

Modeling with Partial Differential Equations – Modelica Language Extension Proposal

Jan Šilar¹ Kristian Stavåker² Marek Mateják¹ Pavol Privitzer¹ Jozef Nagy³

¹First Faculty of Medicine Charles University Prague, Czech Republic

²Department of Computer and Information Science Linköping University Linköping, Sweden

³Prague, Czech Republic

OpenModelica Workshop 2014

ODE and PDE



	ODE	PDE
examples	vibrating mass	vibrating string
	$\frac{d^2x}{dt^2} + kx = 0$	$\frac{\partial^2 u}{\partial t^2} - q \frac{\partial^2 u}{\partial x^2} = 0$
Unknown	function of 1 variable	multi-variable function
(solution)	(here time)	(here time, space coordinate)
derivatives	the only variable <i>dt</i>	at least two variables $\partial t, \ \partial x, \$
conditions	initial	initial and boundary

PDE handling in the context of Modelica



- PDEs are not supported in the Modelica standard
- Approaches to unifying PDE modeling with Modelica exist
- Chapter in Peter Fritzson's Modelica book[1]
- Levon Saldamli proposed in his PhD thesis [2]
 - support for PDE on language level
 - language extension not complete
 - not supported in OM and other tools

We continue this work and propose some modifications and further extensions.

Example – 3D heat transfer with source and PID antrol

- heat transfer in a room
- in middle of right wall temperature sensor
- left wall heating
- PID controller



Mathematical model of heat transfer



PDE:

IC:

$$\begin{aligned} \frac{\partial T}{\partial t} - \alpha \cdot \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) &= 0 \\ \text{IC:} & T(0, x, y, z) &= a - kx \\ \text{BC for left wall (heating)} & \frac{\partial T}{\partial \vec{n}}(t, 0, y, z) &= -\beta \frac{P}{l_x l_y} \\ \text{BC for other walls (insulated)} & \frac{\partial T}{\partial \vec{n}} &= 0 \quad \text{on remaining walls} \end{aligned}$$

BC for left wa

T. temperature – field t, x, y, z ... time and space coordinates l_x, l_y, l_z ... dimensions of the room P ... power of heating \vec{n} ... normal vector of the boundary

Mathematical model of PID controller and heatin



heat sensor

$$T_{s} = T\left(l_{x}, \frac{l_{y}}{2}, \frac{l_{z}}{2}\right)$$

PID controller and heating - ODE

$$e = T_d - T_s$$

$$P = k_p e + k_i \int_0^t e(\tau) d\tau + k_d \frac{d}{dt} e$$

 T_s .. temperature of the sensor placed in middle of the right wall

Modelica model

model heatPID



```
class Room
    extends DomainBlock3D;
    RegionOD sensorPos(shape=shapeFunc, range={{1,1},
                                    \{0.5, 0.5\}, \{0.5, 0.5\}\};
  end Room
  parameter Real lx = 4, ly = 6, lz = 3;
  Room room(Lx=lx, Ly=ly, Lz=lz);
  parameter Real T 0 = {a-k*room.x in room.interior};
  field Real T(domain = room, start = T 0);
 Real Ts, P, eInt;
  parameter Real kp, ki, kd, Td, a, k, alpha, beta;
equation
  pder(T,time) - alpha*(pder(T,x,x) + pder(T,y,y)
                + pder(T,z,z)) = 0 in room.interior;
  pder(T,region.n) = -beta*P/(lx*ly) in room.left;
  pder(T, region.n) = 0 in room.right room.front,
    room.rare, room.top, room.bottom;
 Ts = T in room.sensorPos;
  e = Td - Ts;
  der(eInt) = e;
  P = kp*e + ki*eInt + kd*der(e);
end heatPid:
```

Domain



- We have to represent the room and it's boundaries.
- Subsets of space (1D, 2D or 3D) where fields are defined, equations hold and calculations are performed we call domain.
- There is new built-in type Domain:

```
type Domain

parameter Integer ndim;

replaceable Region interior;

replaceable function shape

input Real u[ndim-1];

output Real coord[ndim];

end shape;

end Domain;
```

- All domains extends this built-in type
- Domain contains regions representing its interior and boundaries. region is also new built-in type.
- Shape-function maps real intervals onto regions and thus defines them (idea from Peter's Book [1]).

Domain example



```
class DomainBlock3D
  extends Domain(ndim=3);
  parameter Real Lx, Ly, Lz, ax, ay, az;
  Coordinate x, y, z ;
  coord = \{x, y, z\}:
  redeclare function shape //impure - not supported
    input Real vx, vy, vz;
     output Real x=ax+Lx*vx, y=ay+Ly*vy, z=az+Lz*vz;
  end shape;
  Region3D interior(shape=shape, interval=\{\{0,1\},\{0,1\},\{0,1\}\});
  Region2D left(shape=shape, interval=\{0, \{0,1\}, \{0,1\}\});
  Region2D bottom(shape=shape, interval=\{\{0,1\},\{0,1\},0\});
  ... //right, top, front, rear
end DomainBlock3D:
```

other options to define domains exist

Coordinates



We used coordinate variables to determine position of points in the room.

Coordinates

- are independent variables (such as time in current Modelica)
- fields are functions of coordinates
- fields may be differentiated with respect to coordinates
- need spacial handling in compiler and runtime

New modifier coordinate - to define coordinates. Usage e.g.

```
coordinate Real x(name="cartesian");
```

The type should be always Real.





