

Starfish Webinar

Source Code Overview

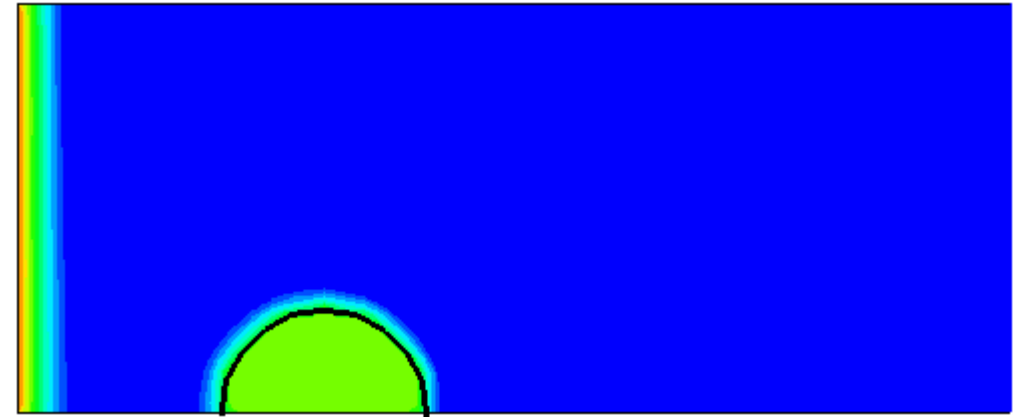
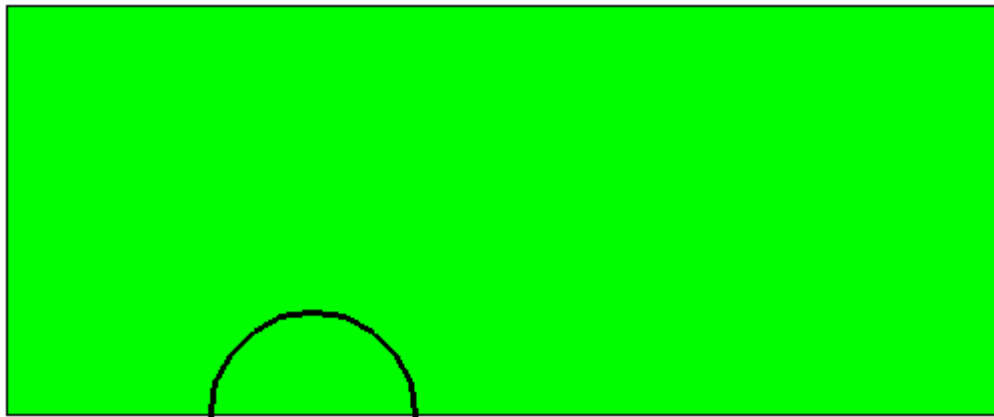
Lubos Brieda, Ph.D.
Particle In Cell Consulting LLC
particleincell.com/starfish



Introduction

- What is Starfish?
 - Two-Dimensional (XY or RZ) Java code for modeling ionized and non-ionized gases
 - Currently mainly a rarefied plasma / gas code but plan is to add support for fluid modeling
 - There are two editions: “regular” and “light”
 - The light edition, Starfish-LE, meant to be an academic tool that you can use to learn about modeling plasmas and rarefied gases and possibly extend with your own models
 - You can download the binary from <https://www.particleincell.com/starfish/> and get the source code from <https://github.com/particleincell/Starfish-LE>
 - There you will also find links to a five step tutorial for getting started as an end user

In this webinar, I want to give you the basics needed to start **developing** in Starfish



Courses

- You may also be interested in visiting <https://www.particleincell.com/courses> to learn more about online courses I offer on various topics related to numerical plasma modeling

Courses

2017 announcement

In 2017 I plan to offer a new course of **fluid modeling of plasmas**. This course will cover the magnetohydrodynamic (MHD) model, as well as smoothed-particle hydrodynamics (SPH) and Vlasov solvers. Stay tuned for more detail. The course will be offered in second half of 2017. The previous courses (PIC Fundamentals/Advanced PIC/Distributed Computing) will not be offered live in 2016, but I plan to re-record and clean up the lectures and be available to help with homework.

2016 courses

In 2016 I offered three courses, which are listed below. Although the courses have now ended, you may still register to obtain access to the lecture recordings, slides, and example codes. I will also be available to assist you with homework assignments.

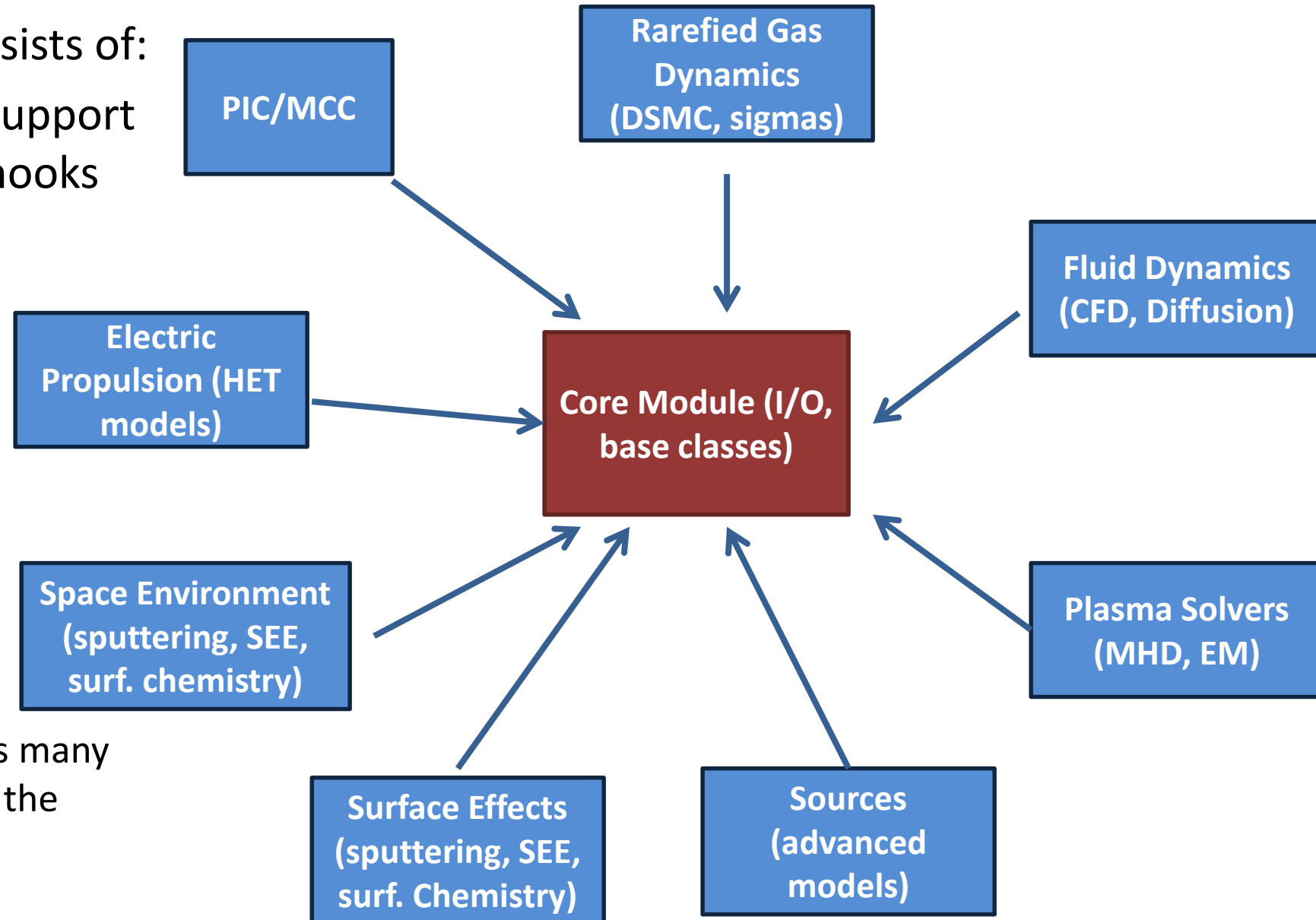
- Fundamentals of the PIC method:** This course introduces the Particle in Cell method using step-by-step approach. We will develop 1D, 3D, and 2D (axisymmetric) codes to simulate plasma sheath, $E \times B$ transport, plasma flow past a charged sphere, and a simple ion gun.
- Distributed Computing for Plasma Simulations:** In this course you'll learn how to develop plasma simulation codes that utilize multiple CPUs and graphic cards to handle larger simulation domains or to obtain results faster. We'll cover multithreading, distributed computing with MPI, and GPU computing using CUDA.
- Advanced PIC techniques:** This course covers topics beyond the scope of the intro course. It covers three main concepts: electromagnetic PIC (EM-PIC), Direct Simulation Monte Carlo (DSMC) collision modeling, and finite element PIC (FEM-PIC).

