FSML: Fusion Simulation Markup Language for Interoperability of Data and Analysis Tools

Svetlana Shasharina and Chuang Li

GRIDL: High-Performance and Distributed Interactive Data Language

(time permitting…)

Svetlana Shasharina, Ovsei Volberg, Peter Stoltz and Seth Veitzer

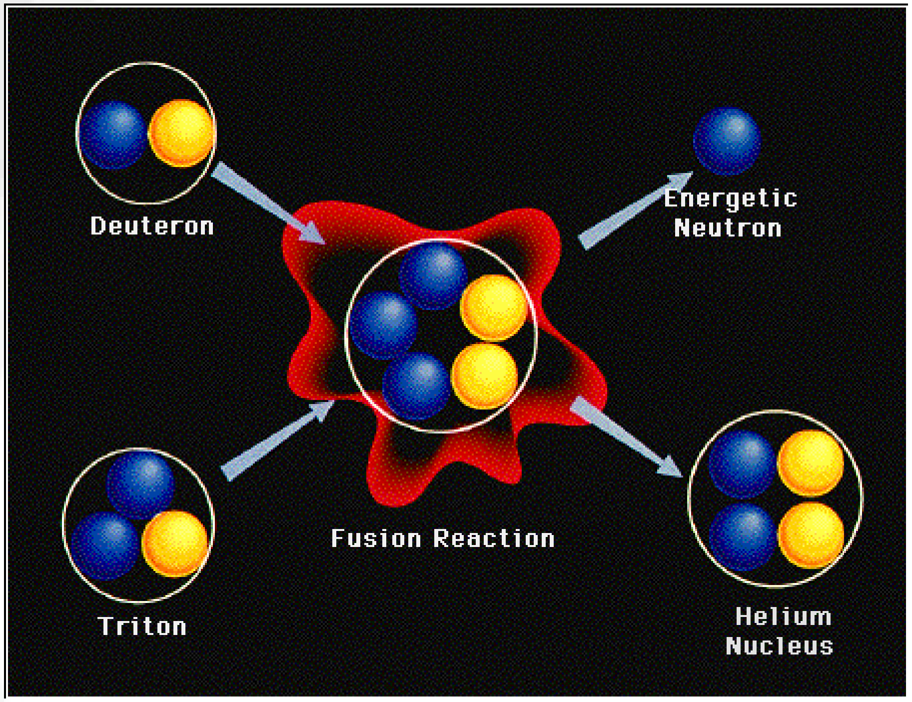
Tech-X Corporation (DOE/SBIR)

CLADE 2005

Overview

- FSML
  - Background
  - Motivation
  - Design
  - Status
- GRIDL
  - Motivation
  - Design of GRIDL
  - Status

The nuclear fusion produces energy:
$D + T \rightarrow (He^4 + 3.53\ MeV) + (n + 14.06\ MeV)$

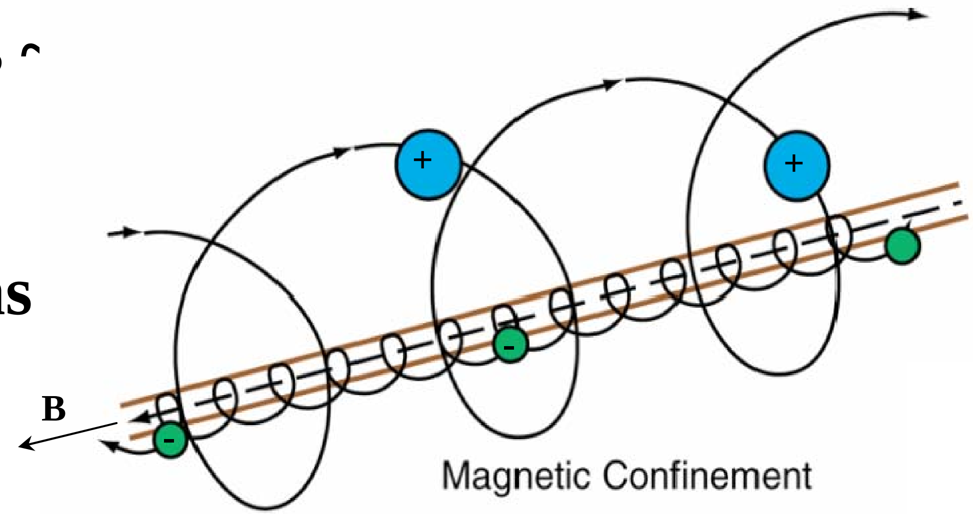


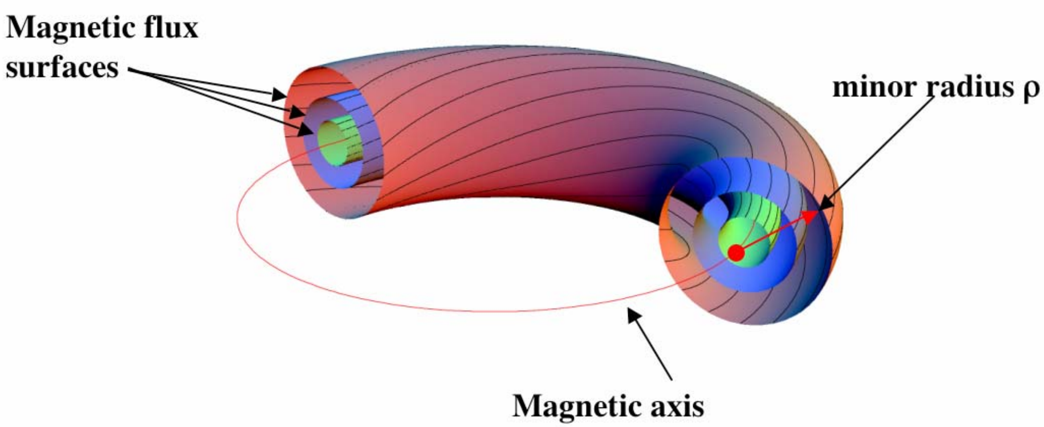
E_n = 14MeV	E_α = 3.5 MeV
Collected at walls	**Deposited in plasma**

Don Batchelor's (ORNL) figure

Heat (to overcome repulsion) and hold particles in magnetic traps

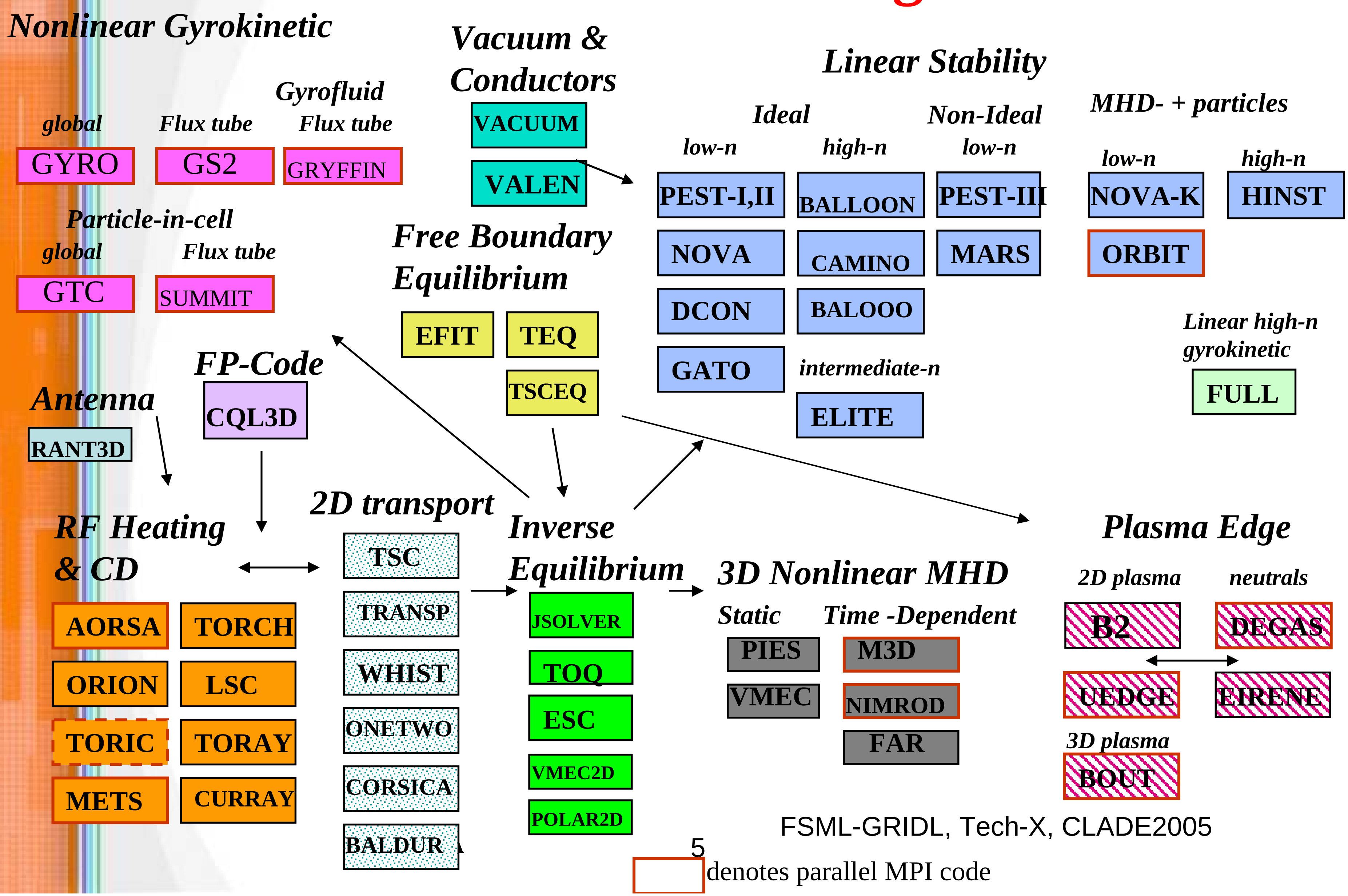
- **We heat the particles so that the average energy is ~ 100,000,000F (plasma)**
- **Then we should contain plasma for many reactions to happen**