Temperature in the room is a field variable

• its value dependes on time and space position (multi-variable function)

new modifier field to define fields, usage e.g.

field Real T(domain=room);

- modelica built-in types or types derived from them allowed only
- domain mandatory attribute to determine definition domain

Field – literal constructor, accessing value



• to set initial value of the temperature, field literal constructor is needed

field parameter Real T_0 = {a-k*room.x in room};

- T_0 is a field constant in time
- its domain is room
- its value is given by the expression depending on the x coordinate
- We have to access value of temperature in the point where the temperature sensor is placed.

T_sensor = T in room.sensorPosition;

- T is field, T_sensor not
- sensorPosition is of type RegionOD represents the point

in – domain and region specification keyword



- in keyword is used also in PDEs and BC to determine on which region (boundary) they hold.
- default region is interior, if it is not specified

```
field Real T, W;
Real T_sensor;
parameter Real lambda, T_out;
Room room; //3D domain, has OD region sensorPosition
equation
W = -lambda*grad(T) in room; //= room.interior (PDE)
pder(T,room.right.n) = 0 in room.right; //BC
T_sensor = T in room.sensorPosition;
//(nonfield-field)
```



We need partial differential operators that are used in PDEs and BCs.

• New pder operator:

pder(u,time) $\sim \frac{\partial u}{\partial t}$, pder(u,room.x) $\sim \frac{\partial u}{\partial x}$, pder(u,room.x,room.y) $\sim \frac{\partial^2 u}{\partial x \partial y}$

- normal derivative (often in BC) pder(u,room.n) $\sim \frac{\partial u}{\partial \vec{n}}$
 - n (normal vector) implicit member of all regions of dimension n – 1 in n-dimensional domain
- vector differential operators gradient, divergence, curl are defined

Accessing coordinate variables



Fields and equations are located outside domain class.
 Coordinates (and normal vector) inside – in equations must be accessed using "."

```
pder(u,omega.x) = 0 in omega.interior;
v*omega.left.n = 0 in omega.left;
```

- One possible shortcut would be to use new keywords dom and reg to refer the domain, resp. region specified with in. E.g.
 pder(u,dom.x) = 0 in omega.interior; v*reg.n = 0 in omega.left;
- Other option allow access coordinates directly without specification of the domain:

pder(u,x) = 0 in omega.interior; v*n = 0 in omega.left;

• if a variable of a same name exists, it has preference and the coordinate must be accessed with "." anyway

Changes over previous extensions - domains



- Domains
 - previously described by defining its boundaries using shape-function. It works well in 2D, but doesn't work in 3D.
 E.g. to build-up the domain on the picture below, it is hard to find shape-functions generating incomplete intersecting square sides and sphere.



• we suggest to use one shape-function to parametrize interior and all boundaries. Complex geometries define in some other way (CSG, import from CAD). Changes – coordinates, in operator, accessing fields



- Coordinates
 - previously no special syntax to define them. There are two predefined arrays for coordinate systems in built-in type domain.
 - we suggest new modifier coordinate to define coordinates so that user can define any number of coordinate systems.
- in operator
 - previously used only in BCs and filed literal constructor
 - we suggest to use it also in PDEs and equations relating field and non-field variables (explained in next point)
- accessing field values in particular point
 - originally in function-like style, e.g. T(1.3, 9.1, 4.7)
 - we suggest to disable this, as it is also not possible to access regular variable in particular time in this way. Use in operator with region of type Region0D to represent the point instead.

Changes – field literal constructor, start values of derivatives



- field literal constructor
 - originally e.g. u = {2*a+b for (a,b) in omega}, where iterator variables (a,b) exist only in constructor expression and represent coordinates in omega. But which coordinate do iterator variables represent if there are more coordinate systems in omega?
 - we suggest u = {2*omega.x+omega.y in omega.interior} instead, where omega.x and omega.y are already defined in omega.
- start value for derivatives of a field
 - higher derivatives of fields are allowed, thus we need to assign initial values to derivatives. We suggest new attributes of a field variables startPrime and startSecond to set start value for first and second derivative. Prospective even higher derivatives must be initialized in initialEquation section.

Changes – differential operators, normal vector, accessing coordinate variables



- differential operators
 - previously der(u) $\sim \frac{\partial u}{\partial t}$, der(u,x) $\sim \frac{\partial u}{\partial x}$
 - we suggest pder(u, time) $\sim \frac{\partial u}{\partial t}$, pder(u, x) $\sim \frac{\partial u}{\partial x}$
- normal vector
 - previously member of domain
 - now member of regions of dimension n-1 in n-dimensional domain i.e. plane in 3D, curve in 2D and points in 1D.
- accessing coordinate variables
 - two possible shortcuts to access coordinates in equations

Conclusions and future goals



- we studied previous extensions
- proposed few changes to eliminate some weaknesses
- added some new extensions

Presented extension – merge of previous and new extensions. What next?

- complete the extension (still several open problems)
- implement support (by compiler, runtime, solver) in OpenModelica (during my PhD implement at least 1D models)
- attempt to standardize it



New ideas welcome.

Thank you.

Bibliography



Peter Fritzson.

Principles of Object-Oriented Modeling and Simulation with Modelica 2.1. Wiley-IEEE Press, 2004.

Levon Saldamli.

A High-Level Language for Modeling with Partial Differential Equations.

PhD thesis, Department of Computer and Information Science, Linköping University, 2006.