Code Overview

- Starfish conceptually consists of:

- Core** library providing support for I/O and main logic hooks
- Numerous **modules** implementing relevant physics

- The modules can be further extended with **plugins**
 - The full version implements many different plugins extending the Starfish-LE capabilities



Source Code

- Start by getting the source code from GitHub: <https://github.com/particleincell/Starfish-LE>

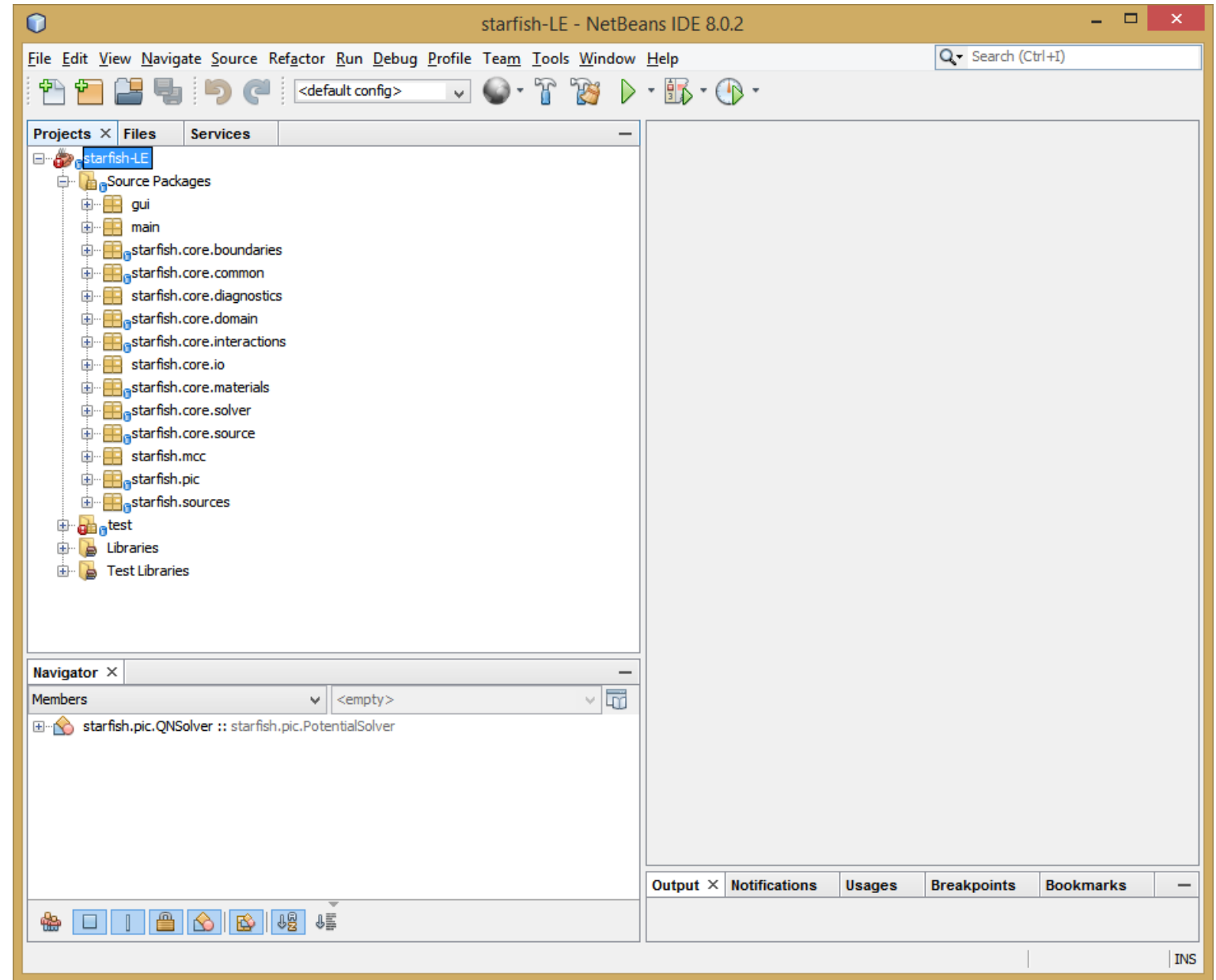
The screenshot shows the GitHub repository page for `particleincell/Starfish-LE`. At the top, there are buttons for 'Branch: master', 'New pull request', 'Create new file', 'Upload files', 'Find file', and a green 'Clone or download' button. Below these, a dropdown menu is open, showing 'Clone with HTTPS' and 'Use SSH' options. The 'Clone with HTTPS' option is selected, showing the URL `https://github.com/particleincell/Starfish-LE` and a copy icon. Below the URL are buttons for 'Open in Desktop' and 'Download ZIP'. The main content area shows a list of files and folders:

File/Folder	Commit Message	Time Ago
<code>dat/tutorial</code>	Initial release (version 0.15)	12 hours ago
<code>nbproject</code>	Initial release (version 0.15)	12 hours ago
<code>src</code>	Initial release (version 0.15)	12 hours ago
<code>test/starfish</code>	Initial release (version 0.15)	12 hours ago
<code>.gitattributes</code>	Added .gitattributes & .gitignore files	13 hours ago
<code>.gitignore</code>	Initial release (version 0.15)	12 hours ago
<code>LICENSE</code>	Initial release (version 0.15)	12 hours ago
<code>README.md</code>	Initial release (version 0.15)	12 hours ago
<code>build.xml</code>	Initial release (version 0.15)	12 hours ago
<code>manifest.mf</code>	Initial release (version 0.15)	12 hours ago
<code>starfish.png</code>	File rename	12 hours ago

- While you can just download a zip file of the entire source, it's better to clone the repo using Git. This will make it easier to receive updates and makes it possible for you to contribute to the project
 - <http://stackoverflow.com/questions/5989893/github-how-to-checkout-my-own-repository#5989998>
 - GitHub Desktop provides easy to use graphical interface to Git: <https://desktop.github.com/>