Don Batchelor's (ORNL) figures

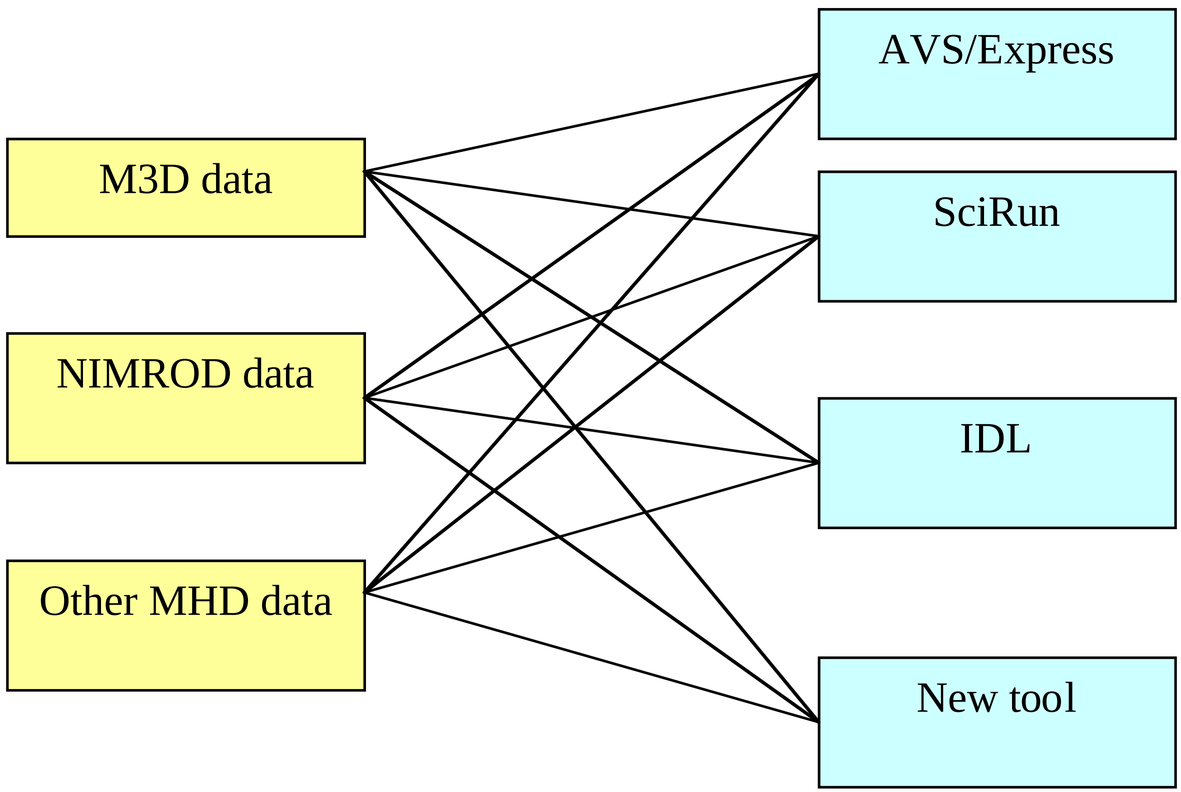
Multiple fusion codes to address aspects of fusion modeling



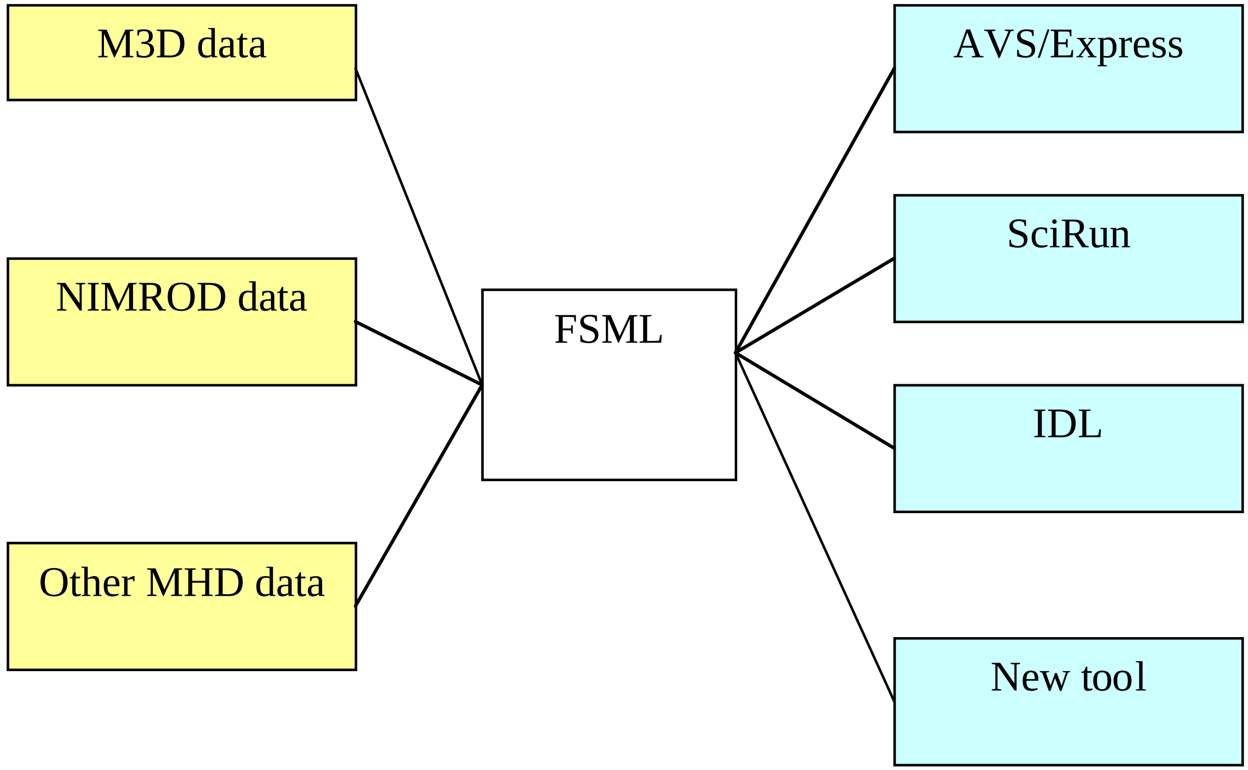
Heterogeneous settings impede integrated modeling and data visualization and analysis in fusion and plasma physics

