Open Source, component based simulation software development using Orcan

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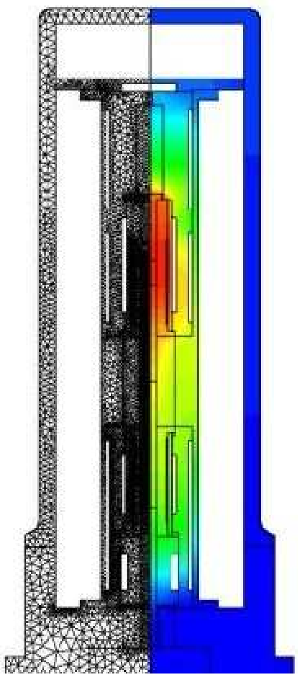
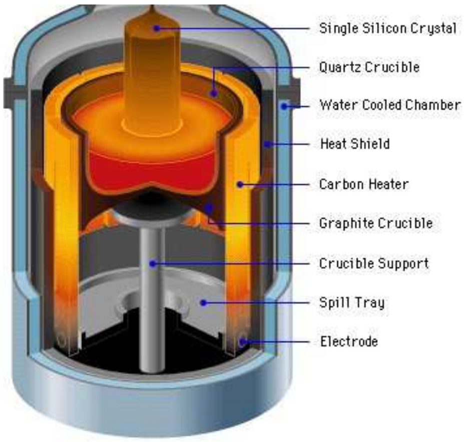
Fraunhofer-Institute IISB, Erlangen

- Development and analysis of crystal growth processes (Si, InP, GaAs, CaF2, oxide crystals, ...)
- Experiments + Simulation
- CrysVUn: TMT for the user support program of the MSL



Background of ORCAN development:

- need to be able to simulate radiative heat transfer in complex 3D geometries – including volume effects (absorption, scattering), and different surface effects (diffuse/ specular reflection, ...), e.g. for optical crystals, szintillators, ...



Options:

- Use a commercial CFD-code ?

  +? most is already done... (however, radiation models are weak)
  - you don't know what is going on behind the scenes
  - difficult to extend
  - expensive, take a lot of learning time: have to select one, and stick to it

- Develop your own proprietary code ?

  - beyond our possibilities: we cannot do everything needed

- Use the wealth of existing open source tools: mesh generators, solvers, geometry handling, visualizations, ...

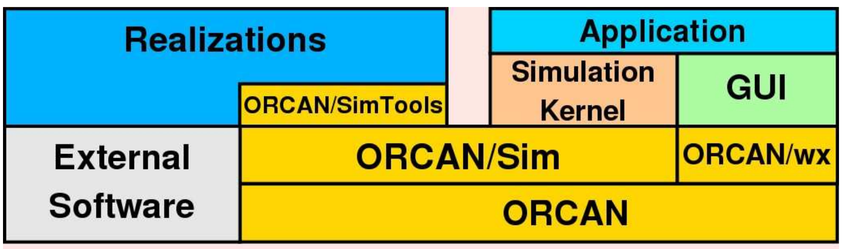
  \+ its free ..
  \+ source code available -> possibility to check what is really done, and to extend the code
  \- no common interfaces: some common software infrastructure needed
  ? how to finance yourself ?
  \- no guaranteed support

Decision:

Create a framework, which hopefully can serve as basis for our future software development:

- separate the task into clearly distinguished components
- easily exchange these components, even on runtime
- allow independent development of components at different sites by clear interface specifications
- no intrinsic dependency on other packages (just C++), platform independent
- supports and simplifies creation of GUI's
- Open Source, in the hope to initiate an exchange of components with other working groups

