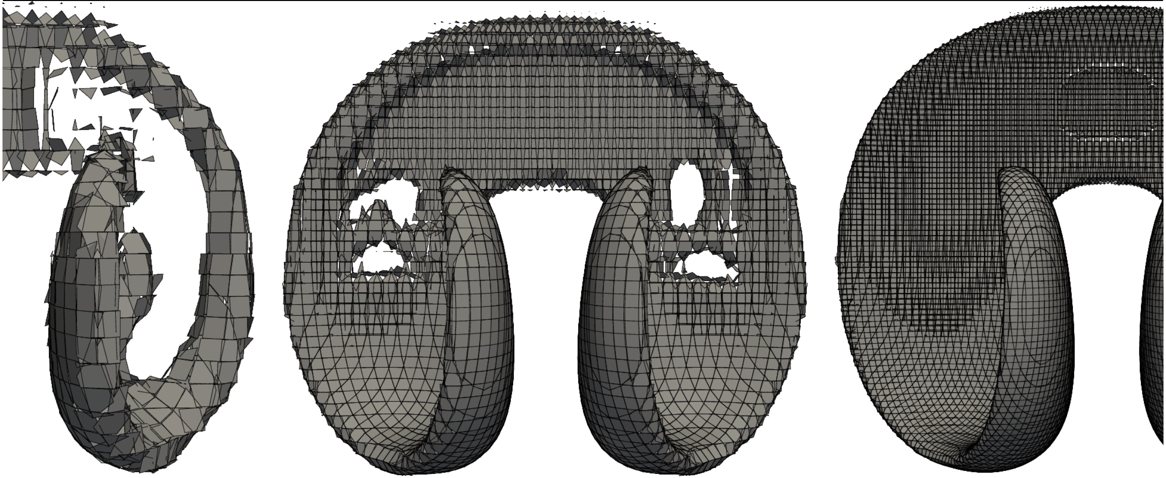
Software Design Patterns in Research Software with examples from OpenFOAM



Disclaimer

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This webinar is about Design Patterns in Research Software, and I'll be using examples from my own work with OpenFOAM, a GPL open-source, but trademarked software:

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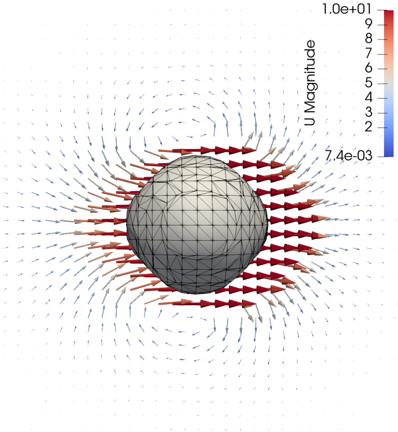
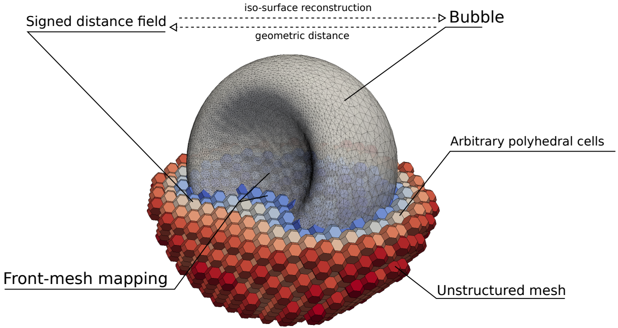


- Fluid phases that do not mix are separated by sharp interfaces (3D surfaces).
- Fluid phases exchange mass, momentum, and energy at fluid interfaces.
- Fluid interfaces deform, break up, and merge.
- **Direct Numerical Simulations** aim to resolve all scales, while ensuring convergence, volume conservation and (parallel) computational efficiency.

Multiphase flows are everywhere

- Fuel-cells, Lab-On-a-Chip, ship/offshore hydrodynamics, coating processes, 3D printing, ...



Level Set / Front Tracking [1, 2, 3, 4] on unstructured meshes [5, 6, 7, 8] **combines**

- Phase-indication (marker field): which fluid phase occupies point $\mathbf{x}$ at time t?
- Signed-distance calculation (redistancing): curvature approximation.
- Front (3D surface mesh) reconstruction: topology changes.
- Point-search operations: vertex-cell (front-mesh) mapping.
- Velocity interpolation.