- Multiple data output formats used in modeling codes
  - HDF5 (M3D, VORPAL, NIMROD)
  - NetCDF (parallel version is gaining popularity)
  - MDSplus (experiment, NIMROD, TRANSP)
- Different data organization even within one format within one type of physics
  - Different presentation of the same variable (potential vs. vector)
  - Different discretization
  - Different names (node-0 vs temperature)
  - Different units
  - Different file structures (nodes, attributes)
- Multiple data analysis and data visualization tools
  - SCIRun (University of Utah)
  - AVS/Express (Advanced Visual Systems)
  - IDL (Research Systems Inc)
  - OpenDX (open source)

MxN solution does not scale: need custom solution to analyze data from each code for each analysis tool



More scalable and maintainable solution is to provide a translation layer for conceptually similar codes



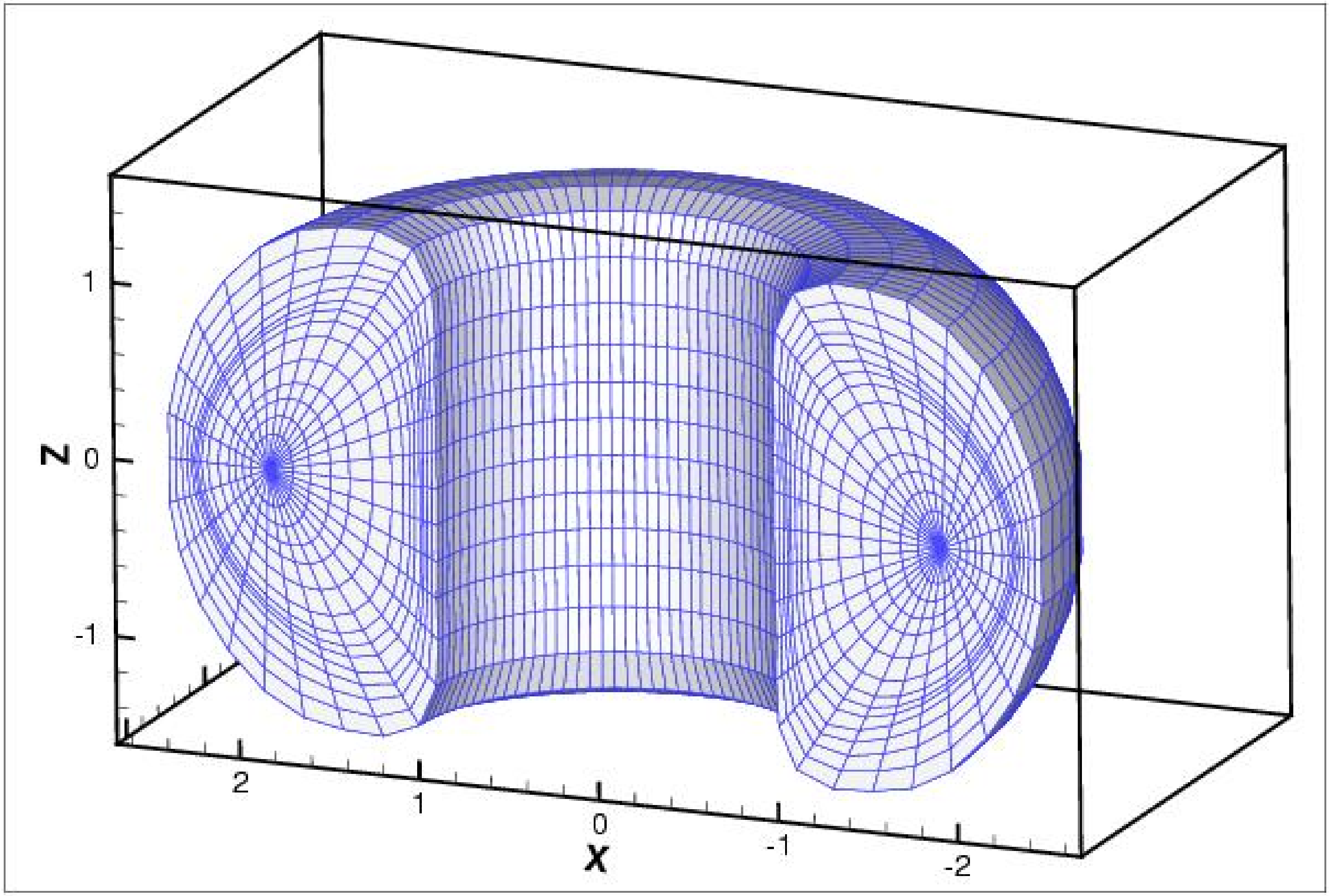
Data from different codes describing the same physics is conceptually the same: allowing domain vocabulary using XML

- **Concise (minimal but full) formulation of some fusion domain data and ways to transform between representations**
  - **A plus for future integrated modeling (big thing in the fusion community for the international device ITER to be built in France)**
- **XML to describe the domain data**
  - **XML is proven interoperability tool**
  - **Schemas can impose what should be present and how many times**
  - **Instances are validated against schema**
  - **Multiple APIs (C, C++, Java)**
  - **Many XML tools exist, wide industry support, Web Services**
  - **All other tools translate to XML and back (UML, Interface Definition Language, SIDL).**
- **Should we move to ontology?**
- **Need to narrow the fusion problem: we chose fusion MHD (magnetohydrodynamics) as our domain and a couple of tools for MHD data analysis and viz. Contradicts the original name (FSML). Might rename to MHDML ☺**

MHD codes (NIMROD and M3D) as foundation for FSML

- **Treat plasma as charged fluids. Fluids are described by velocities and fields (E and B) on a grid.**
- **Solve PDE (extension of non-linear diffusion-type equations for many variables and multiple sources and sinks) and show evolution in time.**
- **Store data in HDF5 (hierarchical binary format suited for multidimensional arrays). Information: values of velocities and fields on a grid organized by time slices.**
- **Attributes and data organization are different in every MHD code using HDF5.**
- **Use different "networks" of SCIRun and AVS/Express.**

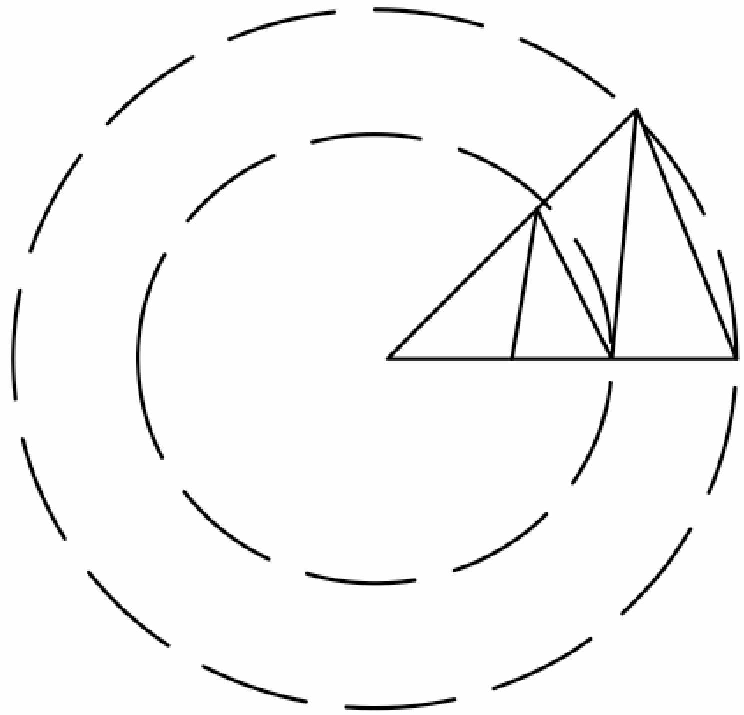
NIMROD uses finite difference in poloidal plane and Fourier in toroidal direction



