An Introduction to the OOMMF eXtensible Solver Class Architecture

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1901-2001
NIST CENTENNIAL

The

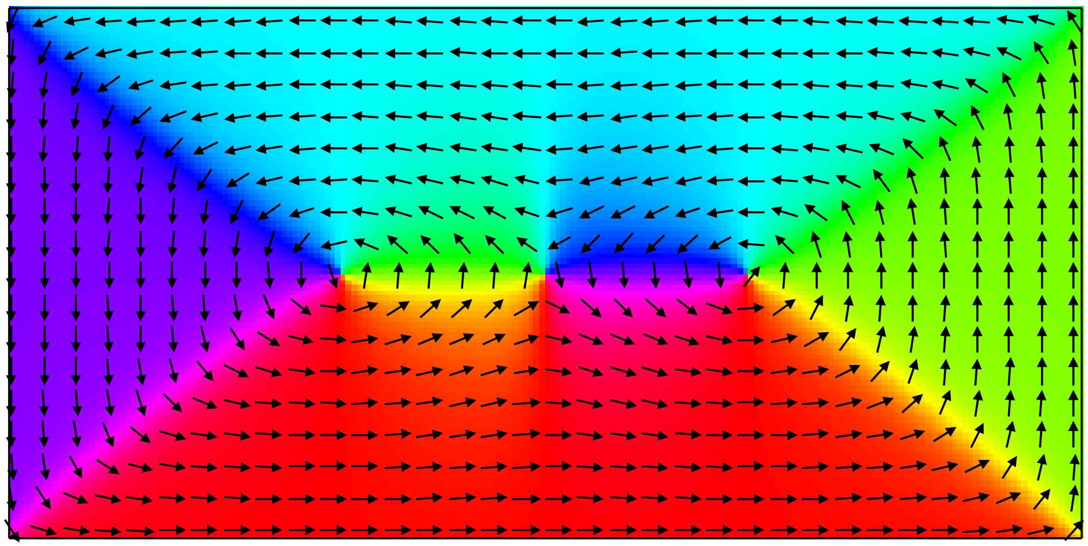
OOMMF

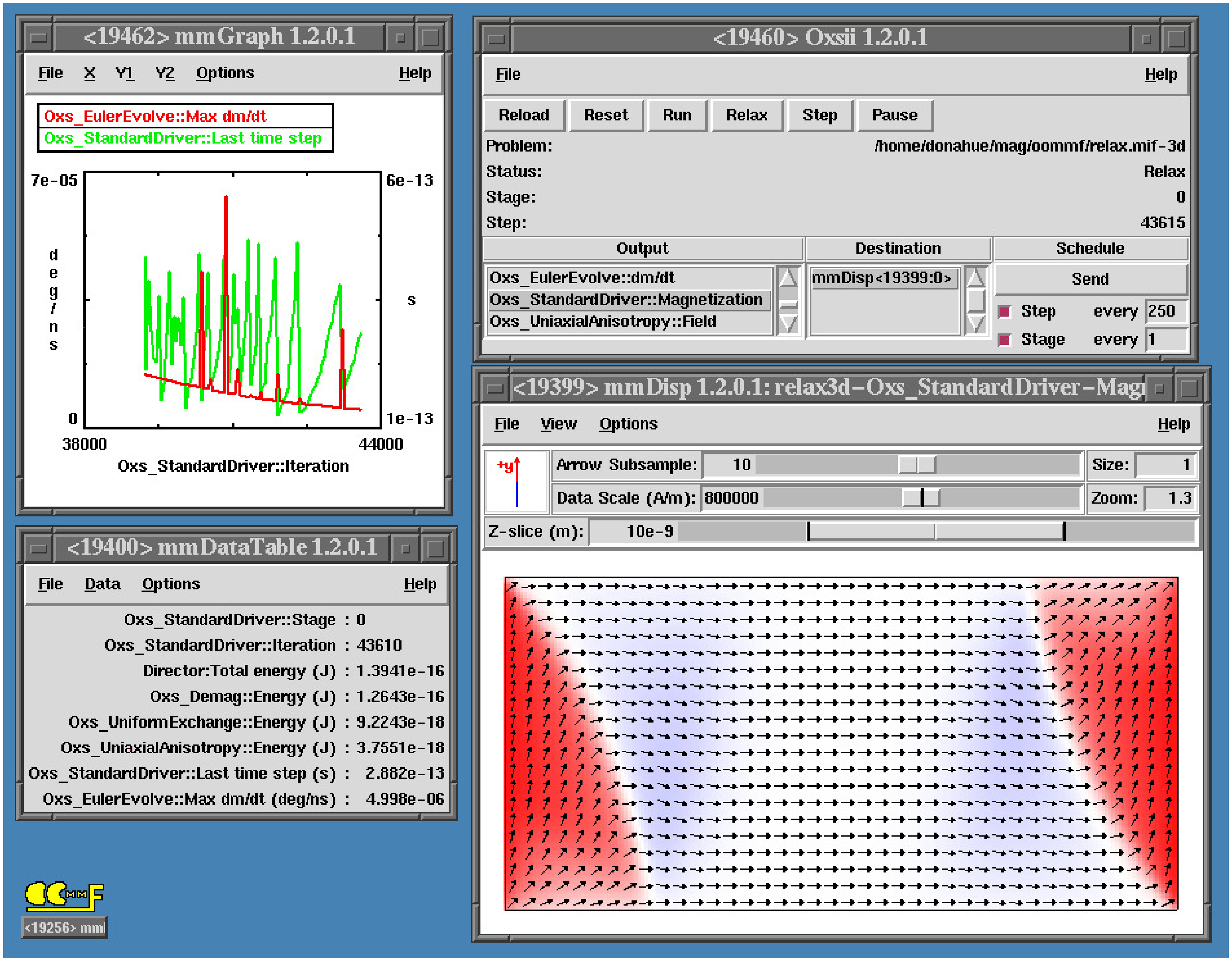
eXtensible

Solver

Remanent Magnetization

1 μm $\times$ 0.5 μm $\times$ 5 nm





<19462> mmGraph 1.2.0.1
File X Y1 Y2 Options Help
Oxs_EulerEvolve::Max dm/dt
Oxs_StandardDriver::Last time step
7e-05
6e-13
deg/ns
s
0
1e-13
38000
44000
Oxs_StandardDriver::Iteration
<19460> Oxsii 1.2.0.1
File Help
Reload Reset Run Relax Step Pause
Problem: /home/donahue/mag/oommf/relax.mif-3d
Status: Relax
Stage: 0
Step: 43615
Output
Destination
Schedule
Oxs_EulerEvolve::dm/dt
Oxs_StandardDriver::Magnetization
Oxs_UniaxialAnisotropy::Field
mmDisp<19399:0>
Send
Step every 250
Stage every 1
<19399> mmDisp 1.2.0.1: relax3d-Oxs_StandardDriver-Mag