Research Software

Unstructured Level Set / Front Tracking Method II

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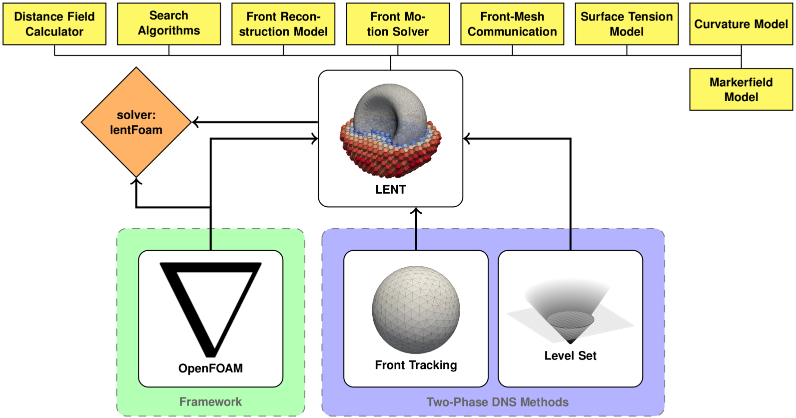
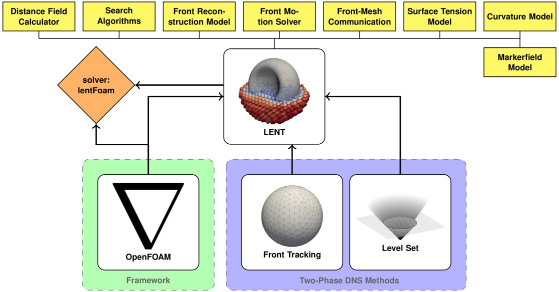


Research software development for LENT is done by Tobias Tolle, Jun Liu, and myself.

Research Software

Unstructured Level Set / Front Tracking Method III



The quality of the method is determined by validation & verification studies.

- There was a another IDEAS/ECP webinar (2021-04-07) that covers a workflow for increasing research software quality in this context.

The sub-algorithms build a hierarchy, whose elements should be interchangeable at runtime without changing existing code.

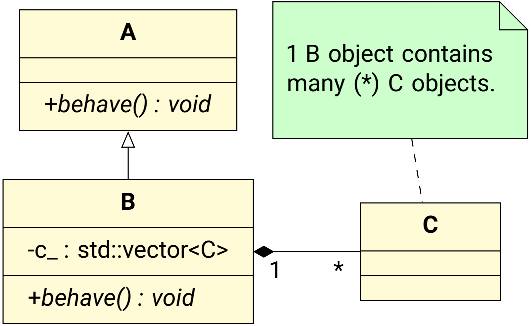
```
lentCommunication
---
// Triangle -> Cell : triangle vertex in cell.
-triangleToCell_: DynamicList<label>
// Vertex -> Cell : vertex in cell.
-vertexToCell_: DynamicList<label>
// Interface cell -> contained triangles (inverse of triangleToCell_)
-interfaceCellToTriangles_: std::map<label, std::vector<label»
// Interface cell -> contained vertices (inverse of vertexToCell_)
-interfaceCellToVertices_: std::map<label, std::vector<label»
// Cell -> Nearest Triangle.
-cellsTriangleNearest_: DynamicList<pointIndexHit>
// Point -> Nearest Triangle.
-pointsTriangleNearest_: DynamicList<pointIndexHit>
---
+update(): void
+updateVertexToCell(): void
+updateInterfaceCellToTriangles(): void
+updateInterfaceCellToVertices() void
```

Cannot talk about the hierarchy without understanding its elements first.

- Complex things (e.g. Front-Mesh communication) are **abstracted** in C++ as User-Defined Types (UDT, **classes**).
- A class **encapsulates** its data (attributes, **data members**).
- A class implements **behavior**: **member functions** that change the data members.
- Access specifiers
  - **+**: accessible from outside (public)
  - **-**: inaccessible from outside (private)
- Private data (**-**) = narrow focus.

Object-Oriented Programming Crash Course II

Dynamic Polymorphism on one slide



Cannot talk about the hierarchy without understanding the interactions between its elements (UML)

- Classes **inherit (derive)** from other classes: A inherits from B.
- Classes **contain (composit) objects** of other classes: A contains C.

Dynamic polymorphism: **addressing an object of the derived class via a pointer to the base class** can be used to set the type of the object **at runtime**.

```
configData input{"path/to/file"};
smart_pointer<A> Aptr = A::New(input);
Aptr->behave(); // B chosen in input!
```

Support programming on a higher-level of abstraction

- A high-level of abstraction is crucial - **thinking in terms of complex objects; not getting lost in low-level details.**
- **Design patterns modularize abstractions' functionality and their interaction:**
  - What do **`parcels`** require from the **`mesh`** in order to **`evolve`**?
  - Which objects are written with **`runTime.write()`**?

```
// Peform mesh changes
mesh.update()

// Update moving reference frame
MRF.update();

// Make the fluxes relative to the mesh-motion
fvc::makeRelative(phi, rho, U);

// Evolve the particle cloud
parcels.evolve();

// Evolve the surface film
surfaceFilm.evolve();

// Write data
runTime.write();
```

Software Design Patterns in Research Software
Examples from OpenFOAM

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Software Design Patterns [9]: code structures that **combine inheritance and composition** and have emerged repeatedly as **best-practice solutions for specific design problems**.