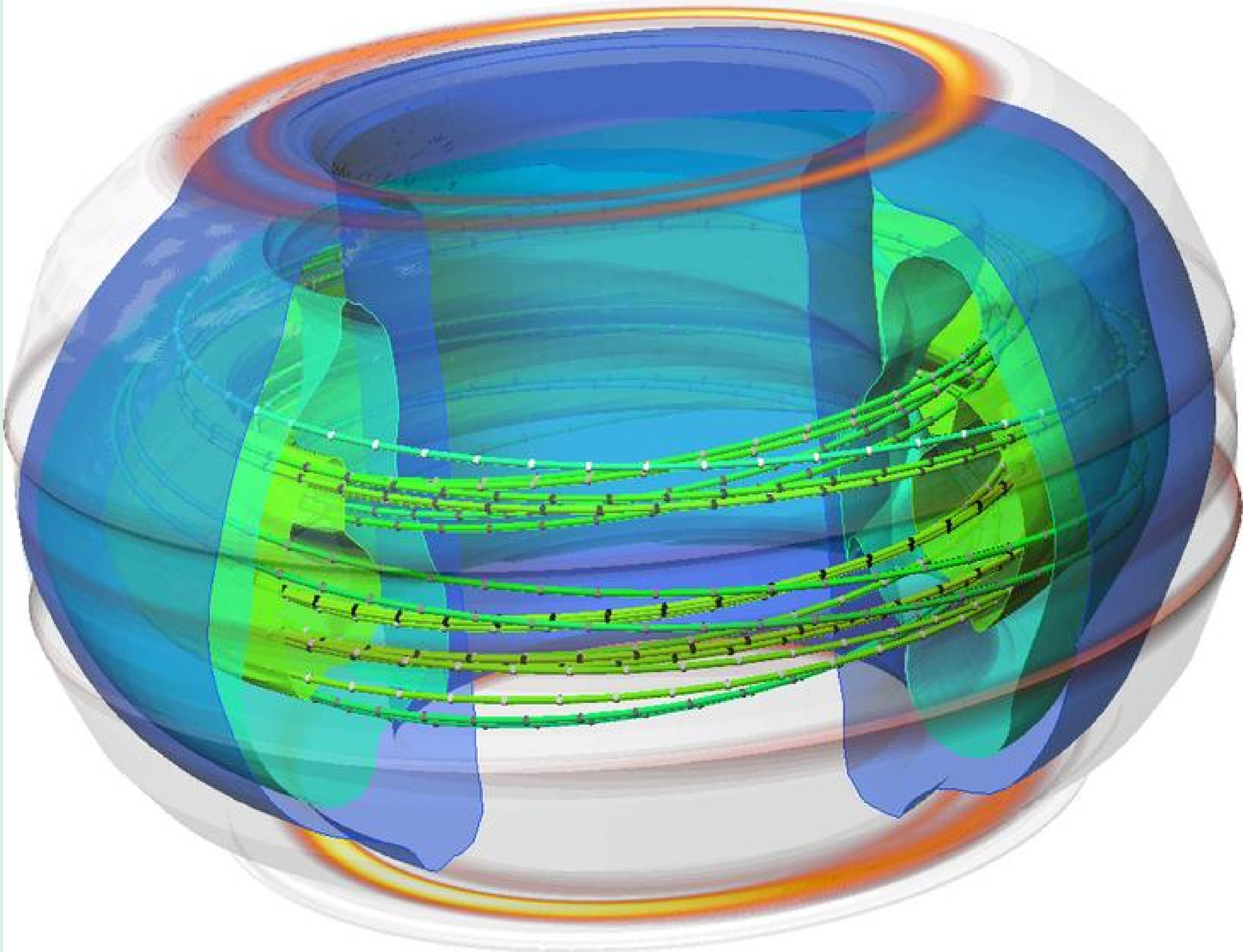
FSML-GRIDL, Tech-X, CLADE2005

Unstructured mesh needs more information

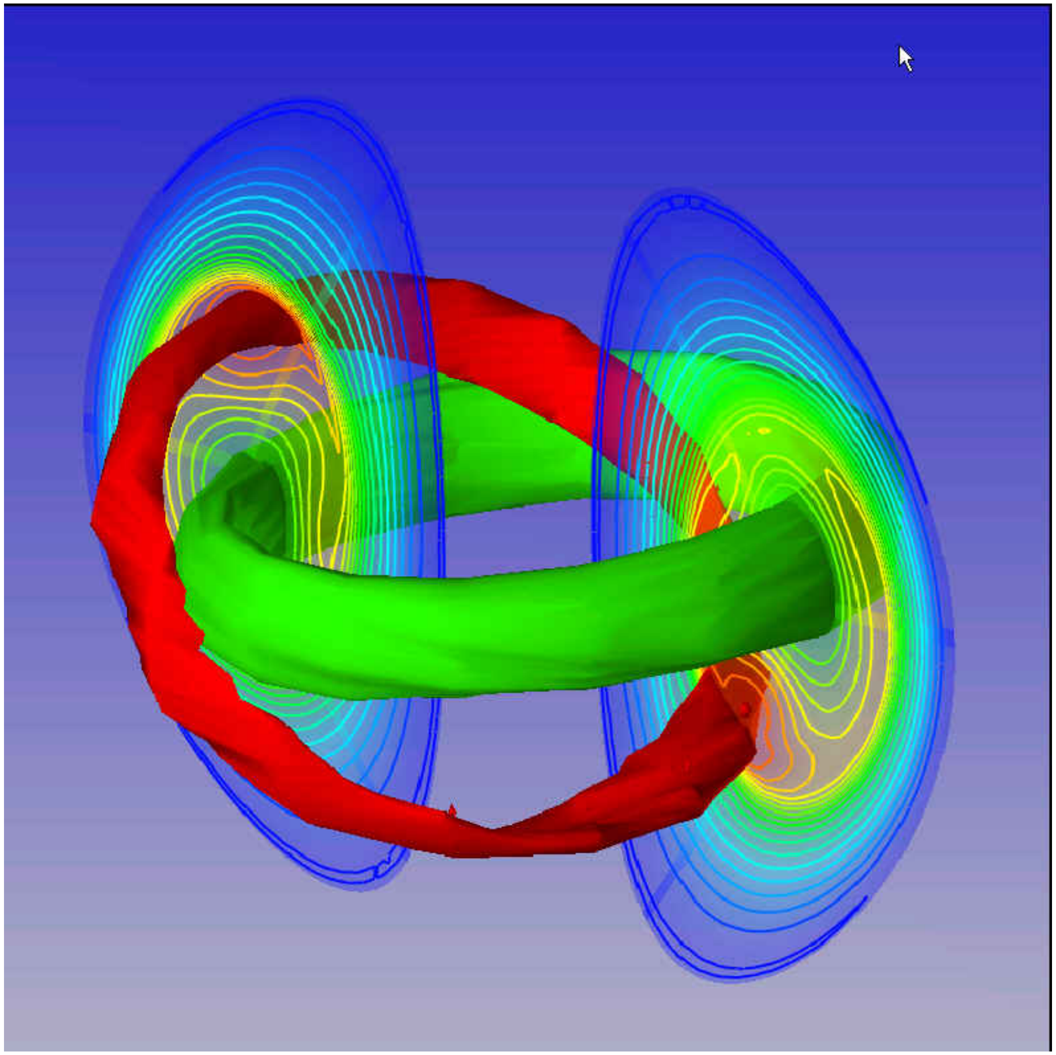
Schematic of the poloidal plane of M3D mesh



SciRun for NIMROD shows heat deposition, temperature isosurfaces, and field lines



AVS/Express shows magnetic surfaces and MHD activity modeled by M3D



MHD data has 3 levels

- Syntax (numerical types) is taken care of HDF5 itself
- Semantic MHD schema will include the unified set of MHD variables (temperature, pressure, velocity, current density, magnetic field, and particles density for all species etc) and geometry information
- Content metadata
  - simulation and publication relevant data (authors, platforms, compilers, goals, notes)
  - connectivity for multiple distributed files (large data might get split and end up at different sites)
  - abbreviated descriptions of data