Open **R**eflective **C**omponent **A**rchitecture

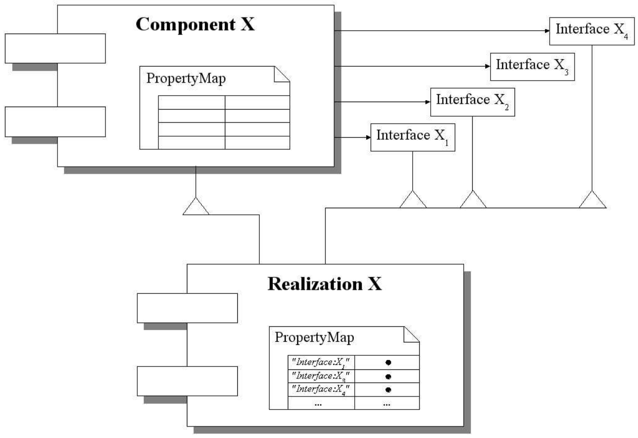


ORCAN: application-independent component management: ObjectServer handles component creation and deletion

Orcan/Sim: a set of component and interface specifications specific for CFD-style simulation applications

Orcan/Wx: a library based on WxWidgets, allows automatic creation of GUI elements based on XML-descriptions, exploiting the reflexivity of Orcan components

Orcan/SimTools: frequently used tools, e.g. polygon class, parsers what is a ''component'' ?



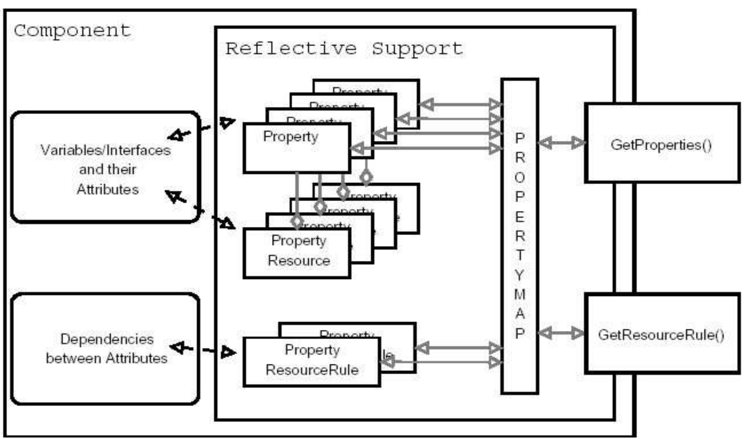
e.g. Mesh component

mandatory interface:	''IMeshCreate" -> functions to build a mesh
optional interface:	''IMeshChange'' -> functions to modify (e.g. refine) an existing mesh