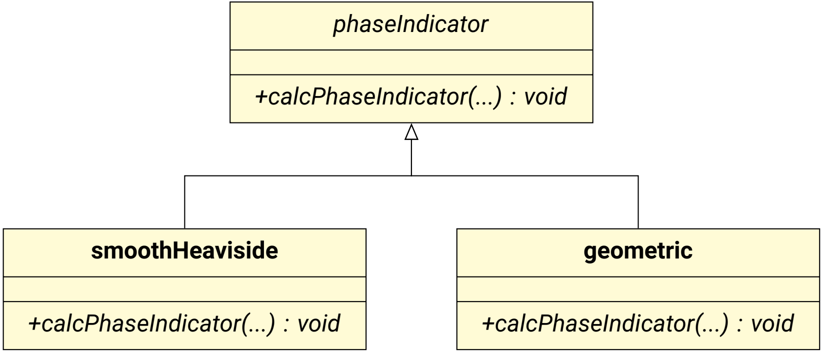
Software Design Patterns (examples from OpenFOAM)

- Template Method: boundary conditions, viscosity models, discretization schemes, ...
- Strategy: transport models, solvers and pre-conditioners, ...
- Observer: dynamic mesh handling, IO synchronization, ...
- OpenFOAM's Creational Pattern: Runtime-Type Selection (RTS), **used everywhere**.

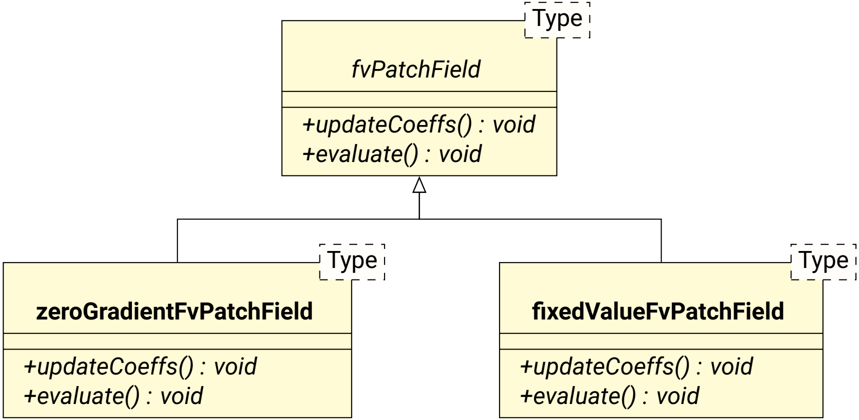
Not covered in this webinar

- Facade: Level Set / Front Tracking (Additional Slides)
- Curiously Recurring Template Pattern (CRTP): Discrete Parcel Method (Additional Slides)

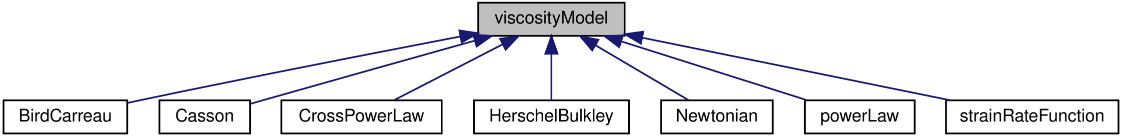
Virtual member function: implements different behavior in a derived class.



OpenFOAM's boundary conditions



Viscosity model hierarchy



and the nu Template Method

```
//      Return the laminar viscosity.
virtual tmp<volScalarField>  nu() const = 0;
```

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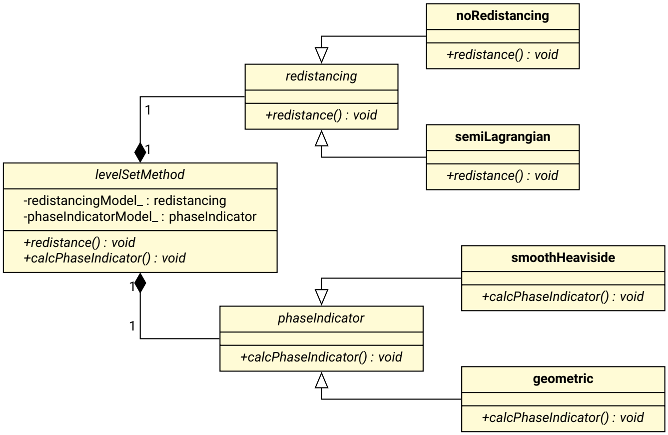
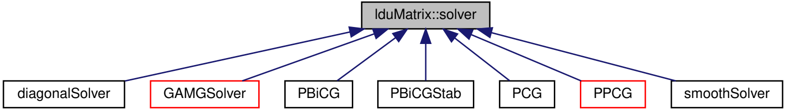
- The Template Method is the virtual member function (method) to be overridden, it has nothing to do with C++ templates.
- **Best practice**: utilize virtual member functions (dynamic polymorphism) to extend existing libraries without modifying them.



- A single class contains different sub-algorithms.
- Sub-algorithms can be selected at runtime.
- Combining sub-algorithms does not require programming.
- Basically the composition of the Template Method for sub-algorithm hierarchies.
- **Best practice**: when unsure about sub-algorithm combinations, implement the Strategy Pattern.