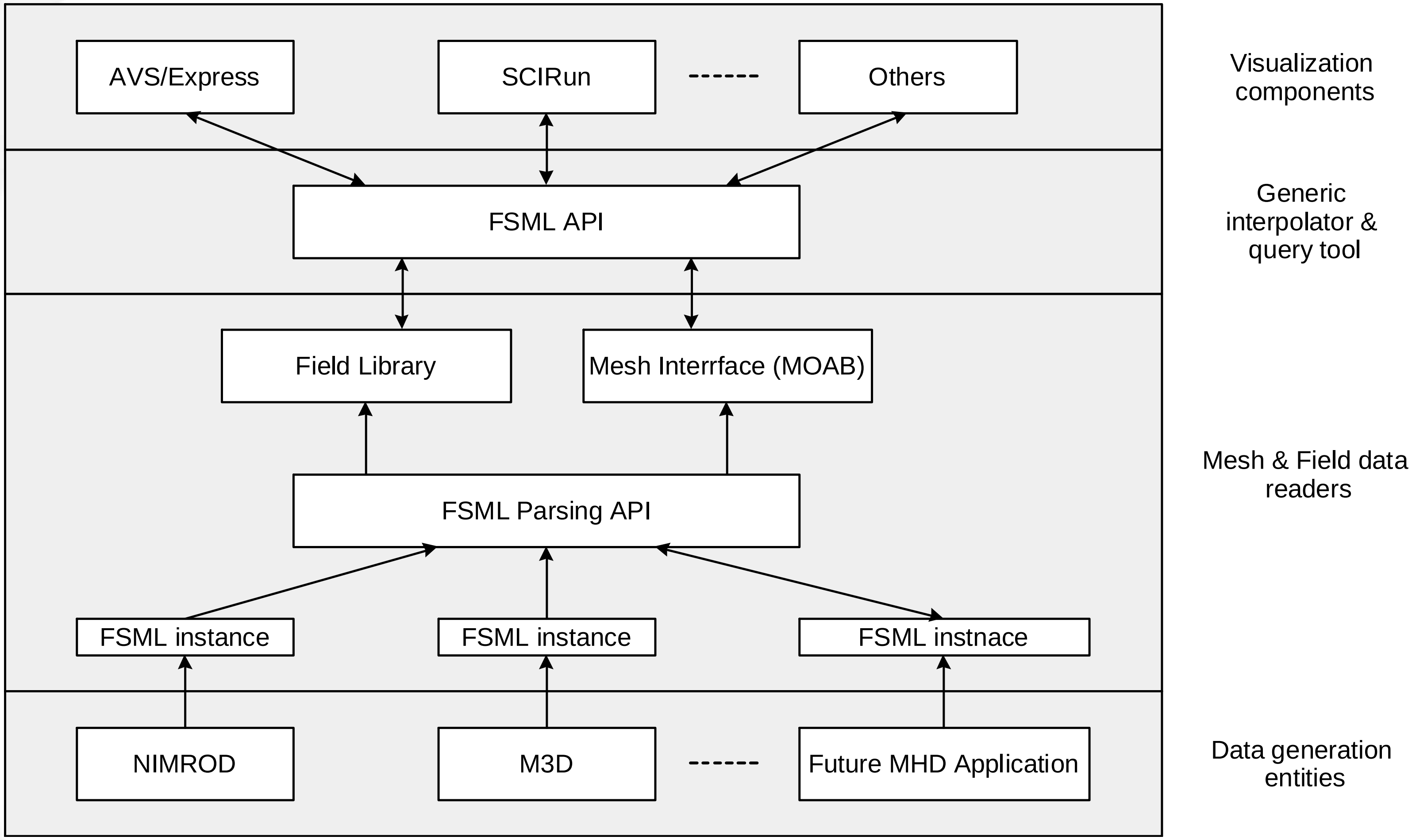
Data analysis and visualization also need

- **Uniform mesh descriptions (dimensionality, nodes and connectivity)**
  - **Structured and unstructured meshes**
  - **Optimization when possible (for structured meshes)**
  - **Problem is of interest to TSTT, the Terascale Simulation Tools and Technology center (MOAB C++ library from Sandia National Laboratory)**
- **Data in arbitrary point (not just on mesh)**
  - **Interpolate in accordance with discretization of the code (not linear interpolation used currently)**
  - **Problem of interest to TSTT (the Field Library)**

Proposed solution for MHD: FSML

- Study MHD codes and their outputs
  - M3D, NIMROD and a European code to be determined
- Develop XML schema for fundamental MHD variables
- Add XML tags for other common content
- C++ API based on the schema and implemented based on XML instances for access of native HDF5 data
- C++ API for uniform access of mesh data (structured and unstructured)
- C++ API for data interpolation for MHD data
- SCIRun and AVS/Express modules wrapping C++ APIs
- Component representation for all elements (for future integrated modeling)

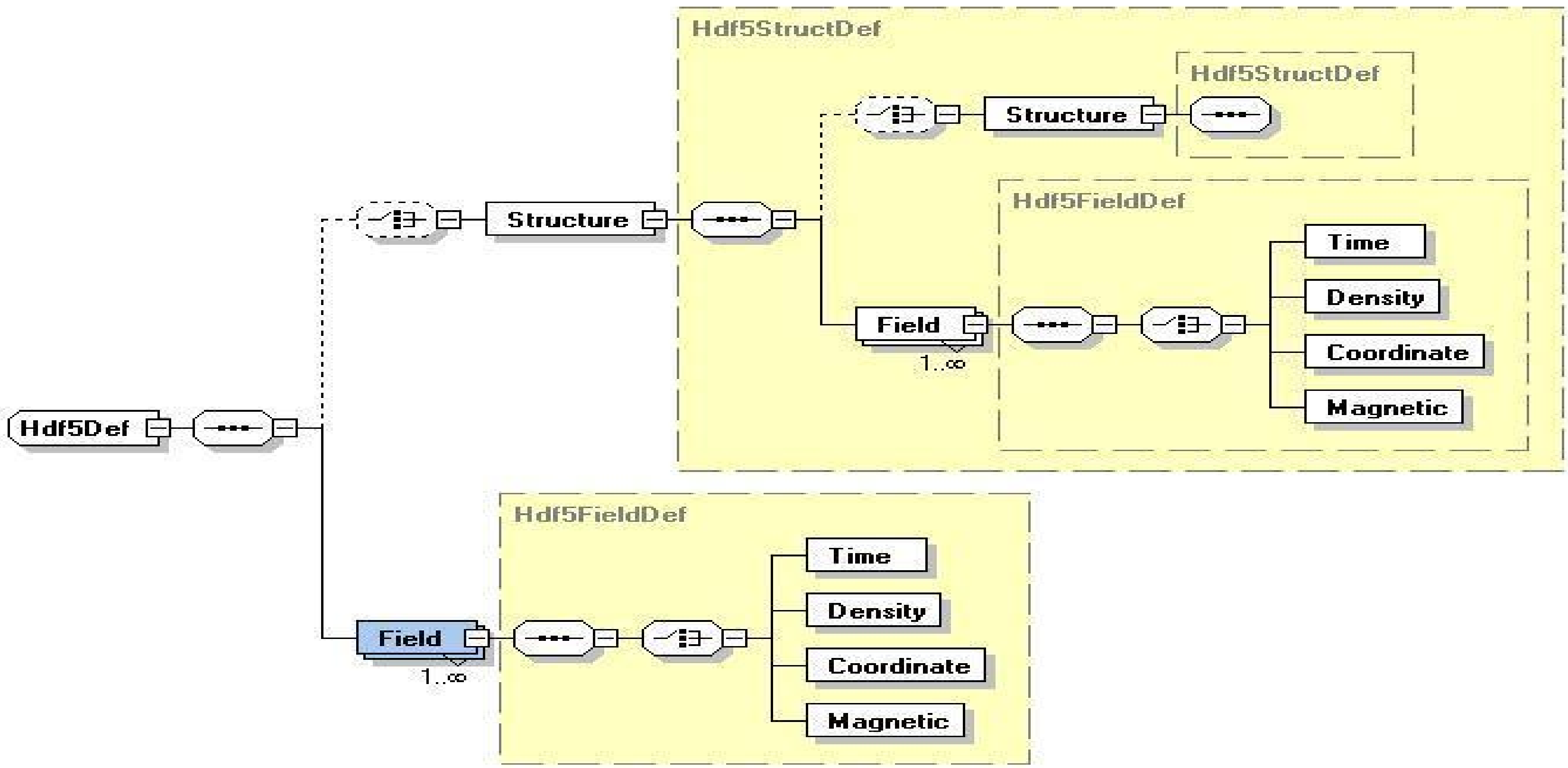
FSML Architecture allows for new MHD codes and new analysis tools