File View Options Help
Arrow Subsample: 10
Size: 1
Data Scale (A/m): 800000
Zoom: 1.3
Z-slice (m): 10e-9
<19400> mmDataTable 1.2.0.1
File Data Options Help
Oxs_StandardDriver::Stage : 0
Oxs_StandardDriver::Iteration : 43610
Director:Total energy (J) : 1.3941e-16
Oxs_Demag::Energy (J) : 1.2643e-16
Oxs_UniformExchange::Energy (J) : 9.2243e-18
Oxs_UniaxialAnisotropy::Energy (J) : 3.7551e-18
Oxs_StandardDriver::Last time step (s) : 2.882e-13
Oxs_EulerEvolve::Max dm/dt (deg/ns) : 4.998e-06
<19256> mml

Testbed Systems

Platform	Compilers
AIX	VisualAge C++ (xlC), Gnu gcc
Alpha/Compaq Tru64 UNIX	Compaq C++, Gnu gcc
Alpha/Linux	Compaq C++, Gnu gcc
Alpha/Windows NT	Microsoft Visual C++
HP-UX	aC++
Intel/Linux	Gnu gcc
Intel/Windows NT, 95, 98	Microsoft Visual C++, Cygwin gcc, Borland C++
MIPS/IRIX 6 (SGI)	MIPSpro C++, Gnu gcc
SPARC/Solaris	Sun Workshop C++, Gnu gcc