Foam::lduMatrix

```
solverPerf = lduMatrix::solver::New
(
    psi.name() + pTraits<Type>::componentNames[cmpt],
    *this,
    bouCoeffsCmpt,
    intCoeffsCmpt,
    interfaces,
    solverControls
)->solve(psiCmpt, sourceCmpt, cmpt);
```

selects a linear solver as a (solution) Strategy.

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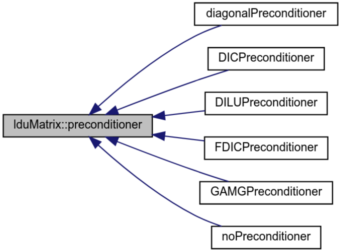
```
autoPtr<lduMatrix::preconditioner> preconPtr =
    lduMatrix::preconditioner::New
    (
        *this,
        controlDict_
    );
```



Each `lduMatrix::solver` selects its pre-conditioner as a (preconditioning) Strategy.

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From GoF Design Patterns Book [9]: ”Define a one-to-many dependency between objects so that when one object changes state, all its dependents are notified and updated automatically.”

Subject

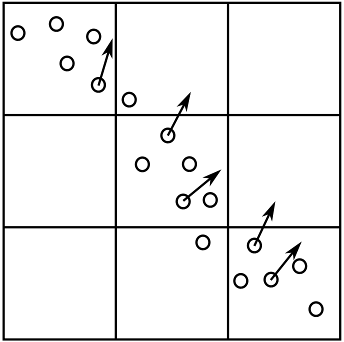
- Has a state that is updated when the subject is modified.
- Forwards the `update` call to a list of its observers.

```
void subject::update()
{
    for (auto& observer : observers_)
        observer.update();
}
```

Observers

- Implement the `update` interface.
- Register themselves to the subject via their constructor.

Example: Particles tracked along Lagrangian trajectories in an Eulerian (background) mesh



- Lagrangian-cloud particles know which cell they are in.
- The **Eulerian mesh is the subject** that changes state.
- **Lagrangian particle cloud is an observer**.
- Vice-versa is also relevant, resulting in 6-way coupling (mass, momentum, energy exchange $\times$ 2).

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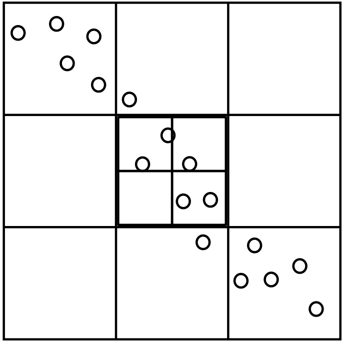
Example: Particles tracked along Lagrangian trajectories in an Eulerian (background) mesh



1. The Eulerian mesh (subject) changes state: it is refined.
2. The Eulerian mesh (subject) updates its observers

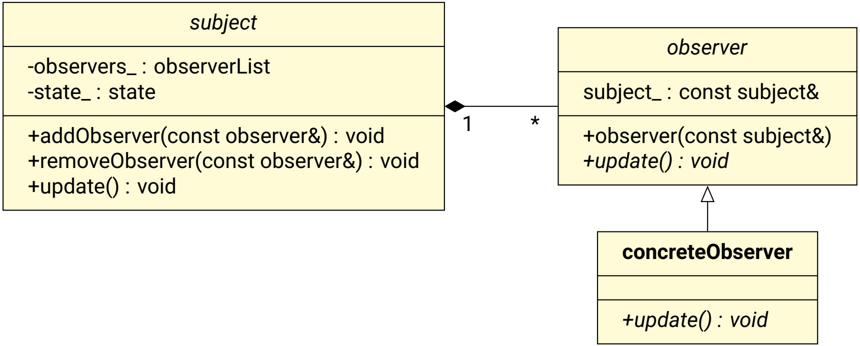
```
for (auto& observer : observers)
    observer.update(cellMap);
```

3. The Lagrangian cloud is an observer

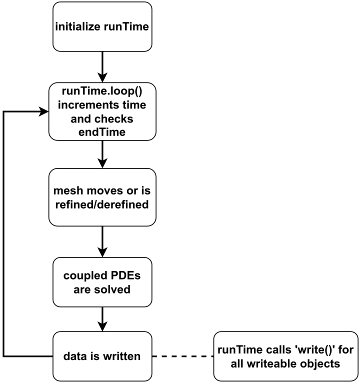
```
for (auto& particle : cloud)
{
    auto found = cellMap.find(particle.cellLabel());
    if (found)
    {
        auto newCellLabel = cloud.find(particle, cellMap);
        particle.setCellLabel(newCellLabel);
    }
}
```