FSML has been prototyped

- **Partial XML schema (temperature, magnetic field, time, geometry) and C++ parsing libraries for the variables**
- **AVS/Express modules to do 3D visualization**

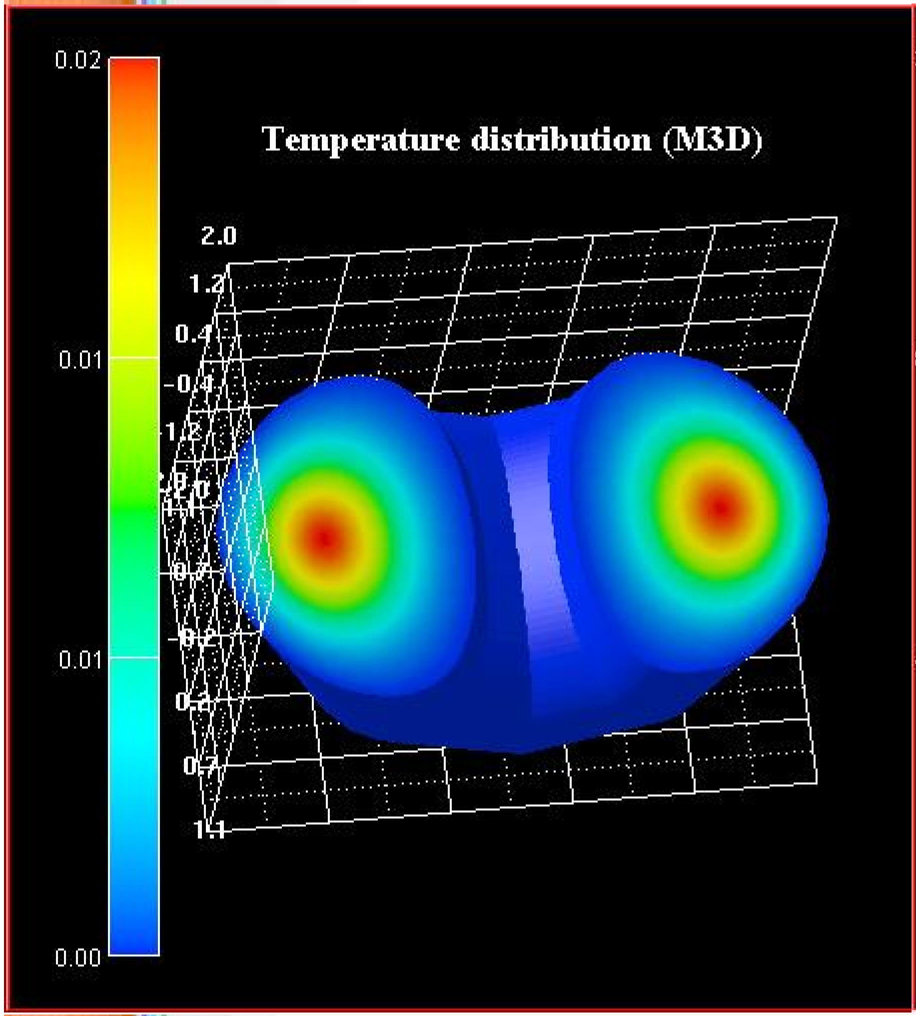
XML schema included several common variables and geometry data

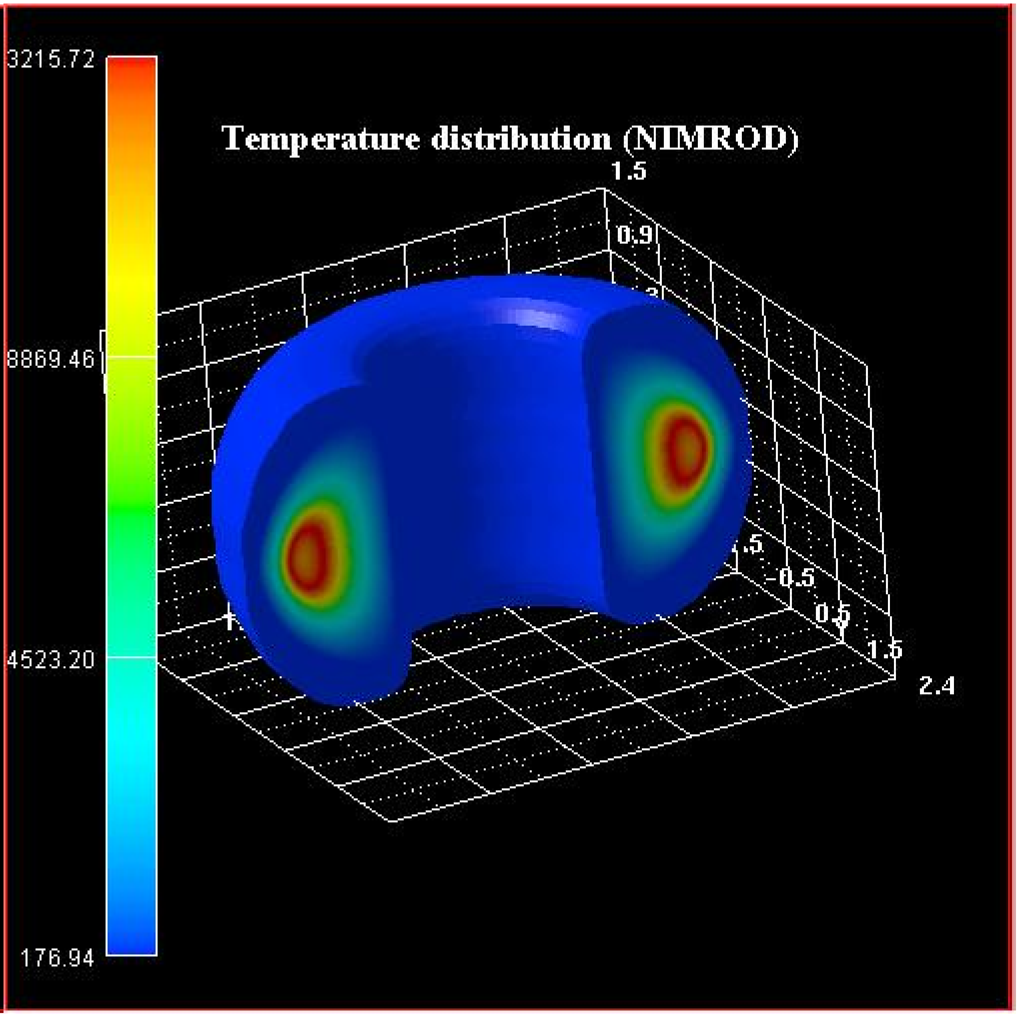


XML instances describe particular codes

```
<?xml version="1.0"?>
<a:FSML xmlns:a="FSML"
   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="FSML FSML.xsd">
   <SyntacticMetaData>
   <Hdf5 application="M3D">
        <Structure name="/" instances="1">
          <Field name="time">
                <Time name="m3d-time", unit="second"/>
          </Field>
        </Structure>
        <Structure name="time_node_data[0]" instances="1"/>
          <Field name="node_data[9]" instances="1">
                <Magnetic name="m3d-magnetic"  unit="Tesla"/>
            </Field>
        </Structure>
        </Hdf5>
   </SyntacticMetaData>
</a:FSML>
```

AVS/Express and SCIRun use uniform API to access all data





Future is great

- **Funding for 2 year project (2 FTE per year) just received from DOE/SBIR (thanks!)**
- **Proceed as described above**

GRIDL: High-Performance and Distributed Interactive Data Language

Svetlana Shasharina, Ovsei Volberg, Peter Stoltz and Seth Veitzer

Tech-X Corporation

See poster at HPDC 2005, July 25, 2005

Overview

- Interactive Data Language
- Design of parallel IDL on a grid
- Design of IDL clients for Web/Grid Service
- Status
- Conclusions