Micromagnetic Equations

Landau-Lifshitz-Gilbert:

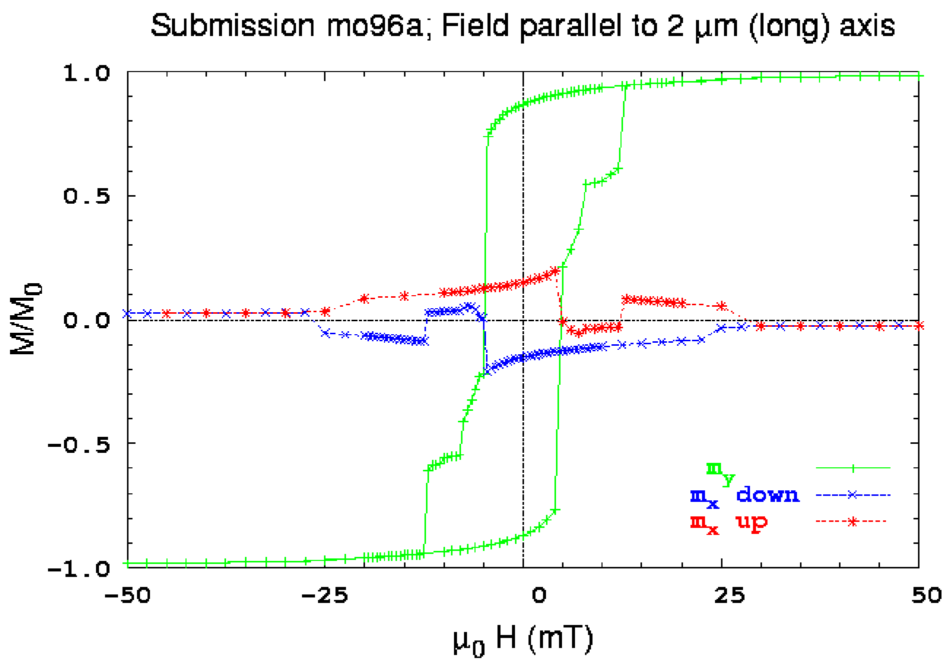
$$\frac{d\mathbf{M}}{dt} = \frac{-\omega}{1+\lambda^2}\mathbf{M}\times\mathbf{H}_{\text{eff}} - \frac{\lambda\,\omega}{(1+\lambda^2)M_{\text{s}}}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})$$

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0}\frac{\partial E_{\text{density}}}{\partial \mathbf{M}}$$

Energies:

$$\begin{aligned}
E_{\text{exchange}} &= \frac{A}{M_s^2}\left(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2\right) \\
E_{\text{anis}} &= \frac{K_1}{M_s^4}(M_x^2 M_y^2 + M_y^2 M_z^2 + M_z^2 M_x^2) \\
E_{\text{demag}} &= \frac{\mu_0}{8\pi}\mathbf{M}(r)\cdot\left[\int_V \nabla\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\,d^3r' \right. \\
&\qquad \left. - \int_S \hat{\mathbf{n}}\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\,d^2r'\right] \\
E_{\text{Zeeman}} &= -\mu_0\mathbf{M}\cdot\mathbf{H}_{\text{ext}}
\end{aligned}$$

Hysteresis Loop Calculations




```
FOR i = 1 to N
   Apply external field i
   WHILE(not equilibrium)
      Take time step
      Calculate energies and fields
   END WHILE(not equilibrium)
END FOR i
```

Cell-Based Calculations

```
FOR cell = 1 to N
   FOR energy = 1 to M
      cell->CalculateEnergy[energy]
   END FOR energy
END FOR cell
```

Energy-Based Calculations

```
FOR energy = 1 to M
   FOR cell = 1 to N
      energy->CalculateEnergy[cell]
   END FOR cell
END FOR energy
```