Software Design Patterns in Research Software

Observer IV



Example: write all data that should be written using the same output frequency



A single

```
runTime.write();
```

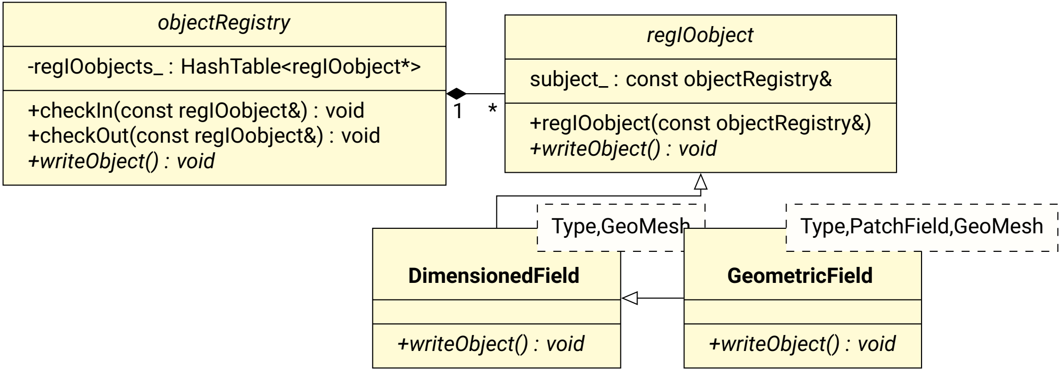
call in the solver application, and

```
for (regIOobject& : regIOobjects)
    regIOobject.writeObject();
```

in the **`Time`** class is better than manually typing

```
if (runTime.writeTime())
{
    alpha.write();
    surfaceMesh.write();
    cloud.write();
    ...
}
```

in a solver application. It is necessary for reactive flows.



`Foam::Time` controls simulation (write) time and it is an `objectRegistry`.
`Foam::Time::write()` loops over all registered fields and writes them to the drive.

Software Design Patterns in Research Software

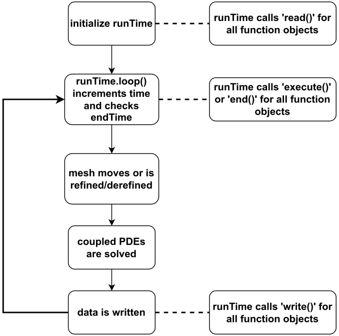
Observer VII

```
while (runTime.loop()) // runTime state
{
    #include "CourantNo.H"

    // Pressure-velocity PISO corrector
    {
        #include "UEqn.H"
        // --- PISO loop
        while (piso.correct())
        {
            #include "pEqn.H"
        }
    }

    laminarTransport.correct();
    turbulence->correct();
    runTime.write(); // runTime state
}
```

- A CFD solver is a procedural application.
- Fields (velocity, pressure, density, temperature, ...) are global variables, modified by FVM differential operators / solution algorithms.
- Observer Pattern simplifies custom post-processing using OpenFOAM Function Objects (not C++ function objects).

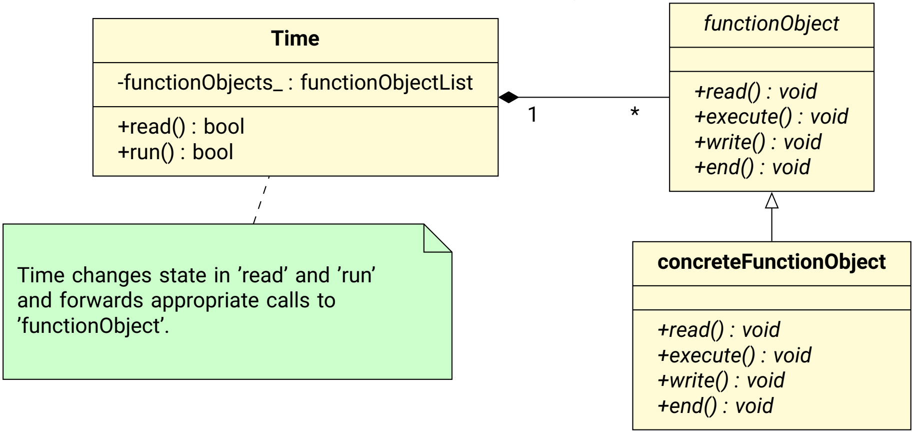
Software Design Patterns in Research Software

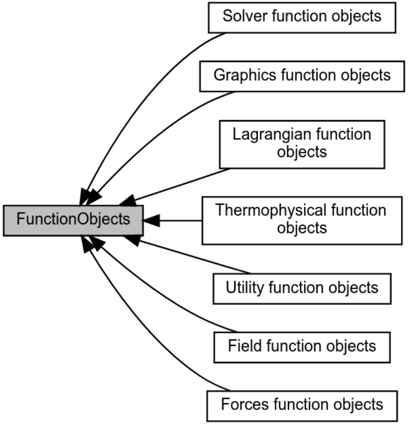
Observer VIII



- **runTime** is the **subject** that changes state:
  - time-step increment
  - reached output time
  - reached end time
- **Function Objects** are the **observers**.
  - They access other (mesh or time) observers and ”work” on them: compute the maximal and minimal temperature, sample the veloity over a line segment, ...
- **OpenFOAM Function Objects change solver behavior without modifying solver application’s source code.**