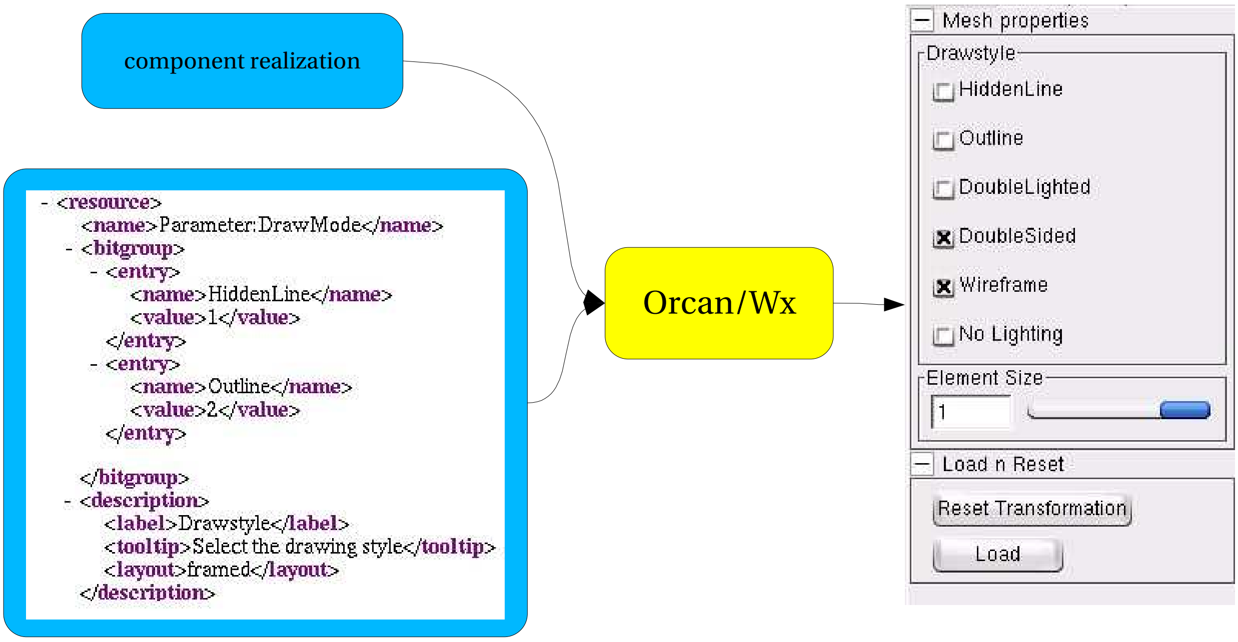
Reflexivity

via an associated ''PropertyMap'', each component realization can be queried for implemented interfaces and specific parameters

Each ''Property'' has associated ''Resources'' and ''Rules'', which are specified in a realization-specific XML file



GUI generation



some currently existing components and realizations:

Geometry — read, e.g. from CAD, perform shape healing,deliver a polygonal appoximation
OCCGeometry: a realization based on OpenCASCADE

Surf/VolMesh — surface and volume meshes, dynamic attributes
SimpleSurfMesh / SimpleVolMesh: own implementations
VtkUGrid: using the VTK mesh implementation

VolMeshGen — volume mesh generation from surface mesh as input
VolMeshGenTetgen: using Tetgen
VolMeshGenGmsh: using Gmsh

Surf/VolMesh Reader/Writer — several formats already available, list is constantly expanding

Visualization — Visualization of scalar or vector attributes on surface or volume meshes
VtkMeshVisualization: using the Visualization Toolkit (VTK)

components and realizations, continued

PDEDiscretizer Discretization of partial differential equations, input: VolMesh and LESSolver
FEMLaplace: discretization of temperature equation using finite element method by J. Haerdtlein, Computer Science 10, University Erlangen/Nuernberg

LESSolver linear equation solver, offers aninterface to build and fill a matrix, and to solve the system
LaspackSparseSolver: uses the Laspack library

MeshCoupling functionality to extract sub-meshes, interpolate/ transfer data between different meshes
SimpleMeshInterpolator (own implementation)
SimpleMeshCoupling (own implementation)

components and realizations, continued

PhotonMapper An efficient ray/tracing based Monte Carlo Method for thermal radiation, capable to take into account basically any effect (different emission/reflection models, absorption, scattering, ...

GPURad radiosity computation with hierarchical clustering and hardware-assisted (GPU) viewfactor computation

Getting component realizations:

```
ocs::VolMeshRef mesh = ocs::VolMesh::New()

ocs::VolMeshRef mesh = ocs::VolMesh::New(“SpecificImplementation”)
```

or: query available implementations, and select one which implements a required interface

Using interfaces:

```
if(mesh.I.TopologyPtr) {
    mesh.I.TopologyPtr->GetNeighbourElements(...)
```

accessing parameters:

```
oc::PropertyMap::iterator r = mesh.GetProperties().begin()
```

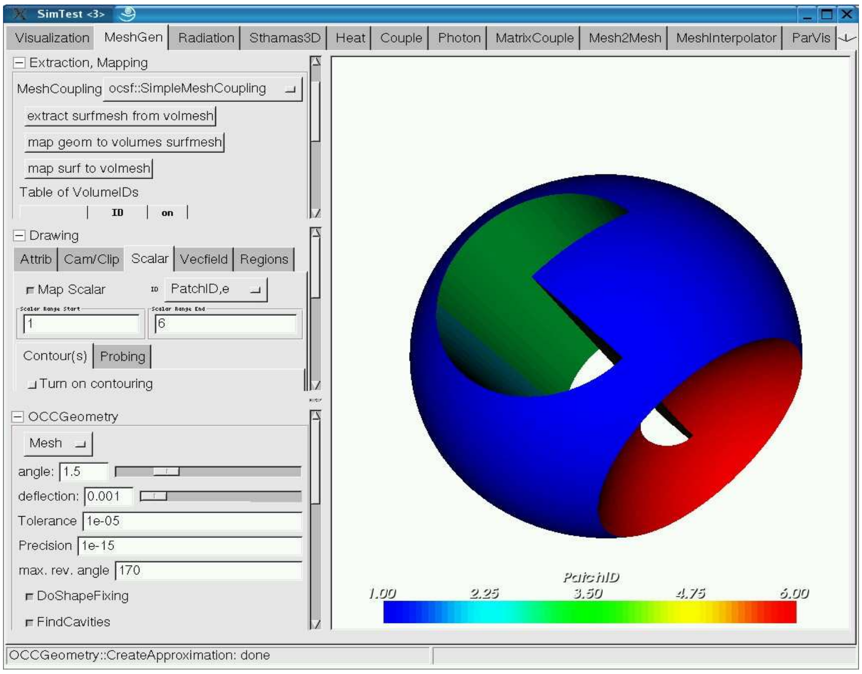
-> iterate over properties, get names and types, modify