Advantages to Energy-Based Approach

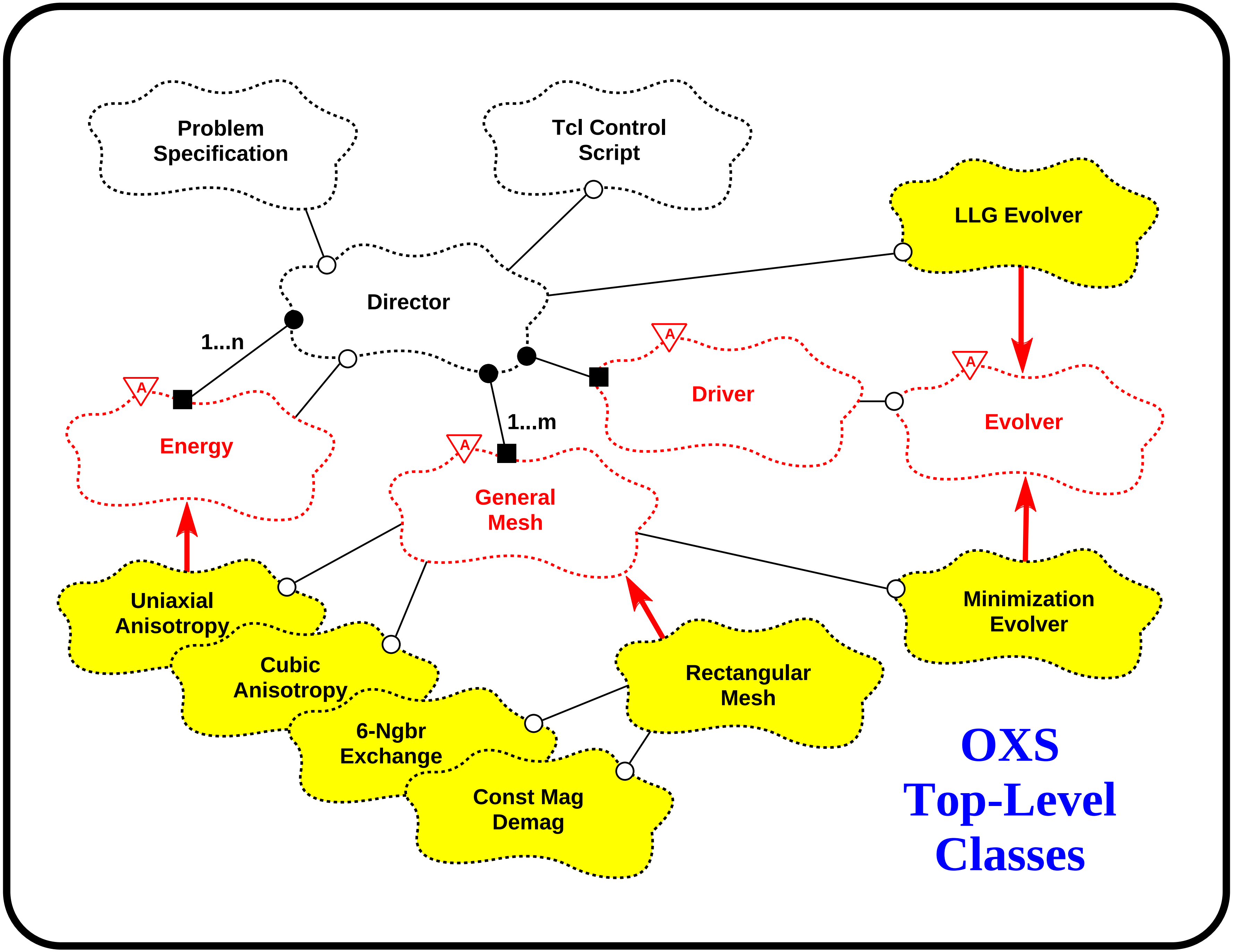
1. Encapsulation of material parameters
2. Efficient demag calculation
3. Typical output requirements
4. Expectations of end users and extension writers

Disadvantages?