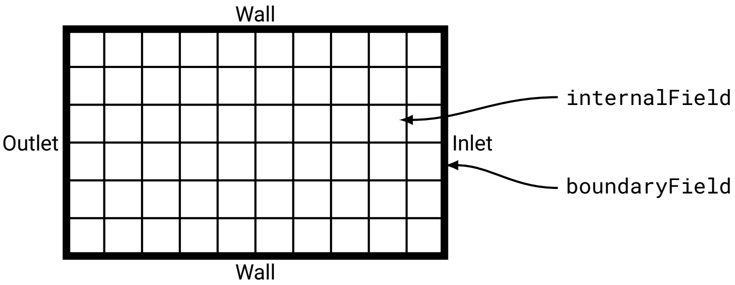
OpenFOAM Function Objects





OpenFOAM Function Objects

- Observer is also used within Function Objects themselves: **`fvMesh`** is an **`objectRegistry`**, FOs fetch objects registered to the mesh and perform live (post-)processing tasks as the simulation runs.
- This saves research time and HPC resources (**green computing**): live post-processing can be used to stop large-scale simulations as soon as the results are too erroneous.



Geometric Fields:

- Values grouped into **`internal`** values and **`boundary patch`** values.
- Internal values associated with **`cell centers`** (alternatively: face centers or cell corner-points), boundary with face centers (alternatively, face corner-points).

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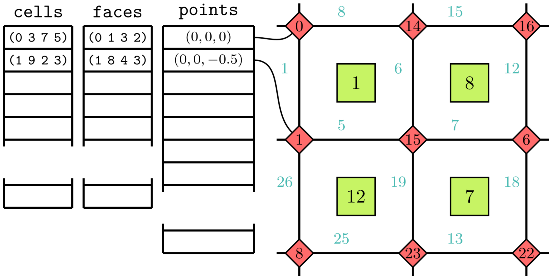

- The mesh connectivity changes with mesh refinement / unrefinement.
  - GeometricFields do not map to the mesh.
- Mesh motion stretches/compresses finite volume faces.
  - Volumetric fluxes change magnitudes.
- Each time the mesh is **updated**, the fields are **updated**.
- `fvMesh` is a `Subject`, `GeometricFields` are the `Observers`.

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Best practice

- Use when the same member function (**`write`**, **`map`**, **`execute`**, **`read`**, **`update`**) must be called for many objects.

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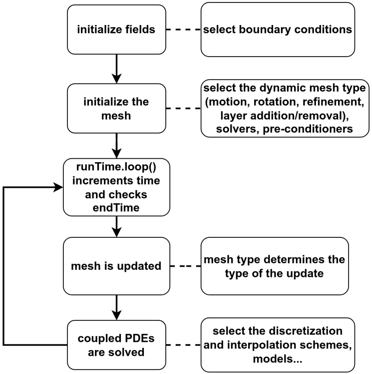

- Using a Creational Pattern to construct objects (select types) at runtime makes the solver application highly configurable.
- No modification to the solver application is required to select boundary conditions, dynamic mesh handling, discretization and interpolation schemes, models, ...

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- Runtime Type Selection (RTS) is OpenFOAM's Creational Pattern.
- **RTS constructs OpenFOAM objects based on user input.**
  - Ease-of-use: RTS tables provide information about available types and their parameters.
  - Simplifies research: "constructing" the PDE discretization and solution via configuration files.
- OpenFOAM's RTS in a nutshell:
  - RTS stores a class-static hash-table that maps strings to a virtual member function pointer.
  - This so-called RTS table is initialized for the base class in its implementation file.
  - The RTS table is extended in implementation files of derived classes.
  - The RTS code is generated using preprocessor macros
    - RTS declaration and definition
    - RTS table extension

- **Best practice:** if a research software provides a creational pattern, learning how to use it simplifies testing and saves time in research, compared to hacking your own ”if-then-else” code for different types.

OpenFOAM RTS macros expanded with **gcc -E**: no need to learn how this works to use it

```
typedef autoPtr<implicitSurface> (*ITstreamConstructorPtr)( ITstream is );
typedef ::Foam::HashTable <ITstreamConstructorPtr, ::Foam::word, ::Foam::Hash<::Foam::word> > ITstreamConstructorTableType;
typedef ::Foam::HashTable < std::pair<::Foam::word,int>, ::Foam::word, ::Foam::Hash<::Foam::word> > ITstreamConstructorCompatTableType;
static ITstreamConstructorTableType* ITstreamConstructorTablePtr_;
static std::unique_ptr<ITstreamConstructorCompatTableType> ITstreamConstructorCompatTablePtr_;
static ITstreamConstructorCompatTableType& ITstreamConstructorCompatTable();
static void ITstreamConstructorTablePtr_construct(bool load);
static ITstreamConstructorPtr ITstreamConstructorTable(const ::Foam::word& k);
template<class implicitSurfaceType> struct addAliasITstreamConstructorToTable {
explicit addAliasITstreamConstructorToTable ( const ::Foam::word& k, const ::Foam::word& alias, const int ver ) {
    ITstreamConstructorCompatTable() .set(alias, std::pair<::Foam::word,int>(k,ver));
}
};
template<class implicitSurfaceType> struct addITstreamConstructorToTable {
    static autoPtr<implicitSurface> New ( ITstream is ) {
        return autoPtr<implicitSurface>(new implicitSurfaceType (is));
    } explicit addITstreamConstructorToTable ( const ::Foam::word& k = implicitSurfaceType::typeName ) {
        ITstreamConstructorTablePtr_construct(true);
        if (!ITstreamConstructorTablePtr_->insert(k, New)) {
            std::cerr << "Duplicate entry " << k << " in runtime table " << "implicitSurface" << std::endl;
            ::Foam::error::safePrintStack(std::cerr);
        }
    } ~addITstreamConstructorToTable() {
        ITstreamConstructorTablePtr_construct(false);
    } addITstreamConstructorToTable (const addITstreamConstructorToTable&) = delete;
    void operator= (const addITstreamConstructorToTable&) = delete; };
```