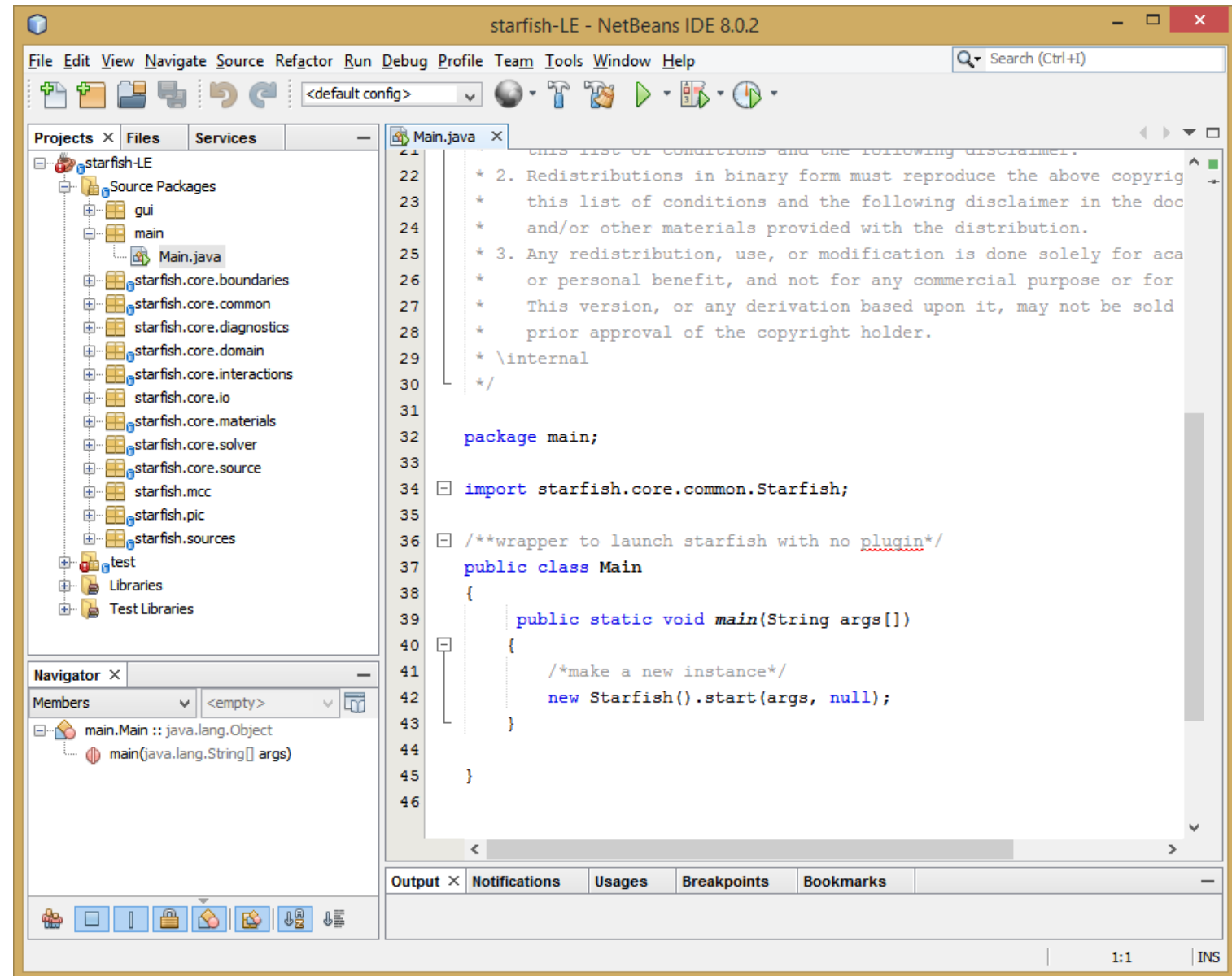
Netbeans

- I use Netbeans for the development environment but Eclipse should work just as well
- This image shows the package layout



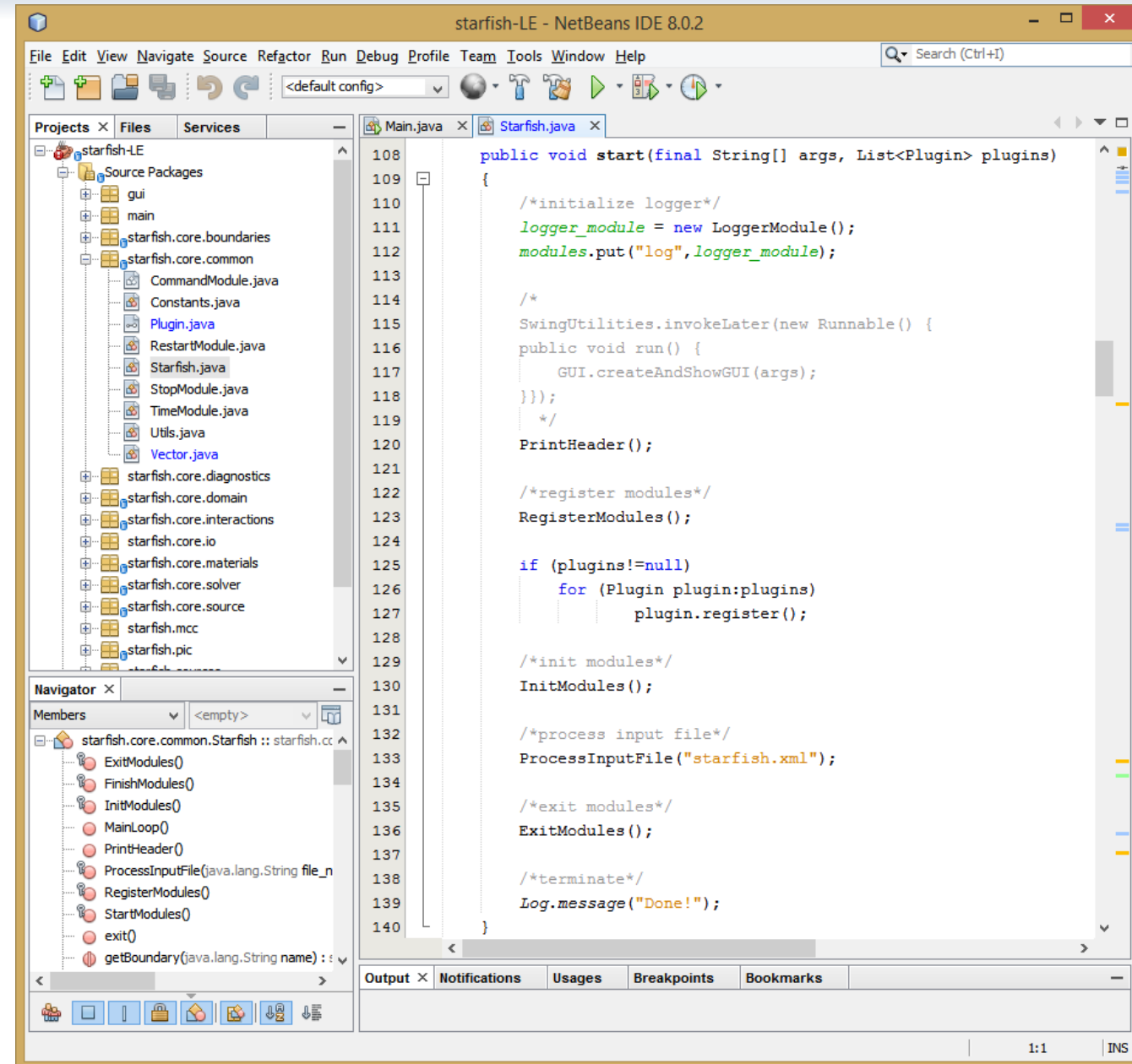
Main

- Just as any Java program, Starfish execution begins in a function called “main”
- This function is defined in Main.java located in package **main**
- This function instantiates a new object of type Starfish and then calls that object’s **start** method.