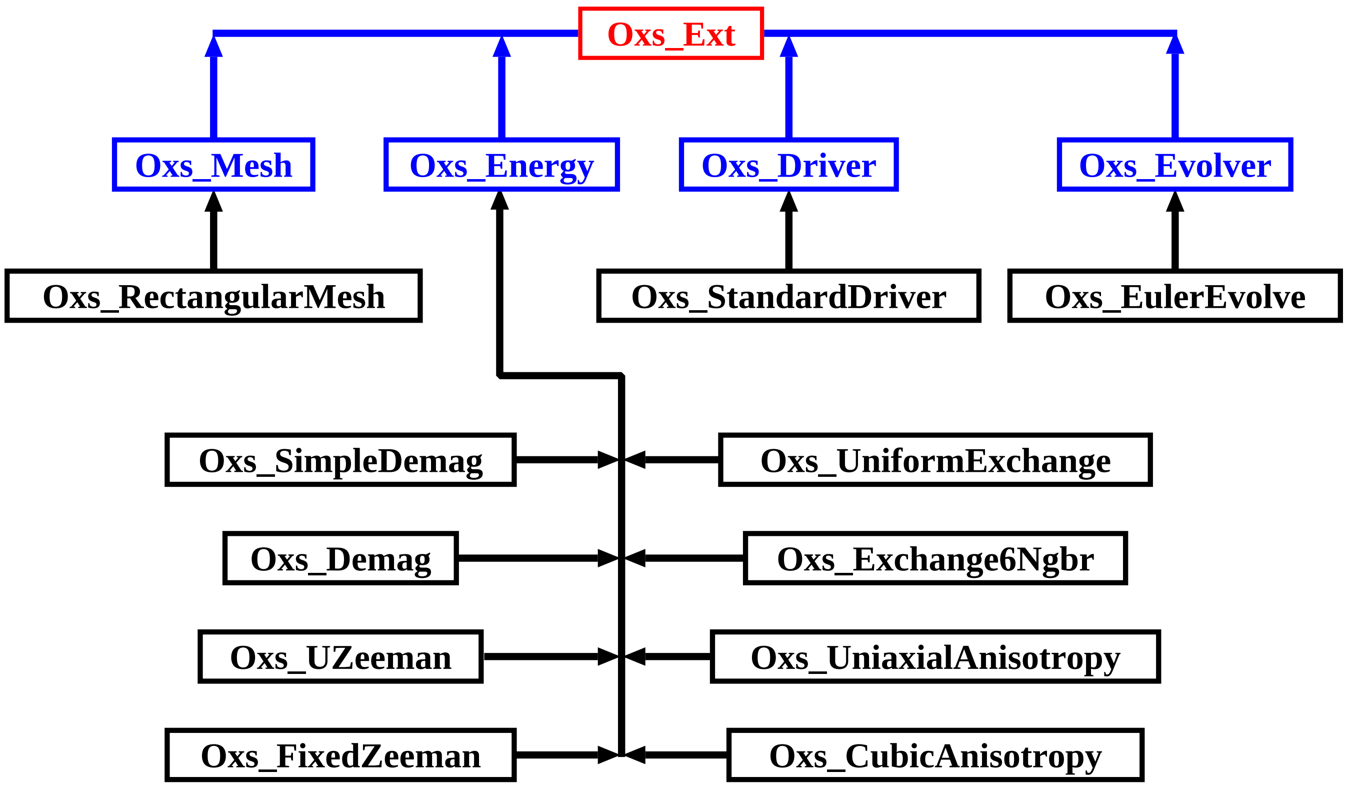
- Exposure of mesh details
- Shared material parameters
- Multiple spin array traversals

