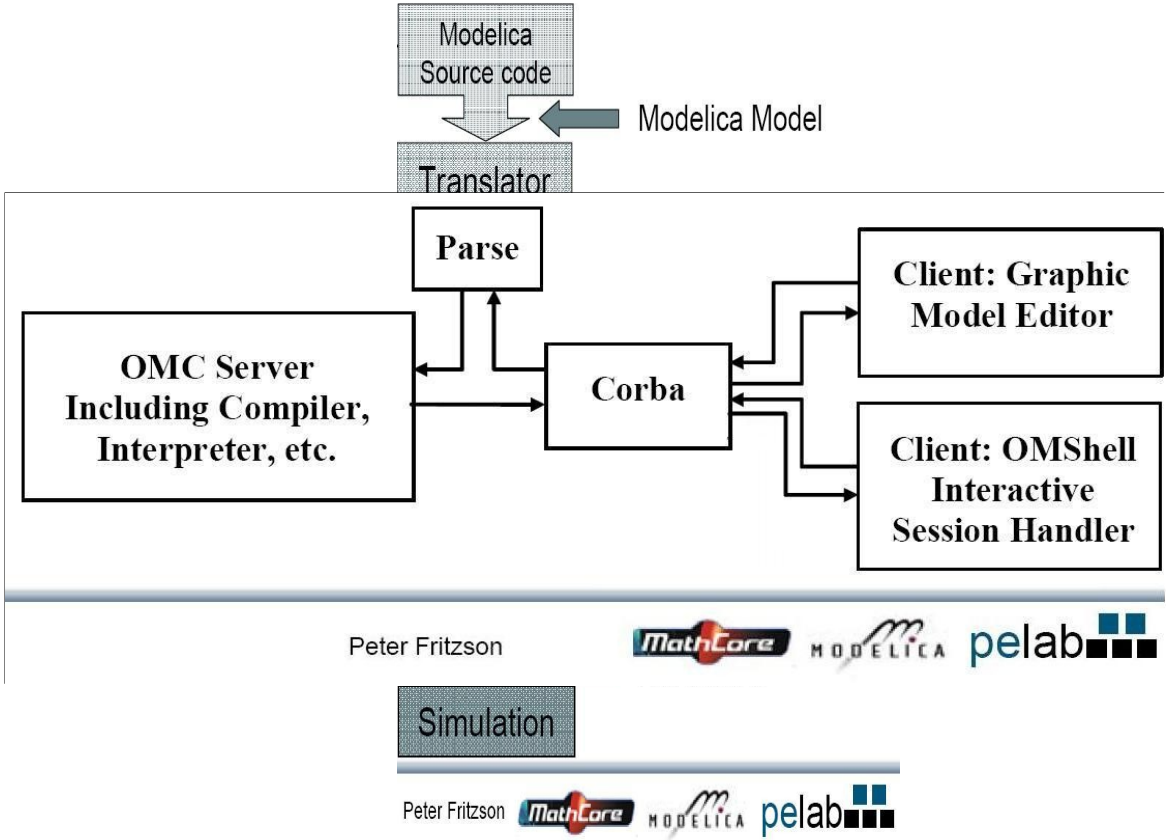
Modeling with Modelica

$$S_1 + S_2 \rightarrow P \equiv$$

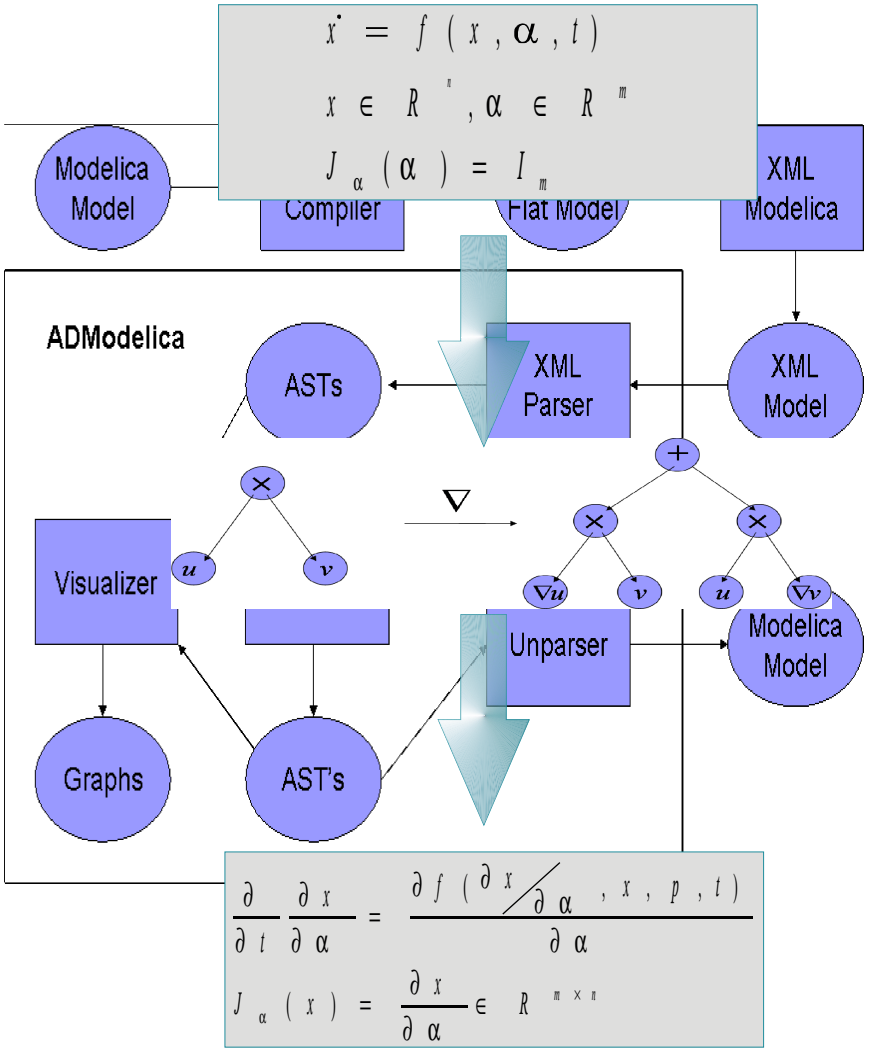
```
connector Metabolite
    Concentration C;
    Parameter Integer M,N;
    Reaction Rin[N]   "in  reactions";
    Reaction Rout[M] "out reactions";
equation
    der(C) = sum(Rin.v) - sum(Rout.v);
end Metabolite;

connector Reaction
    ReactionRate v;
    Parameter Integer M,N;
    Metabolite S[N] "substrates";
    Metabolite P[M] "products";
    Parameter Real alpha;
    ... // other parameters
equation
    v = ... ; // a kinetic formula
end Reaction;
```

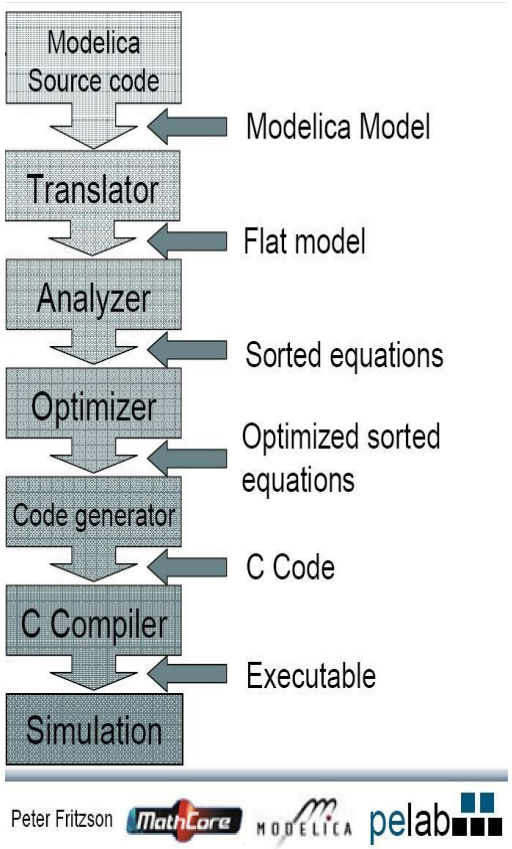
```
Model BiUniReaction
    Metabolite S1 (N=0,M=1,C=1);
    Metabolite S2 (N=0;M=1,C=1);
    Metabolite P(N=1,M=0,C=0);
    Reaction   r(N=2,M=1,pplus=.5,pneg=.5);
end
    connect(S1 , r.S[1]);
    connect(S2 , r.S[2]);
    connect(P , r.P[1]);
    connect( r, S1.Rout[1] );
    connect( r, S2.Rout[1] );
    connect( r, P.Rin[1]);
end BiUniReaction
```

OpenModelica Environment



ADModelica


$\dot{x} = f(x, \alpha, t)$
$x \in R^n, \alpha \in R^m$
$J_\alpha(\alpha) = I_m$
Modelica Model
Compiler
Flat Model
XML Modelica
ADModelica
ASTs
XML Parser
XML Model
Visualizer
Unparser
Modelica Model
Graphs
AST's
$\frac{\partial}{\partial t}\frac{\partial x}{\partial \alpha} = \frac{\partial f(\partial x/\partial \alpha, x, p, t)}{\partial \alpha}$
$J_\alpha(x) = \frac{\partial x}{\partial \alpha} \in R^{m \times n}$


Modelica Source code
Modelica Model
Translator
Flat model
Analyzer
Sorted equations
Optimizer
Optimized sorted equations
Code generator
C Code
C Compiler
Executable
Simulation
Peter Fritzson
MathCore
MODELICA
pelab