Start

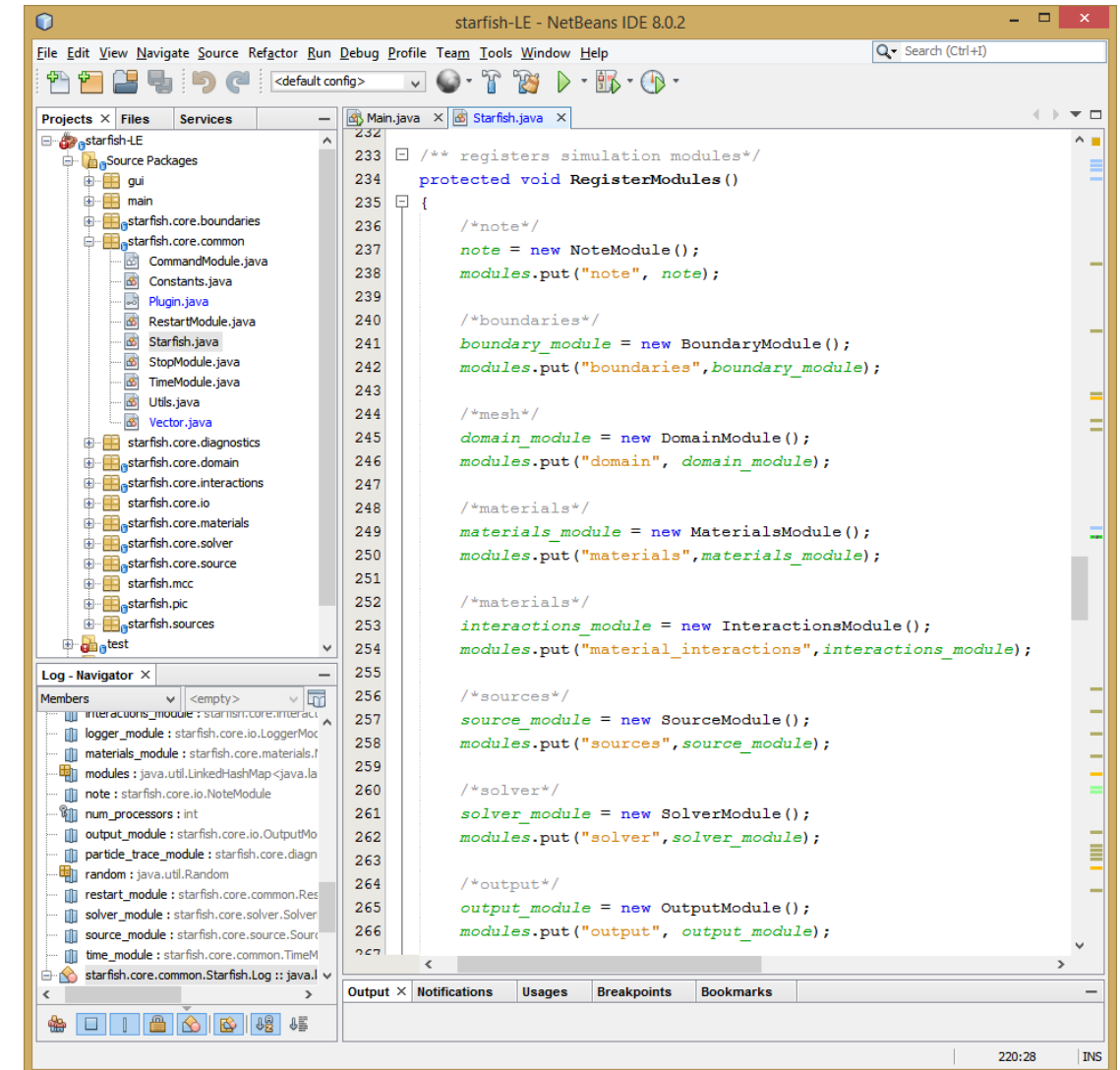
- This **start** method is located in Starfish.java located in package **starfish.core.common**
- It starts by instantiating a **LoggerModule**. This logger is how the rest of code prints information and error messages
- Next the header with version and copyright info is printed
- Next all default modules are registered
- Plugins are registered next, if any
- The modules are then initialized
- The code then reads file called **starfish.xml** and performs commands as specified – this is the “meat” of the simulation
- ExitModules let’s modules perform clean up actions
- Finally, “Done” is printed to the screen



RegisterModules

```
/*iterable list of registered modules, using LinkedHashMap to get predictable ordering*/  
static LinkedHashMap<String,CommandModule> modules = new LinkedHashMap<String,CommandModule>();
```

- Starfish modules are stored in a HashMap called modules. The accessor (key) is a string identifying the module name. All modules are derived from base class **CommandModule**
- **RegisterModules** is also defined in Starfish.java
- As you can see, this function simply adds (using put) various modules to the hash map
 - Some modules are first instantiated into a member variable – this is so other functions can use these modules without going through the hash map



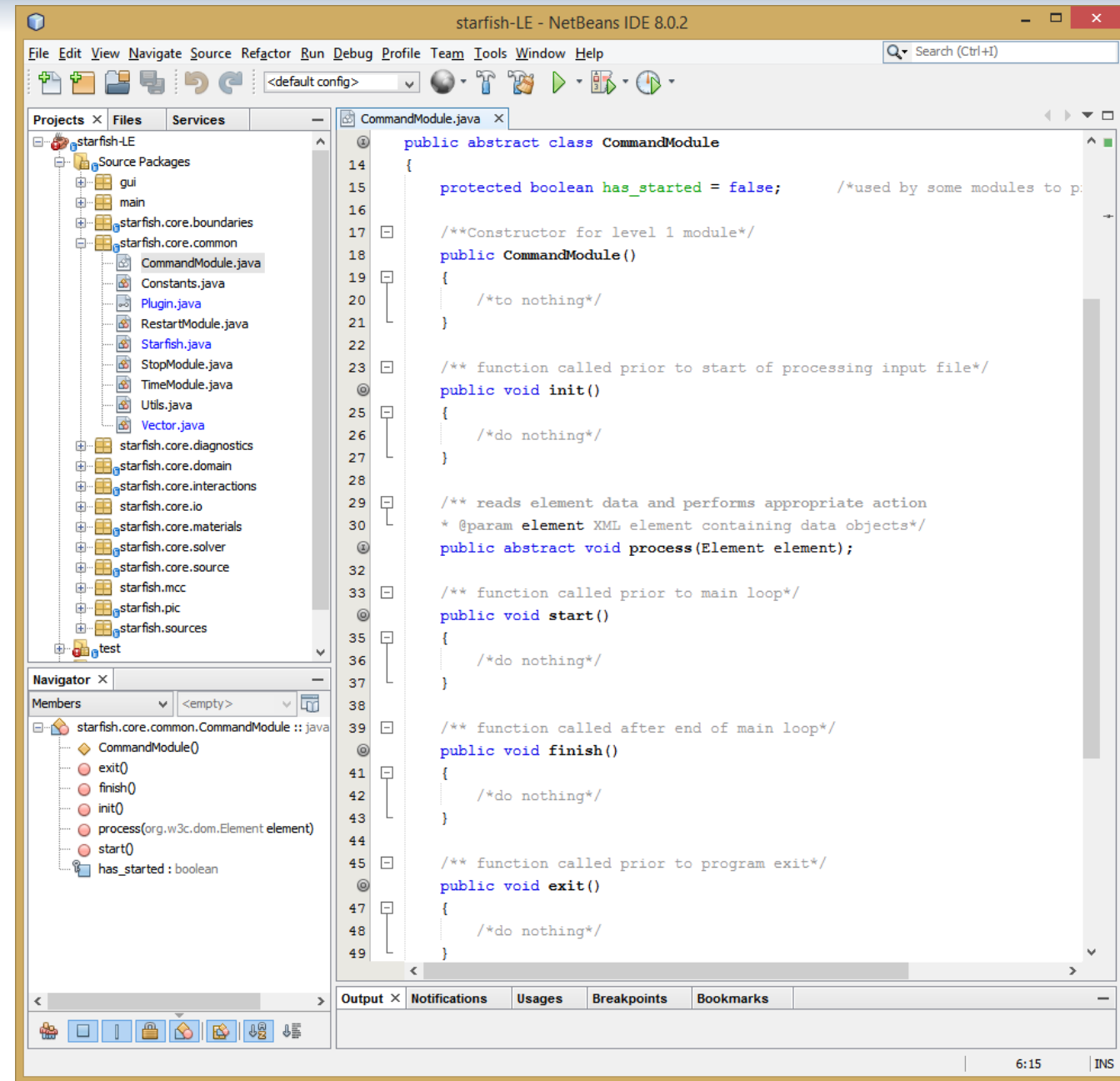
Modules

- Here is the list of currently defined modules in the order of appearance

Module	Purpose	Module	Purpose
note	Adds user defined message to the log file	time	Controls time step and code termination
boundaries	Loads line segments defining surface geometry and contains math functions for line-line intersections	load_field	Support for loading magnetic (and other) fields
domain	Generates computational mesh(es)	restart	Support for restarting simulation
materials	Loads definition of solid or gas materials	stop	Terminates the code (useful for debugging)
material_interactions	Handles surface interactions, chemistry, and collisions	starfish	Provides simulation main loop
sources	Contains mass injection algorithms	particle_trace	Output of a single particle to a file
solver	Various field solvers (such as Poisson)	animation	Generates output files at user defined interval
output	Functions for generating output files	averaging	Data averaging