Mesh Downcasting in Oxs_Demag

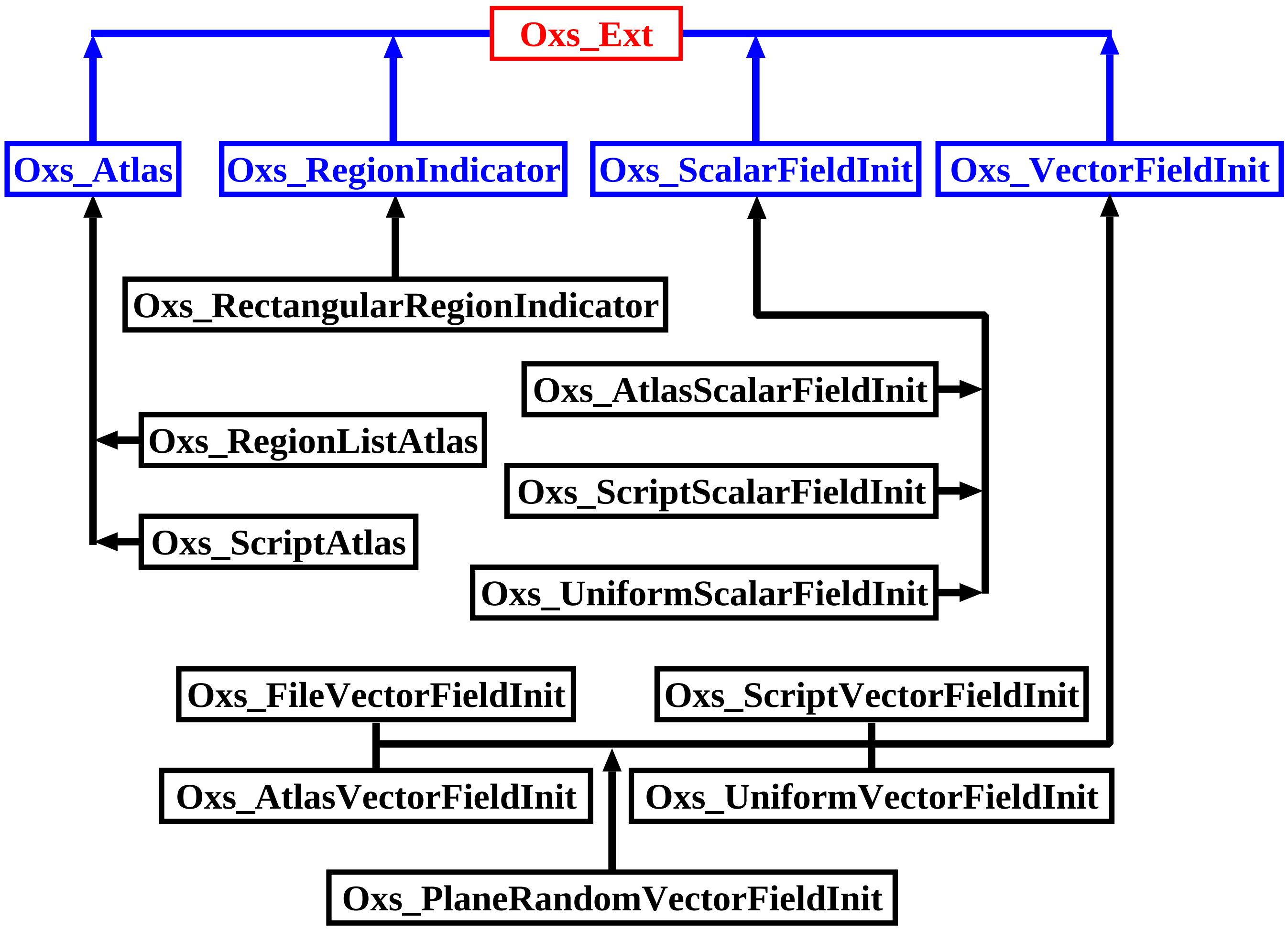
```
void Oxs_Demag::FillCoefficientArrays
                (const Oxs_Mesh* genmesh) const
{ // This routine is conceptually const.
  const Oxs_RectangularMesh* mesh
    = dynamic_cast<const Oxs_RectangularMesh*>(genmesh);
  if(mesh==NULL) {
    string msg=string("Object ")
      + string(genmesh->InstanceName())
      + string(" is not a rectangular mesh.");
    throw Oxs_Ext::Error(msg.c_str());
  }

...
```


Problem Specification
Tcl Control Script
LLG Evolver
Director
1...n
Driver
Evolver
Energy
1...m
General Mesh
Uniaxial Anisotropy
Cubic Anisotropy
6-Ngbr Exchange
Const Mag Demag
Rectangular Mesh
Minimization Evolver
A
OXS
Top-Level
Classes

