

IFEM - getting started

Knut Morten Okstad

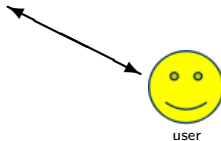
SINTEF ICT, Department of Applied Mathematics

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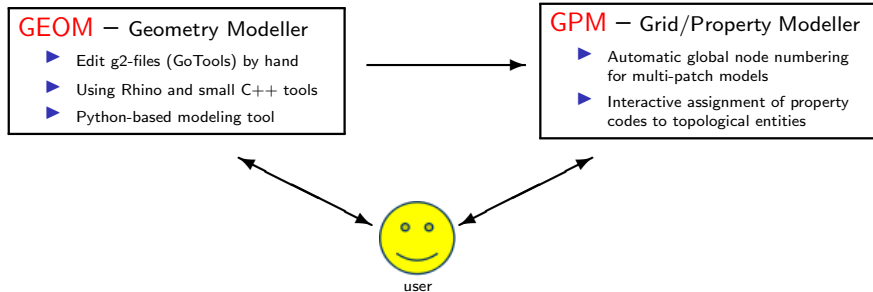
IFEM module overview

GEOM — Geometry Modeller

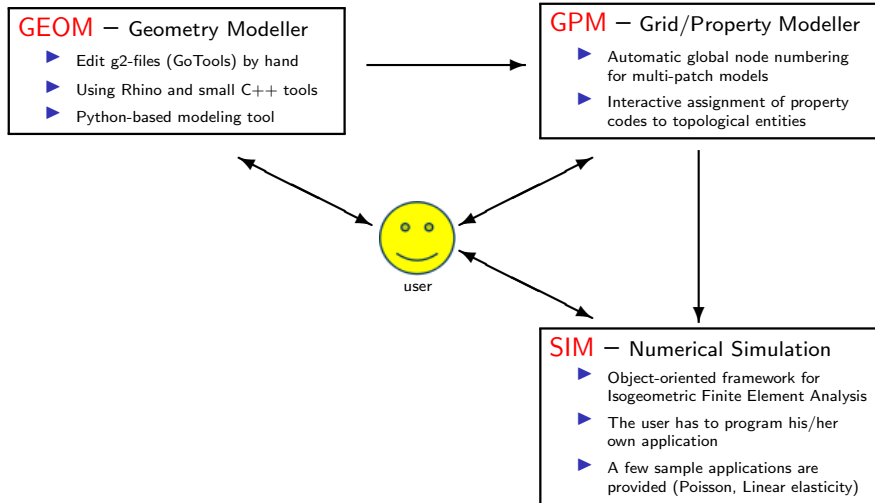
- ▶ Edit g2-files (GoTools) by hand
- ▶ Using Rhino and small C++ tools
- ▶ Python-based modeling tool



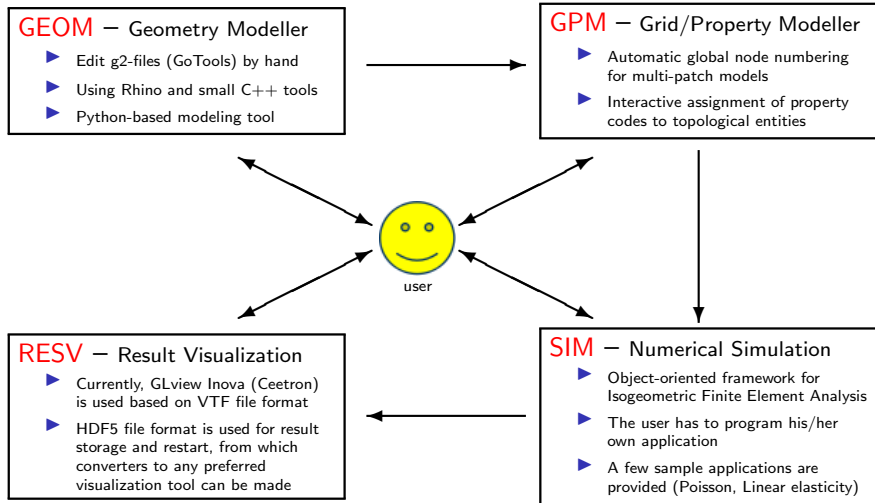
IFEM module overview



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Major class hierarchies of the SIMulation environment

1. NonLinSIM - Nonlinear simulation driver

- ▶ Administers time/load step loop of the solution algorithm
- ▶ Newton iteration loop, convergence check, configuration update

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 - ▶ Interface to equation solvers (direct/iterative, serial/parallel)
 - ▶ Sub-classes for various linear equation solver packages

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 - ▶ Administers the element loop and numerical integration loop within a block (spline patch)
 - ▶ Sub-classes depending on discretization (Splines/NURBS, Lagrange, Spectral)
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 - ▶ Administering the integration point loop with
 - ▶ Subclass **User/Application level** problem