Intro to Modules

- All modules extend from base class **CommandModule**
 - In starfish.core.common
- This base class defines five functions that need to be overloaded as needed:
 - **process**: called when command tag is encountered in starfish.xml input file
 - **init**: called by InitModules before simulation main loop starts
 - **start**: called at the start of the main loop
 - **finish**: called at the end of the main loop
 - **exit**: called by ExitModules just prior to code termination
- Why two initialization functions?
 - Some modules depend on others – for instance material interactions module needs material list to be initialized



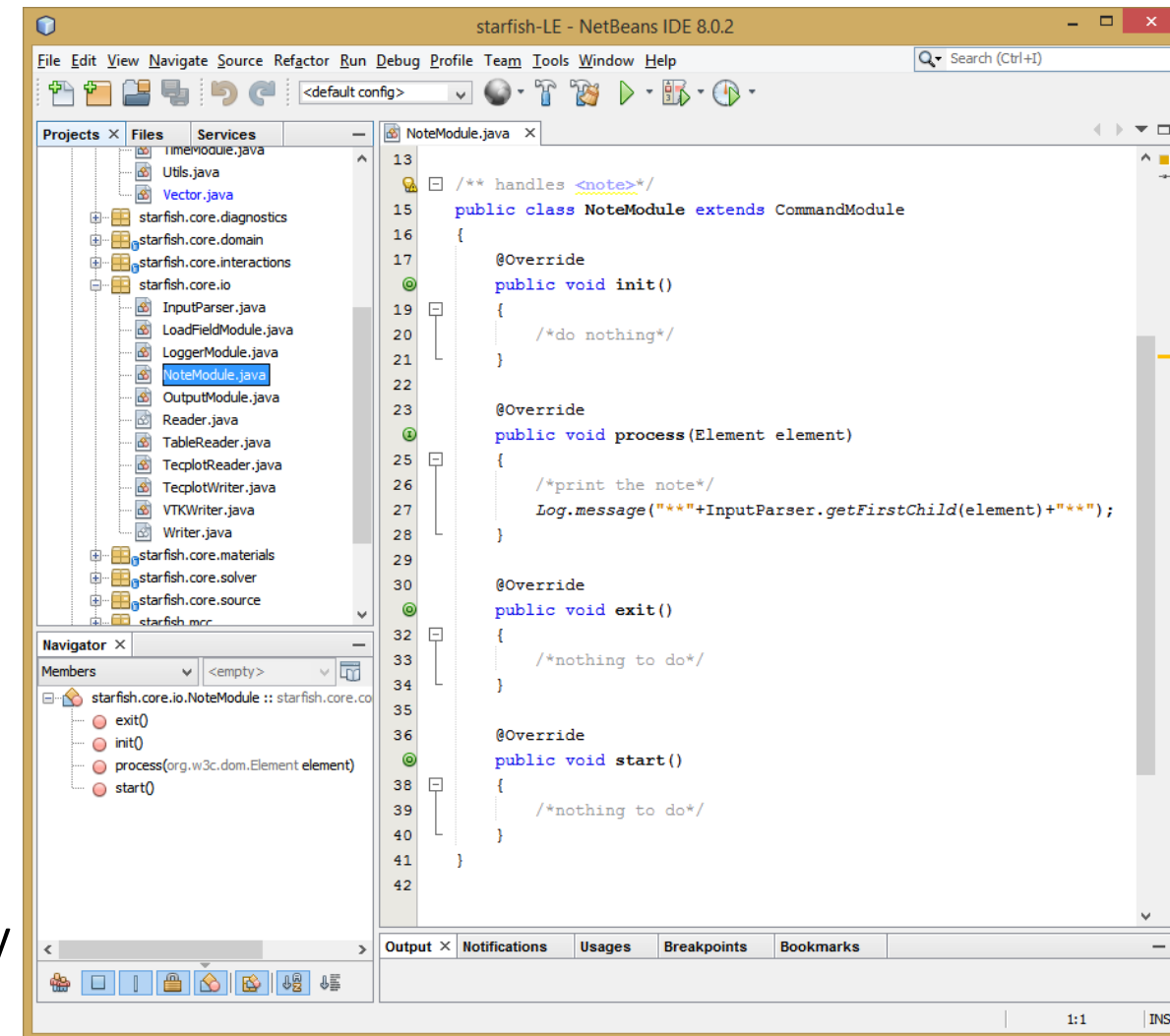
Example: Note Module

- As an example, let's take a look at the Note Module
- This module's process function is called when **<note>** tag is encountered in starfish.xml

```
<simulation>
<note>Starfish Tutorial: Part 1</note>
```

- Only the process method does anything, and that's simply to call **Log.message(..)** with the message given by **InputParser.getFirstChild(element)**
 - In this case this will be "Starfish Tutorial: Part 1"
- The argument to the process method of all modules is the XML element for the handled tag
 - This element can contain many additional child tags as well as attributes. **InputParser** class provides handy accessor methods

```
/*note*/
note = new NoteModule();
modules.put("note", note);
```