a minimalistic, but working, application (showing Commands):

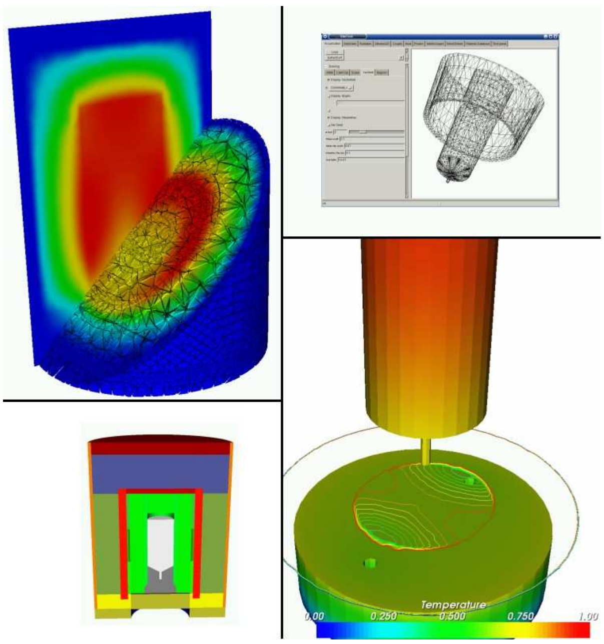
```
#include <ocs/SurfMesh.hh>
#include <ocs/SurfMeshWriter.hh>


int main(int argc, char** argv) {
   ocs::SurfMeshRef surfmesh= ocs::SurfMesh::New();
   oc::File infile("inputfile");
   ocs::SurfMeshReaderRef reader =
                       ocs::SurfMeshReader::New("ocsf::SurfMeshBinaryReader");
   reader.SetInput(infile);
   reader.SetOutput(surfmesh);
   reader.Execute();

   ocs::SurfMeshWriterRef writer =
                       ocs::SurfMeshWriter::New("ocsf::SurfMeshUnvWriter");
   writer.SetInput(surfmesh);
   reader.SetOutput(“outputfile);
   reader.Execute();

  return 0;
```

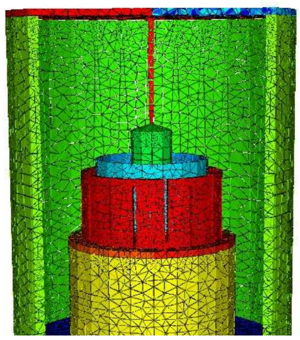
SimTest

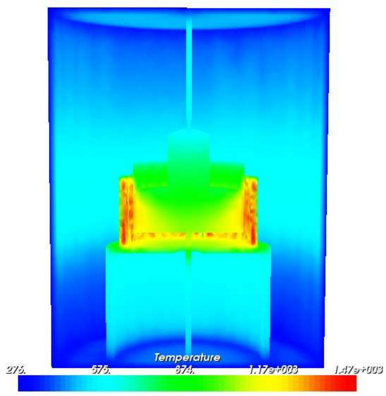
an example- and component testing application