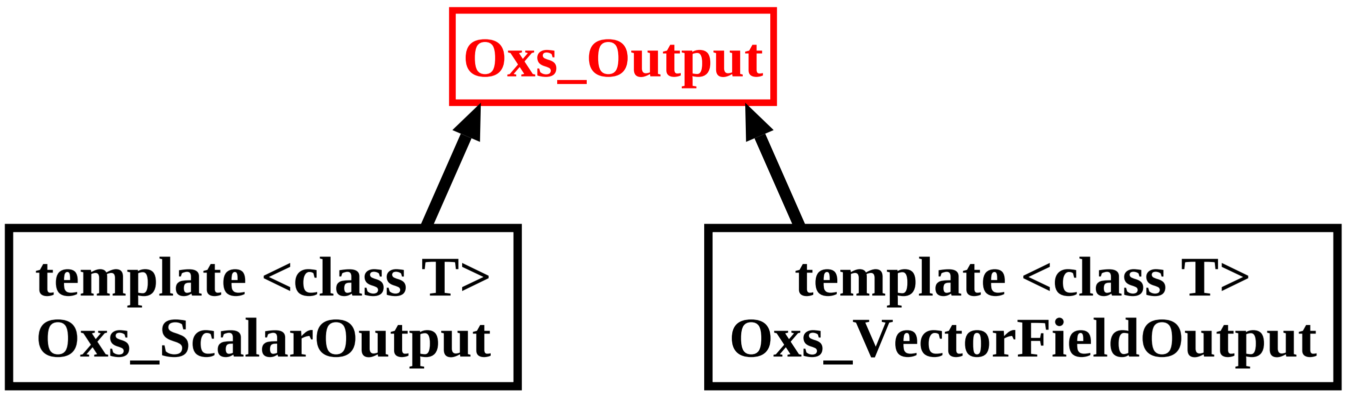
Oxs_Ext Main Tree



Oxs_Ext Support Tree



Oxs_Output Hierarchy



Sample MIF 2.0 File

```
# MIF 2.0

Specify Oxs_SimpleDemag {}

Specify Oxs_UniformExchange:NiFe {
  A  13e-12
}

Specify Oxs_EulerEvolve {
  alpha 0.5
  start_dm 0.01
}
```

```
Specify Oxs_SectionAtlas:atlas {
   world { Oxs_RectangularSection {
     xrange {1e-9 301e-9}
     yrange {0 200e-9}
     zrange {-1d-9 19e-9}
   }}
}

Specify Oxs_RectangularMesh:mesh {
  cellsize {10e-9 10e-9 10e-9}
  atlas :atlas
}
```

```
Specify Oxs_UniaxialAnisotropy {
  K1 { Oxs_UniformScalarFieldInit { value  6.2831853e4 } }
  axis { Oxs_RandomVectorFieldInit {
     min_norm 1
     max_norm 1
  } }
}
```

```
Specify Oxs_StandardDriver {
 evolver Oxs_EulerEvolve
 min_timestep 1e-18
 max_timestep 1e-9
 stopping_dm_dt 0.01
 mesh :mesh
 Ms { Oxs_UniformScalarFieldInit { value 8e5 } }
 m0 { Oxs_ScriptVectorFieldInit {
      script  {SineSpin 5}
      norm  1
 } }
}
```

```
proc SineSpin { freq x y z xmin ymin
                zmin xmax ymax zmax } {
    global pi
    set xspan [expr $xmax - $xmin]
    set mult [expr 2*$pi*$freq/$xspan]
    set vx [expr sin($mult*$x)]
    set vy [expr cos($mult*$x)]
    set vz 0
    return "$vx $vy $vz"
}
```