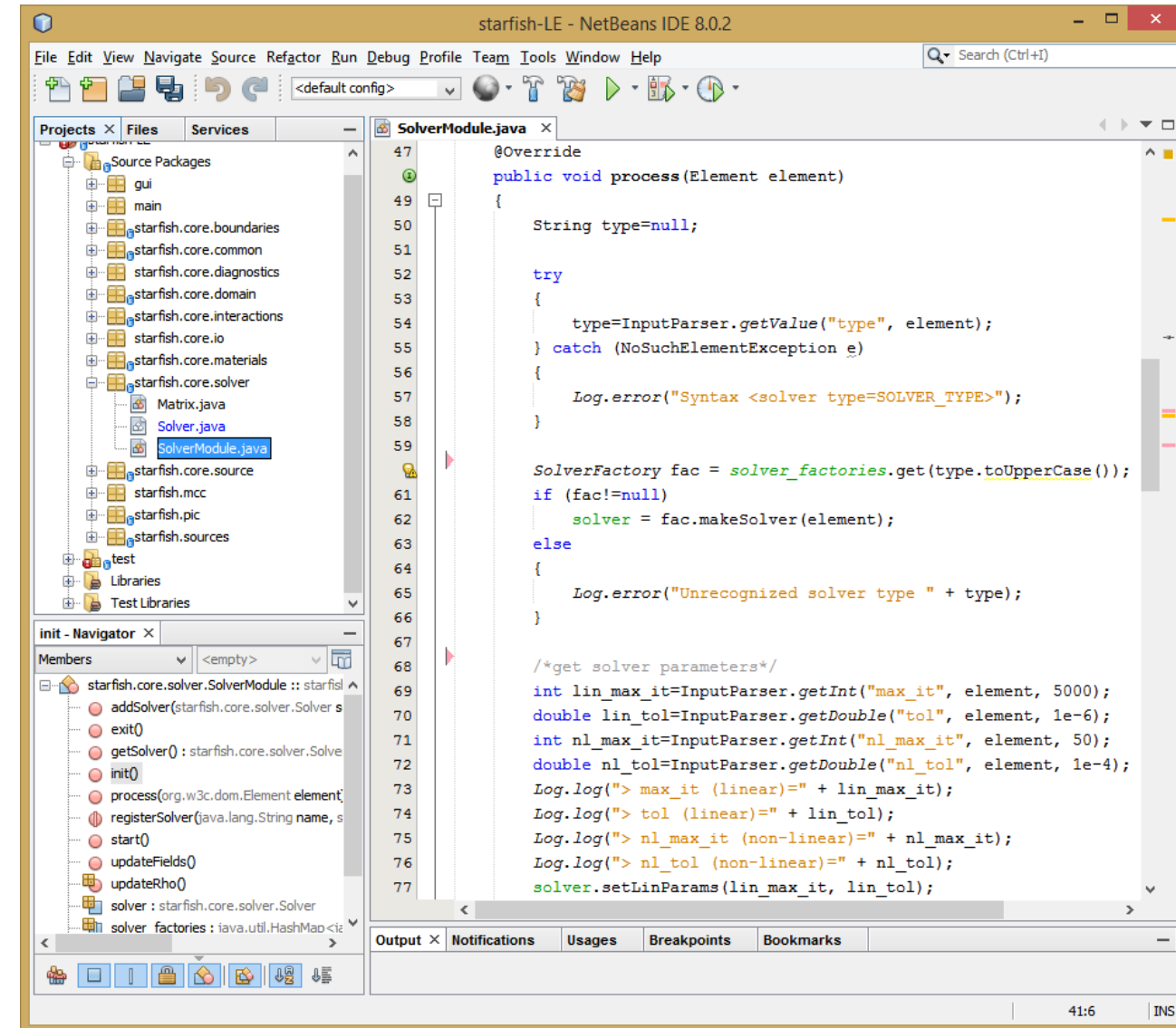


Second Example: Solver

- We now consider a more complex example: the `<solver>` tag
 - In `SolverModule.java` in `starfish.core.solver`

```
<!-- set potential solver -->
<solver type="poisson">
  <n0>1e12</n0>
  <Te0>1.5</Te0>
  <phi0>0</phi0>
  <max_it>1e4</max_it>
  <nl_max_it>25</nl_max_it>
  <tol>1e-4</tol>
  <nl_tol>1e-3</nl_tol>
  <linear>false</linear>
</solver>
```

- `InputParser.getValue/getInt/getDouble...` provide easy way to obtain data regardless of whether it was defined as an *attribute* (type) or *child elements* (n0, Te0...)



Solver Module

- Starfish implements modularity using object oriented programming
- You already saw an example with the modules extending base CommandModule
- Another example is Solver module
- The string provided for “type” is used to retrieve a **SolverFactory** from a hash map
- This factory then generates a solver object that derives from the base **Solver** class
- At no point does the actual solver module know (or care!) what type of a solver the user specified
- Different solver types are registered in **init**
 - You may want to write a **plugin** to register additional solvers

```
try
{
    type=InputParser.getValue("type", element);
} catch (NoSuchElementException e)
{
    Log.error("Syntax <solver type=SOLVER_TYPE>");
}

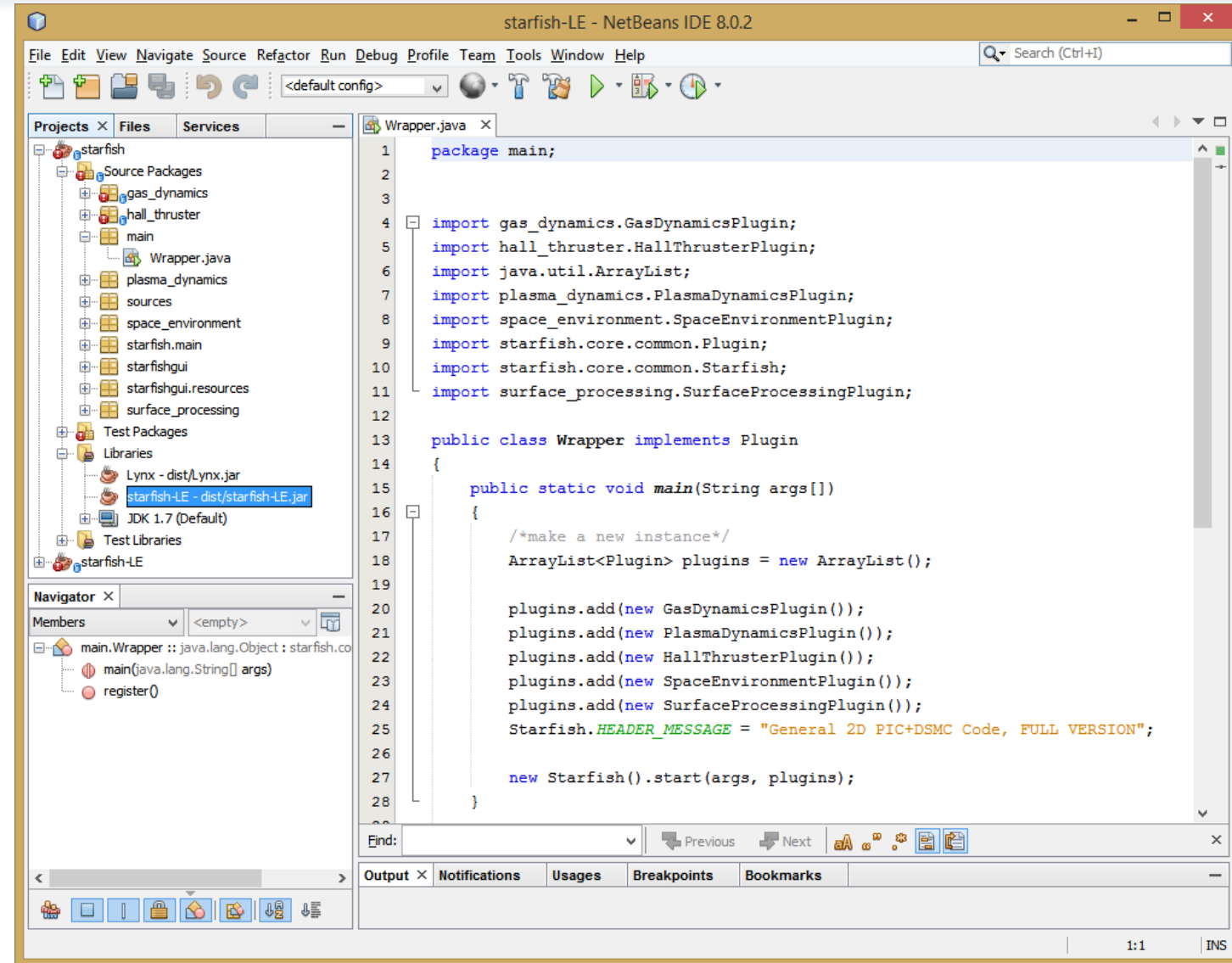
SolverFactory fac = solver_factories.get(type.toUpperCase());
if (fac!=null)
    solver = fac.makeSolver(element);
else
{
    Log.error("Unrecognized solver type " + type);
}
```

```
@Override
public void init()
{
    registerSolver("CONSTANT-EF", ConstantEF.constantEFSolverFactory);
    registerSolver("QN", QNSolver.boltzmannSolverFactory);
    registerSolver("POISSON", PoissonSolver.poissonSolverFactory);
}
```


Plugins

- The easiest way to extend Starfish LE is using **plugins**
 - This is in fact how the full version Starfish code works
- Create a new project and add starfish-LE as a dependency under Libraries
- Define new “main” in which you assemble an ArrayList of **Plugin**, then pass this list to **Starfish().start**
- **Register** method of each plugin will be called after **RegisterModules**
 - Your plugin could for instance call

```
SolverModule.registerSolver("my_solver", mySolverFactory);
```