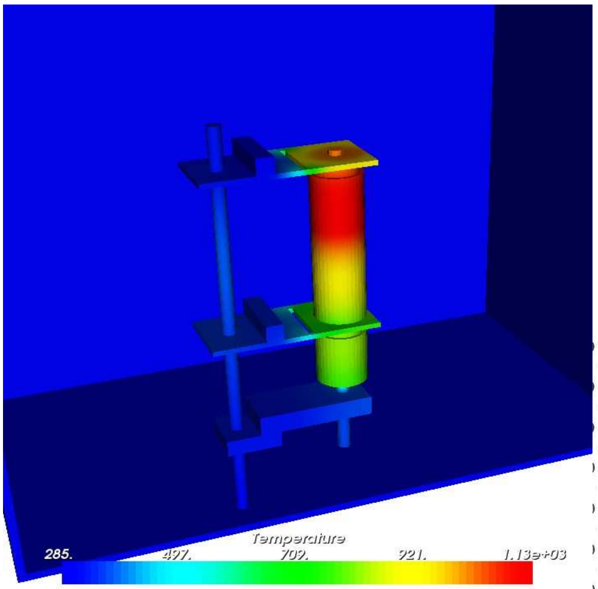


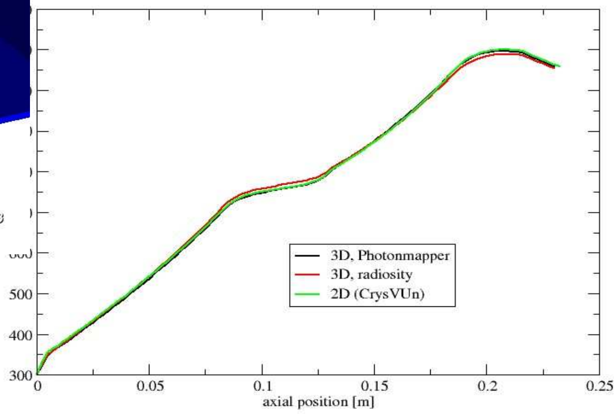
colorful pictures: coupled conducion + radiation











<u>currently used external components/tools/libraries:</u>

- OpenCASCADE (www.opencascade.com) : Geometry handling, shape healing, Cad import
- Vtk (Visualization Toolkit, www.kitware.com) Visualization of mesh data
- Laspack (www.tu-dresden.de/ mwism/skalicky/laspack/laspack.html): sparse matrices, LES solver
- Finite Element discretization from LSS 10
- WxWidgets (www.wxwidgets.com) platform-independent GUI-toolkit

<u>grid generators:</u>

- Gmsh (www.geuz.org/gmsh)
- Tetgen (tetgen.berlios.de)
- Netgen (www.hpfem.jku.at/netgen/)
- noffset3d (http://www.synopsis.com/products/tcad/tcad.html)

Work in progress:

- generic coupling with other solvers

  Block-Newton coupling:
  H.G. Matthies, J. Steindorf: Partitioned but stronlgy coupled iteration schemes for nonlinear fluid-structure interaction *Computers and Structures 80 (2002) 1991-1999*

$$\begin{pmatrix} D_x f(x,y) & D_y f(x,y) \\ D_x g(x,y) & D_y g(x,y) \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = -\begin{pmatrix} f(x,y) \\ g(x,y) \end{pmatrix}$$

$$f(x,y) = x - F(x,y) = 0$$

$$D_x f(x,y) \approx \frac{f(x+\Delta h, y) - f(x,y)}{h}$$

$$g(x,y) = y - G(x,y) = 0$$

still work in progress:

- integration of OpenFOAM (www.opencfd.co.uk/openfoam/) via coupling interface

  OpenFoam (Open Field Operation and Manipulation) is a VERY impressive set of C++ libraries for very general CFD and multiphysics simulations

- Extension of the Photon Mapping module to participating media (absorption, refraction, scattering, ..)

Conclusions

- Framework itself is set up and in a quite stable state
- Possibility to build useful applications has been demonstrated

Outlook

- load modules across network – GRID integration ???
- convince some more people to use it, and exchange components
- Orcan will not be the last say ... but we believe that the future in numerical simulation will belong to modular and open systems

This work was supported by the German Federal Ministry of Education and Research (BMBF)
Grant Number 0327324A