Sample Header File

```
/* FILE: simpleanisotropy.h
 *
 * Simple uniaxial anisotropy, derived from Oxs_Energy class.
 *
 */

#ifndef _OXS_SIMPLEANISOTROPY
#define _OXS_SIMPLEANISOTROPY

#include "energy.h"
#include "meshvalue.h"
#include "simstate.h"
#include "threevector.h"

/* End includes */
```

```
class Oxs_SimpleAnisotropy:public Oxs_Energy {
private:
  REAL8m K1;
  ThreeVector axis;
public:
  virtual const char* ClassName() const; // ClassName() is
  /// automatically generated by the OXS_EXT_REGISTER macro.
  Oxs_SimpleAnisotropy(const char* name,  // Child instance id
       Oxs_Director* newdtr, // App director
       Tcl_Interp* safe_interp, // Safe interpreter
       const char* argstr);  // MIF input block parameters
  virtual ~Oxs_SimpleAnisotropy() {}
  virtual void GetEnergyAndField(const Oxs_SimState& state,
                  Oxs_MeshValue<REAL8m>& energy,
                  Oxs_MeshValue<ThreeVector>& field) const;
};
#endif // _OXS_SIMPLEANISOTROPY
```

Sample Source Code File

```
// FILE: simpleanisotropy.cc

#include "nb.h"
#include "simpleanisotropy.h"

// Oxs_Ext registration support
OXS_EXT_REGISTER(Oxs_SimpleAnisotropy);

/* End includes */
```

```
// Constructor
Oxs_SimpleAnisotropy::Oxs_SimpleAnisotropy(
  const char* name,     // Child instance id
  Oxs_Director* newdtr, // App director
  Tcl_Interp* safe_interp, // Safe interpreter
  const char* argstr)   // MIF input block parameters
  : Oxs_Energy(name,newdtr,safe_interp,argstr)
{
  // Process initialization string
  K1 = GetRealInitValue("K1");
  axis = GetThreeVectorInitValue("axis");
  axis.SetMag(1.0);
  VerifyAllInitArgsUsed();
}
```

```
void Oxs_SimpleAnisotropy::GetEnergyAndField
(const Oxs_SimState& state,
 Oxs_MeshValue<REAL8m>& energy,
 Oxs_MeshValue<ThreeVector>& field
 ) const
{
  const Oxs_MeshValue<REAL8m>& Ms_inverse = *(state.Ms_inverse);
  const Oxs_MeshValue<ThreeVector>& spin = state.spin;
  UINT4m size = state.mesh->Size();

  REAL8m field_mult = (2.0/MU0)*K1;
  for(UINT4m i=0;i<size;++i) {
    REAL8m dot = axis*spin[i];
    field[i] = (dot*field_mult*Ms_inverse[i]) * axis;
    energy[i] = -K1*dot*dot;
  }
}
```

Sample Specify Block

```
Specify Oxs_SimpleAnisotropy {
  K1 530e3
  axis { 1 1 0 }
}
```

Adding a New Energy Term

1. Copy sample `.h` and `.cc` files to `oommf/app/oxs/local`.
2. Change names.
3. Add new code.
4. Run `pimake`.
5. Add new term to `MIF` input file.

NB: Modify no files from OOMMF distribution!

Standard Cubic Anisotropy:

$$E_{\text{anis}} = \frac{K_1}{M_s^4}\left(M_x^2 M_y^2 + M_y^2 M_z^2 + M_z^2 M_x^2\right)$$

Extended Cubic Anisotropy:

$$E_{\text{anis}} = \frac{K_1}{M_s^4}\left(M_x^2 M_y^2 + M_y^2 M_z^2 + M_z^2 M_x^2\right) + \frac{K_2}{M_s^6}\left(M_x^2 M_y^2 M_z^2\right)$$

OOMMF Directory Layout

oommf

- **app**
  - mmarchive, mmhelp, mmsolve2d
  - mmdisp, mmlaunch, omfsh
  - mmgraph, mmpe, oxs
  - mmdatatable, mmsolve, pimake
- **config**
  - cache, local, persons
  - features, names
- **doc**
  - giffiles, psfiles
  - pngfiles, userguide
- **pkg**
  - if, net, ow
  - nb, oc, vf

OXS Subdirectory Layout

- **oommf**
  - **app**
    - **oxs**
      - **base**
      - **ext**
      - **local**
      - **examples**

Web Pages

- Home Page:

  `http://math.nist.gov/~MDonahue/`

- OOMMF:

  `http://math.nist.gov/oommf/`

- μMAG:

  `http://www.ctcms.nist.gov/~rdm/mumag.org.html`