Plugins

- Here is actual example of the gas dynamics plugin from the full version
 - It registers new material type, based on the diffusion equation
 - Registers DSMC as new material interaction
 - Also registers new collision cross-section sigma

```
package gas_dynamics;

import starfish.core.common.Plugin;
import starfish.core.interactions.InteractionsModule;
import starfish.core.materials.MaterialsModule;

public class GasDynamicsPlugin implements Plugin
{
    @Override
    public void register()
    {
        /*add new material types*/
        MaterialsModule.registerMaterialType("FLUID_DIFFUSION", FluidDiffusion.FluidDiffusionParser);

        /*add new interactions*/
        InteractionsModule.registerInteraction("DSMC", DSMC.DSMCFactory);

        /*add cross-section*/
        InteractionsModule.registerSigma("Bird463", SigmaPlus.makeSigmaBird463);
    }
}
```


Solvers

- The SolverModule contains function called **updateFields**
- This function is called by the Starfish main loop at every time step. The function in turn calls **update** for the defined solver type
- We will now take a look at the simplest solver used in PIC, quasi neutral Boltzmann inversion, $\phi = \phi_0 + kT_{e,0} \ln\left(\frac{n_i}{n_0}\right)$
- Defined in QNSolver.java in starfish.pic
- The factory reads in appropriate values from the input file and instantiates object of type QNSolver (derived from Solver)
- It then returns this object

```
public void updateFields()
{
    /*update rho*/
    updateRho();

    /*call solver*/
    solver.update();

    /*update electric field*/
    solver.updateGradientField();
}
```

```
public static SolverModule.SolverFactory boltzmannSolverFactory = new SolverModule.SolverFactory()
{
    @Override
    public Solver makeSolver(Element element)
    {
        double n0=InputParser.getDouble("n0", element);
        double Te0=InputParser.getDouble("Te0", element);
        double phi0=InputParser.getDouble("phi0", element);
        Solver solver=new QNSolver(n0, phi0, Te0);

        /*log*/
        Starfish.Log.log("Added BOLTZMANN solver");
        Starfish.Log.log("> n0 =" + n0 + " (#/m^3)");
        Starfish.Log.log("> T0 =" + Te0 + " (eV)");
        Starfish.Log.log("> phi0 =" + phi0 + " (V)");

        return solver;
    }
};
```

QN Solver

- Starfish stores mesh-based quantities in object of type Field2D. This object defines functions for interpolation and also getData which returns double[][] containing the actual node values.
- The domain module automatically generates fields to store charge density ρ and potential ϕ
- Each mesh node is also classified as DIRICHLET, OPEN, etc...

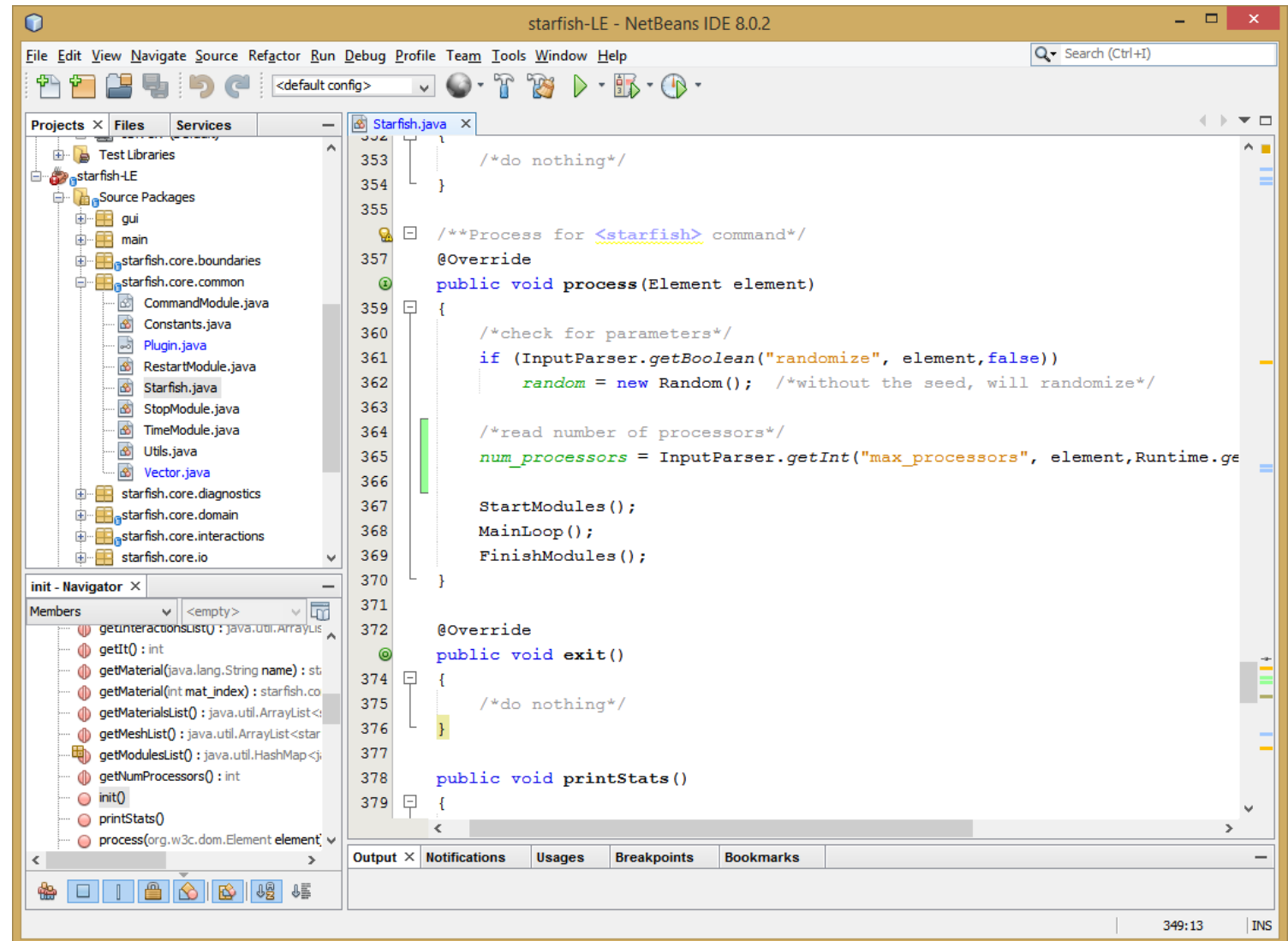
```
@Override
public void update()
{
    for (Mesh mesh:Starfish.getMeshList())
    {
        int ni = mesh.ni;
        int nj = mesh.nj;
        double phi[][] = Starfish.domain_module.getPhi(mesh).getData();
        double rho[][] = Starfish.domain_module.getRho(mesh).getData();

        for (int i=0;i<ni;i++)
            for (int j=0;j<nj;j++)
            {
                if (mesh.nodeType(i, j) == NodeType.DIRICHLET)
                    continue;

                double ion_den = rho[i][j]/Constants.QE;
                if (ion_den>0)
                    phi[i][j] = phi0 + kTe0*Math.log(ion_den/den0);
                else
                    phi[i][j] = phi0 + kTe0*Math.log(1e-10);          /*bac
            }
        }
    }
}
```

Starfish Module

- The simulation is started by the **process** function of StarfishModule
 - Handles <starfish> tag
- First calls **start** on all modules
- The simulation main loop then starts
- The **finish** function is then called



Main Loop

- The main loop performs the typical operations expected in a PIC/DSMC code:
 - Mass is injected into the simulation domain
 - Densities of different material species are computed at a new time step
 - Interactions between different materials are considered
 - Fields are updated to compute forces
 - Restart data is saved as needed
 - Averaging and file output is also performed as needed
- The above steps repeated until some stopping condition
 - Maximum number of time steps is reached
 - Simulation reaches steady state