Interactive Data Language (IDL) is a powerful visualization and analysis tool

- 4GL: scripting and high-level (built on C)
- Well-suited for N-dimensional arrays
- Interworks with C/C++, Fortran, and Java
- Well established in scientific community
  - Fusion community uses IDL interface to access and analyze experimental data
  - Plasma physics simulations (VORPAL: 3D code) make 2D plots, 3D objects and movies using IDL
  - Volumetric MRI data (Los Alamos biophysics and co-registration codes at Ohio Kettering center)
  - Earth sciences
  - Military applications

Scientific computing is parallel and distributed

- **3D simulations are large and need multiple processors (possibly distributed): high-performance in a regular sense and on a grid**
- **Data (computational and experimental) is distributed and large (terabytes produced in remote experiments and simulations)**
- **Data analysis is distributed and massive**
- **Many levels of parallelisms and interactivity:**
  - **Some directives need to be parallel**
  - **Some should happen on one processor in an interactive mode (finalization of data analysis)**

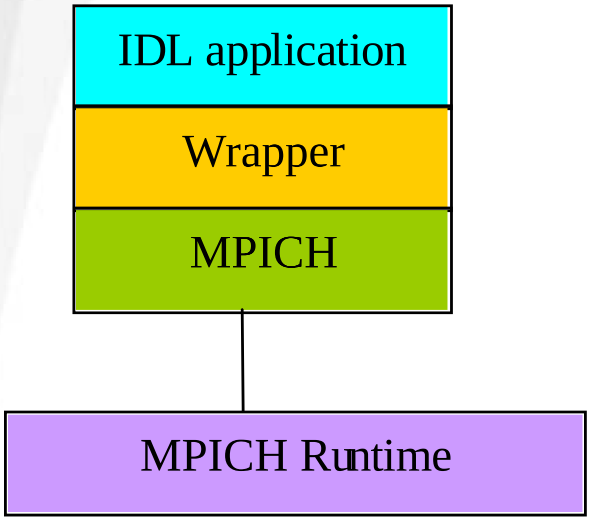
Solutions (high-performance computing and Grids) exist

- **Grids:**
  - **Globus:**
    - GT3 (and pre GT3): secure running remote jobs
    - GT4: Web Services for scientific computing
  - **Web Services:**
    - Distributed client-server using Web technologies
- **MPI: parallel computing**
- **MPICH-G2: MPI on a grid**
- **Grids and MPI have not addressed 4GLs and IDL in particular**

GRIDL: merging parallel distributed computing with IDL

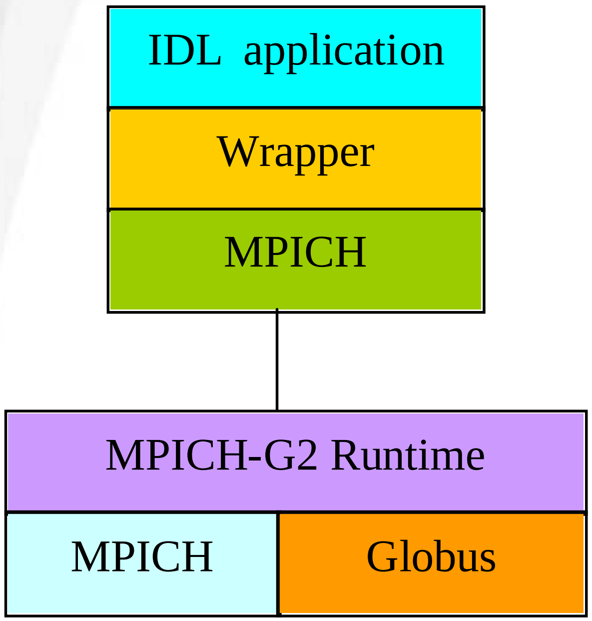
- **Parallel IDL**
  - **Running parallel IDL applications on clusters, supercomputers and grids**
- **IDL clients for Web Services**
- **6 months of prototype work funded by DOE so far**

Parallel IDL uses external C



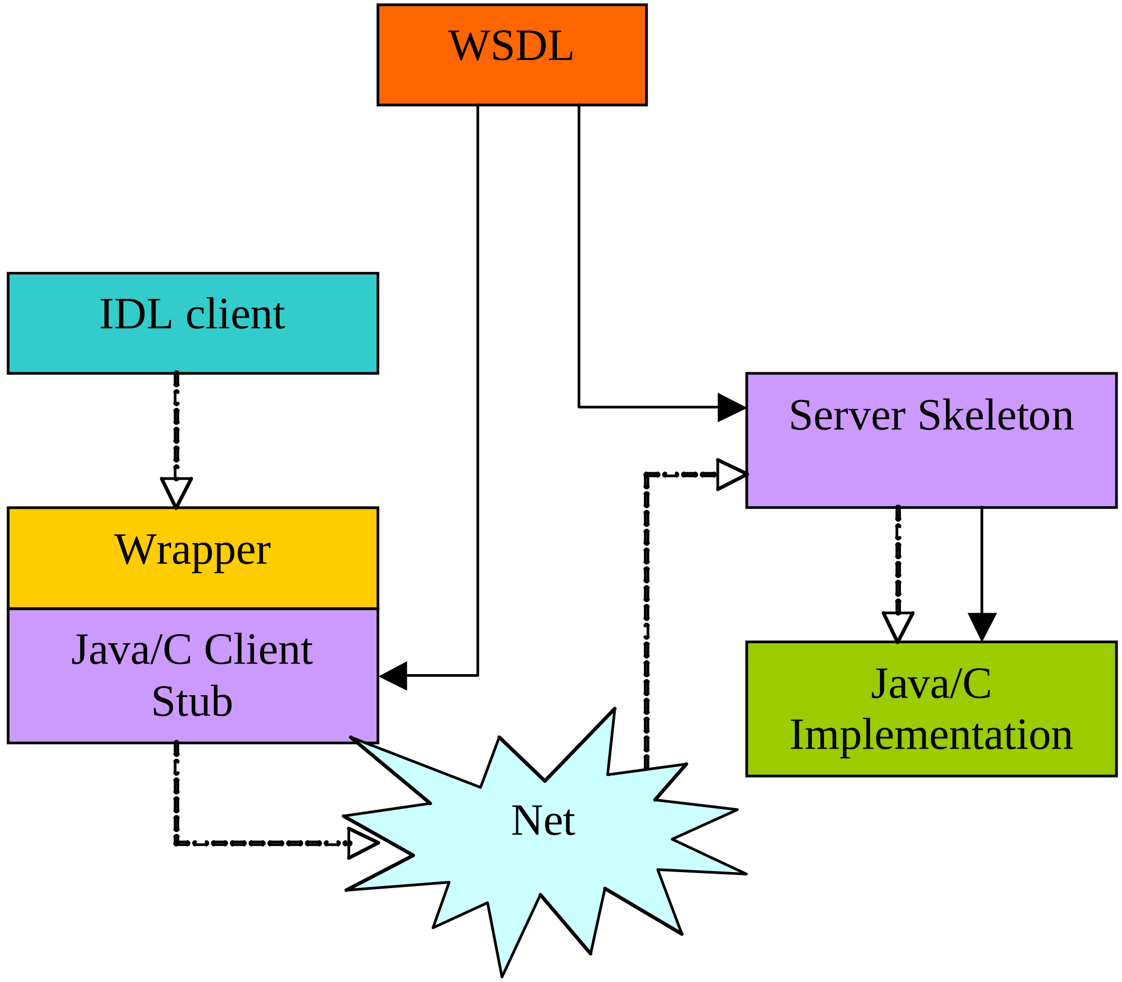
- **Dynamically Loadable Modules allow IDL to call external C functions by wrapping them.**
- **Wrapping C implementation of MPI exposes MPI in IDL**

Parallel IDL on a Grid design uses external C and MPICH-G2



- **MPICH-G2: MPICH using Globus underneath**
- **Wrapping MPICH now allows to run parallel IDL on a grid**

IDL client wraps generated stub (C or Java)



Status

- **DLMaker: prototype tool for automation of IDL wrapping of generic external C code**
- **Testing parallel IDL on a simple grid**
- **Playing with gSoap (wrapping of C++ clients of gSoap Web Services into IDL)**
- **Playing with Globus (wrapping Java clients of GT3.2 Web Services using Java-IDL bridge)**