Software Design Patterns in Research Software

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Software Design Patterns [9]: design structures that **combine inheritance and composition** and have emerged repeatedly as **best-practice solutions for specific design problems**.

Software Design Patterns (examples from OpenFOAM)

- Template Method: boundary conditions, viscosity models, discretization schemes, ... ✓
- Strategy: transport models, solvers and preconditioners, ... ✓
- Observer: dynamic mesh handling, IO synchronisation ✓
- OpenFOAM's Creational Pattern: Runtime-Type Selection (RTS), **used everywhere**. ✓

Not covered in this webinar

- Facade: Level Set / Front Tracking (Additional Slides)
- Curiously Recurring Template Pattern (CRTP): Discrete Parcel Method (Additional Slides)

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```
fvScalarMatrix TEqn
(
      fvm::ddt(T)
    + fvm::div(phi, T)
    - fvm::laplacian(DT, T)
 ==
      fvOptions(T)
);
TEqn.solve();
```

We didn't cover everything, but

- **Type Lifting** for geometric fields and differential operators "+" **generic traits** for tensor rank calculation "+" **Template Method** and **RTS** for discretization and interpolation schemes + **Strategy** and **RTS** for linear solvers "="
  OpenFOAM's Domain-Specific Language for Partial Differential Equation discretization.

- Design Patterns speed up research, if there is a high degree of methodological uncertainty: we don’t know which algorithms will work, in which combination.
- Avoiding dogmatism: not every design question has to be answered by a pattern.
- When dealing with legacy research code, it helps a lot understand its design principles: cargo-cult programming is quicker, but can tank research projects in the long-run.

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Funded by the German Research Foundation (DFG) - Project-ID 265191195 - CRC 1194

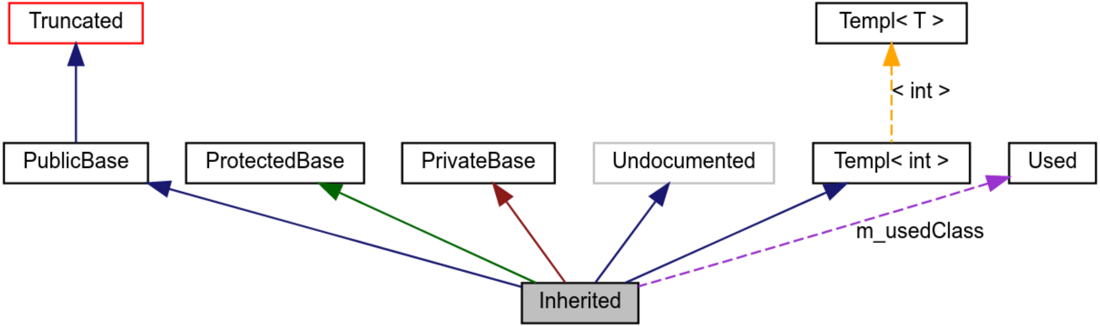
CRC 1194

Interaction between Transport and Wetting Processes

Z-INF sub-project (Prof. Dr. rer. nat. Dieter Bothe, Prof. Dr. Christian Bischof)

Additional Slides and References

OpenFOAM’s UML legend



C++ Generic Programming in OpenFOAM (crash course) I

Useful techniques

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OpenFOAM uses Generic Programming (GP) for type lifting and traits.

- **Type lifting:** same code is **re-used without modification** with completely unrelated types. In OpenFOAM, everything is type-lifted for all tensors (scalar, vector, tensor, symmetric tensor, spherical tensor).
- **Template specialization:** e.g. specializing a fixed value **tensor** boundary condition as a **scalar** total pressure boundary condition.
- **Traits:** determine the tensor rank of the return type of $\nabla \mathbf{v}$ (used in differential operators).

C++ Generic Programming in OpenFOAM (crash course) II

C++ templates: `if-then-else` for types

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```
template<class Type>
Type sum(const UList<Type>& f)
{
    if (f.size())
    {
        Type Sum = pTraits<Type>::zero;
        TFOR_ALL_S_OP_F(Type, Sum, +=, Type, f)
        return Sum;
    }
    else
    {
        return pTraits<Type>::zero;
    }
}
```

template(Merriam Webster dictionary)

- a gauge, **pattern, or mold** (such as a thin plate or board) used as a **guide to the form of a piece being made**
- a molecule (as of DNA) that serves as a **pattern for the generation of another** macromolecule (such as messenger RNA)
- something that establishes or **serves as a pattern**

C++ Generic Programming in OpenFOAM (crash course) III

Type Lifting

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```
template<class Type>
class fixedValueFvPatchField
:
    public fvPatchField<Type>
{
```

- A boundary condition class template is type-lifted all tensors.
- The same is done for arithmetic field operators, discretization schemes, ...