Main Loop

- This is what it looks like in practice

```
/**simulation main loop*/
public void MainLoop()
{
    Log.message("Starting main loop");

    restart_module.load();

    /*compute initial field*/
    solver_module.updateFields();

    while(time_module.hasTime())
    {
        /*add new particles*/
        source_module.sampleSources();

        /*update densities and velocities*/
        materials_module.updateMaterials();

        /*perform material interactions (collisions and
        interactions_module.performInteractions();

        /*solve potential and recompute electric field*/
        solver_module.updateFields();
```

```
        /*save restart data*/
        restart_module.save();

        /*save animations*/
        animation_module.save();

        /*save average data*/
        averaging_module.sample();

        printStats();

        /*advance time*/
        time_module.advance();
    }/*end of main loop*/

    /*save average data*/
    averaging_module.sample();

    /*check if we have reached the steady state*/
    if (!time_module.steady_state)
        Log.warning("The simulation failed to reach
        steady state!");
```

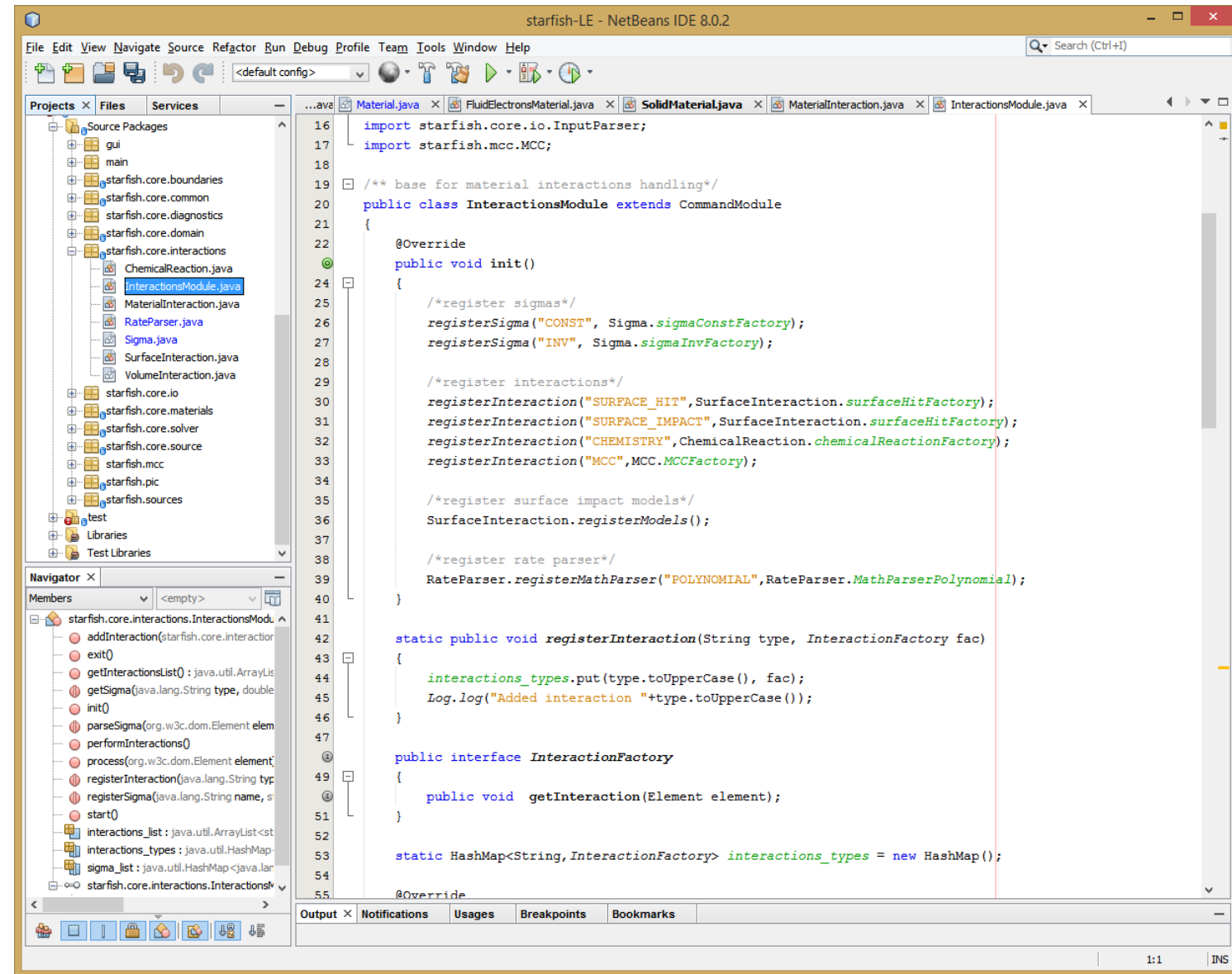
Materials

- The **updateMaterials** function is another example of modularity afforded by object oriented programming
- While Starfish is mainly used for kinetic simulations, the code is not hardwired for this
- Even in a PIC simulation, we merely care about the **density** (and possibly velocities/temperature) of different species, $\rho = \sum_i q_i n_i$
 - The kinetic push of particles $\vec{x}^{k+1} = \vec{x}^k + \vec{v}^{k+0.5} \Delta t$ is only an intermediary step to compute n^{k+1}
- Starfish implements this abstraction in the sense that every material type implements an **update** function which computes the new density, temperature, and bulk velocities at the new time step
 - For kinetic materials, this implies performing the push followed by scatter
 - For fluid materials, this may imply advancing Navier-Stokes solutions forward by Δt

```
/**updates densities of all flying materials*/  
public void updateMaterials()  
{  
    for (Material mat:materials_list)  
        mat.update();  
}
```

Material Interactions

- Interaction between different species is handled by InteractionModule
- Starfish-LE supports three types of interactions: surface impact, chemistry, and MCC
- Full version adds DSMC
- **Surface impact** is an interaction between a material (kinetic or fluid) and a surface boundary: example would be surface recombination or sputtering
- **Chemistry** is a fluid-fluid type interaction. Only the density fields (may be computed from particles) come to play and are used to compute rate constants. Example would be ionization.
- **MCC** is a particle-fluid interaction. The source material must be kinetic and the target is not affected.



```
16 import starfish.core.io.InputParser;
17 import starfish.mcc.MCC;
18
19 /** base for material interactions handling*/
20 public class InteractionsModule extends CommandModule
21 {
22     @Override
23     public void init()
24     {
25         /*register sigmas*/
26         registerSigma("CONST", Sigma.sigmaConstFactory);
27         registerSigma("INV", Sigma.sigmaInvFactory);
28
29         /*register interactions*/
30         registerInteraction("SURFACE_HIT", SurfaceInteraction.surfaceHitFactory);
31         registerInteraction("SURFACE_IMPACT", SurfaceInteraction.surfaceHitFactory);
32         registerInteraction("CHEMISTRY", ChemicalReaction.chemicalReactionFactory);
33         registerInteraction("MCC", MCC.MCCFactory);
34
35         /*register surface impact models*/
36         SurfaceInteraction.registerModels();
37
38         /*register rate parser*/
39         RateParser.registerMathParser("POLYNOMIAL", RateParser.MathParserPolynomial);
40     }
41
42     static public void registerInteraction(String type, InteractionFactory fac)
43     {
44         interactions_types.put(type.toUpperCase(), fac);
45         Log.log("Added interaction "+type.toUpperCase());
46     }
47
48     public interface InteractionFactory
49     {
50         public void getInteraction(Element element);
51     }
52
53     static HashMap<String, InteractionFactory> interactions_types = new HashMap();
54
55     @Override
```

Members

- addInteraction(starfish.core.interaction)
- exit()
- getInteractionsList(): java.util.ArrayLi
- getSigma(java.lang.String type, double
- init()
- parseSigma(org.w3c.dom.Element elem
- performInteractions()
- process(org.w3c.dom.Element element)
- registerInteraction(java.lang.String typ
- registerSigma(java.lang.String name, s
- start()
- interactions_list: java.util.ArrayList<st
- interactions_types: java.util.HashMap
- sigma_list: java.util.HashMap<java.lar
- starfish.core.interactions.Interactions

Conclusion

- That is all for today
- Please visit <https://www.particleincell.com/starfish/> for more information or to contact me with questions