DLMaker works for simple types

- **Input: .h file with C signatures**

```
extern "C" {
void pro(double ,int, float);
int func(int, float);
}
```

- **Output: what is needed for exposing these C functions into IDL (C wrapper, registration code, DLM description). Allows:**

```
pro testmodule
pro, 2, 3, 1
y = func3(1, 3)
end
```

Need more sophisticated DLMaker capable of:

- “In” and “out” variables with correct memory allocation (need extra information in the input file similar to CORBA’s Interface Definition Language or SIDL)
- IDL-type allocations of temporaries
- Produce IDL keywords (some arguments should go there: types)
- Specializing to particular web services compiler (wrappers should deal with return variables and static variables correctly – WS-compiler specific!)
- So far, we hand-wrapped C functions used in MPI and Web Services examples

Simple MPI wrapper can be produced by our DLMaker

```
static IDL_VPTR IDL_MPI_COMM_SIZE
(int argc, IDL_VPTR argv[]){
  IDL_VPTR tmp = IDL_Gettmp();
  int size;
  MPI_Comm_size(MPI_COMM_WORLD,&size);
  tmp->type = IDL_TYP_LONG;
  tmp->value.l = size;
  return tmp;
}
```

Parallel IDL looks like MPI then

```
pro testmodule, x
   rank=mpi_comm_rank()
   nproc=mpi_comm_size()
   help, rank
   help, nproc
end
```

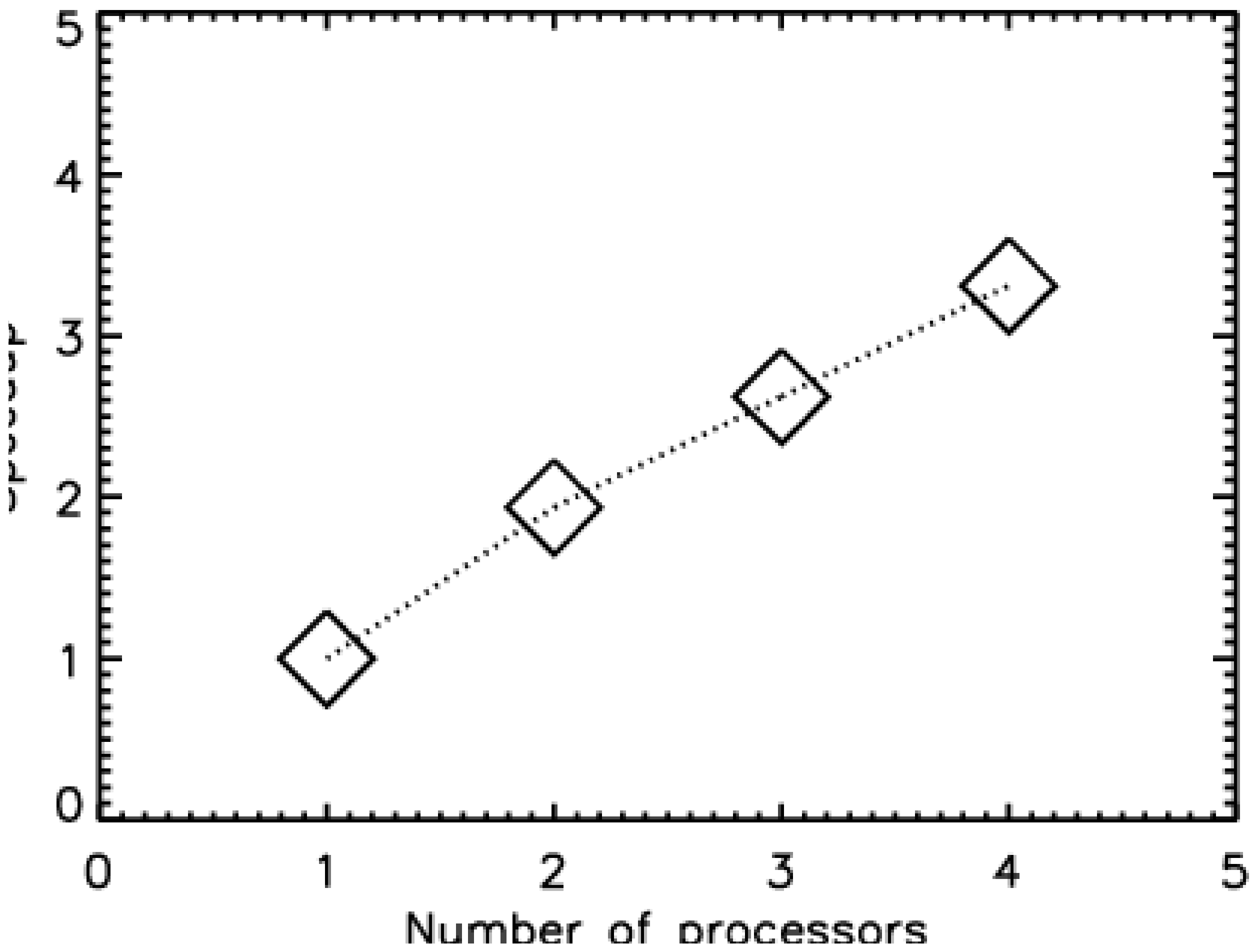
Parallel IDL needs a C driver to do `mpirun`

```
// startMPI.cxx
int main(int argc, char** argv) {
  int errorValue;
  MPI_Init(&argc,&argv);
  errorValue = IDL_Init(IDL_INIT_QUIET, &argc, argv);
  errorValue = IDL_ExecuteStr("testmodule, 1");
  MPI_Finalize();
  errorValue = IDL_Cleanup(0);
  return errorValue;
}
```

```
mpirun -np 4 -v startMPI
```

Speedup is linear

LAN grid with 2 dual processors nodes (MPICH-G2 v. 1.2.6 and Globus 3.2, gcc3.43 and IDL v.6.1)



IDL clients for gSoap Web Service needed hand-wrapping

Interface:

```
int wsidlhello__simproc1(int x, struct
  wsidlhello__simproc1Response {} *out);
```

Wrapper:

```
void IDL_simpro1(int argc, IDL_VPTR* argv){
  int x = argv[0]->value.i;
  // gSoap runtime environment initialized
  struct soap soap;
  soap_init(&soap);
// Call the method
soap_call_wsidlhello__simproc(&soap,
  "grid.txcorp.com:18084", NULL, x,0);
  // Clean up
  soap_end(&soap);
}
```

Working with Java clients and using Java-IDL bridge was straightforward

- **GT3.2**
- **IDL 6.1 (or higher)**
- **Set paths as needed**
- **IDL client mirroring Java client**

Java client:

```
public class Client{
      public static void main(String[] args){
// Get command-line arguments
         URL GSH = new java.net.URL(args[0]);
         int a = Integer.parseInt(args[1]);
// Get a reference to the MathService instance
         MathServiceGridLocator mathServiceLocator = new
   MathServiceGridLocator();
         MathPortType math =
   mathServiceLocator.getMathServicePort(GSH);
// Call remote method 'add'
         math.add(a);
// Get current value through remote method 'getValue'
         int value = math.getValue();
      }
}
```

IDL client creates java objects and uses the bridge to delegate to them:

```
pro CLIENT
; URL for the service
  gsh = OBJ_NEW("IDLJavaObject$URL", "java.net.URL",
   "http://64.240.154.9:8090/ogsa/services/MathService")
; Service Locator
  mathLoc = OBJ_NEW("IDLJavaObject$LOC",
   "com.txcorp.stubs.MathService.service.MathServiceGridLocator")
; Get the port using service locator and service handle
  math = mathLoc->getMathServicePort(gsh)
; Invoke the method
  math->add, 7
  res = math->getValue()
; Clean
  OBJ_DESTROY, gsh
  OBJ_DESTROY, mathLoc
end
```

Conclusions

- **Need more powerful and specialized tool for generation of IDL wrappers from C descriptions (for MPI and particular C Web Services).**
- **Need to wrap more MPI routines using the tool**
- **GT4 working with MPICH-g2**
- **Could use IDL-Java bridge to create IDL clients for Java Web Services. Works really well.**
- **Other 4GLs?**
- **Currently need new funding :-)**