```cpp
#define makePatchTypeFieldTypedef(fieldType, type) \
    typedef type##FvPatchField<fieldType> \
        CAT4(type, FvPatch, CAPITALIZE(fieldType), Field);

class totalPressureFvPatchScalarField
:
    //     fixedValueFvPatchField<scalar>
    public fixedValueFvPatchScalarField
```

- Specialized boundary conditions for pressure, temperature, velocity,...

C++ Generic Programming in OpenFOAM (crash course) V

Traits I

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```
template<class Type>
tmp
<
    GeometricField
    <
        typename outerProduct<vector,Type>::type,
        fvPatchField,
        volMesh
    >
>
grad (const tmp<GeometricField<Type, fvsPatchField, surfaceMesh>>& tssf)
{
    ...
```

- The return-type of the gradient function template is determined based on the argument.
- The gradient of a scalar field is a vector field.

C++ Generic Programming in OpenFOAM (crash course) VI

Traits II

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```
template<class arg1, class arg2>
class outerProduct
{
public:

    typedef typename typeOfRank
    <
        typename pTraits<arg1>::cmptType,
        direction(pTraits<arg1>::rank) + direction(pTraits<arg2>::rank)
    >::type type;
};
```

- Traits determine the component types of scalars, vectors, tensors.
- Component type and rank traits promote outer product type.
- **One only needs this if the research involves extending the set of differential operators.**
- **Type-lifting is enough for 99% of research using OpenFOAM.**

Combining Object-Oriented and Generic Programming

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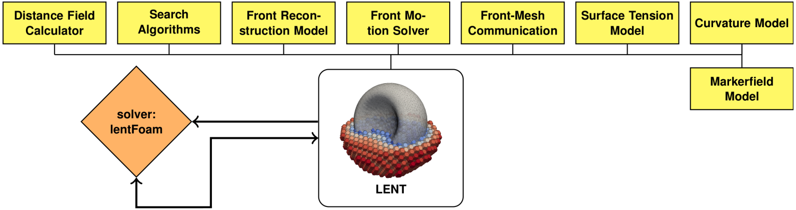
```
template<class Type>
class inletOutletFvPatchField
:
    public mixedFvPatchField<Type>
{

protected:

    // Protected data

        //- Name of flux field
        word phiName_;
```

- OpenFOAM combines Generic and Object Oriented Programming.
- Makes sense: e.g. the **inlet-outlet** boundary condition **is a mixed boundary condition**, and it **behaves exactly the same way for different tensors**.
- Using OOP here for the tensor **Type** is much more cumbersome and potentially slower than using type lifting.



Facade hides the complexity of sub-algorithms, for example, the order of execution:

```
void lent::advect()
{
    frontReconstructionModel->reconstructFront(); // Updates Front-Mesh communication.
    frontMotionSolver->evolveFront(); // Front-Mesh Comm. update, using Search Algorithms.
    distanceFieldCalculator->calcSignedDistances();
}
```

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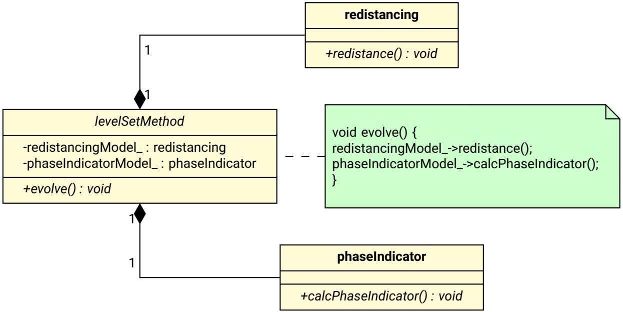

Best practice: implement sub-algorithms as Strategies, test them individually, then integrate them in a specific execution order using Facade.

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```
template<typename Parameter>
class MyType
    : public Parameter
```

- Class template inheriting from its template parameter.
- Used in generic programming for policy-based design: extending the host class (**`MyType`**) interface by inheriting from the template parameter (**`Parameter`**).

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Curiously Recurring Template Pattern (CRTP) is **couriously recurring and nested** for the Lagrangian / Eulerian Discrete Parcel Method.

```
template<class CloudType>
class ReactingCloud
:
    public CloudType,
    public reactingCloud
{
```

```
namespace Foam
{
    typedef ReactingCloud
    <
        ThermoCloud
        <
            KinematicCloud
            <
                Cloud<basicReactingParcel>
            >
        >
    > basicReactingCloud;
}
```

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