ASM class hierarchy - *the Isogeometry level*

ASMbase

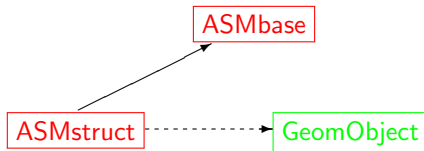
→ 'is-a' relationship

- - -> 'has-a' relationship

IFEM classes

GoTools classes

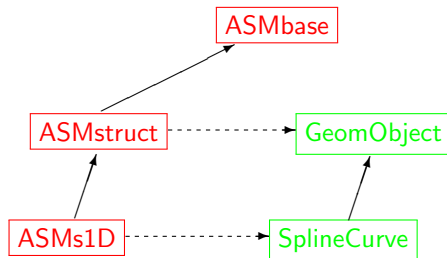
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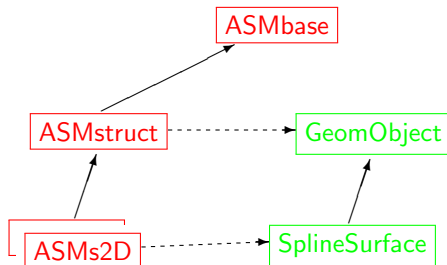
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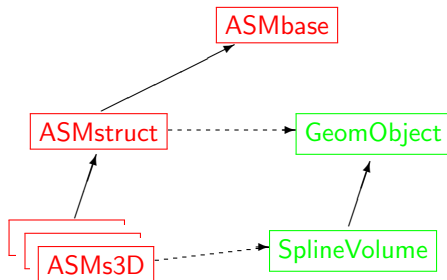
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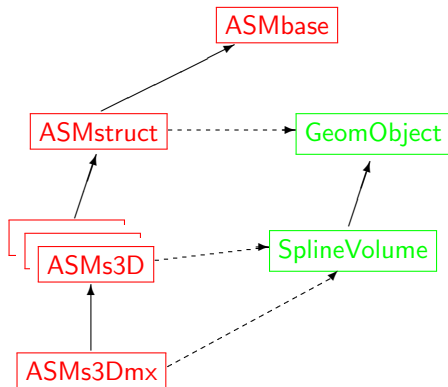
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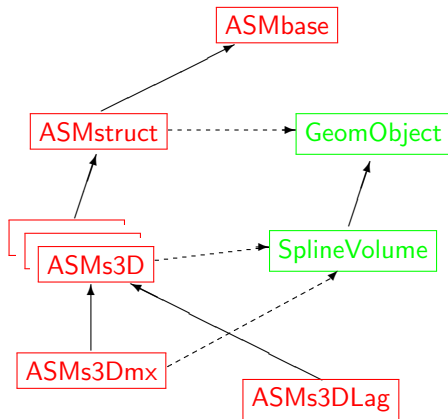
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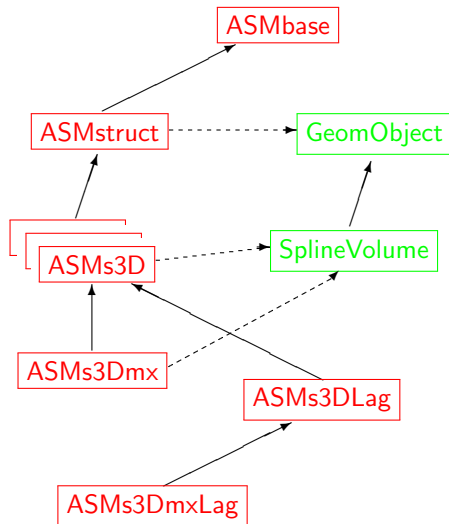
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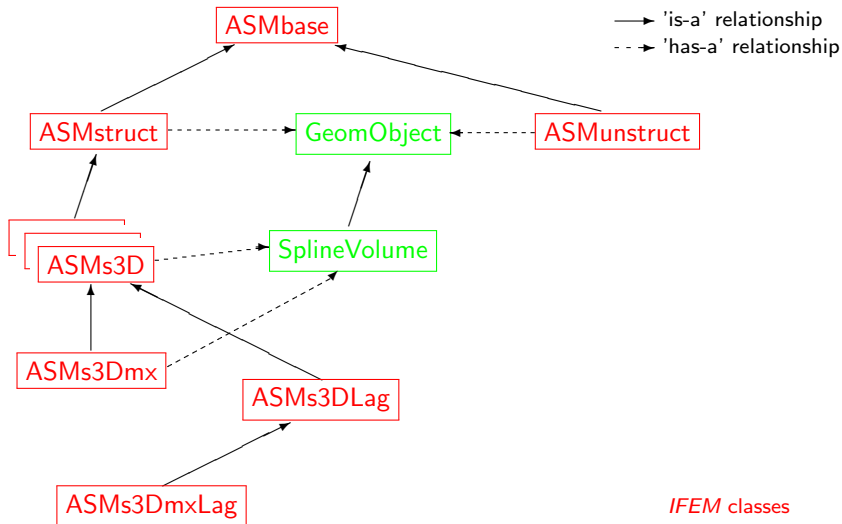
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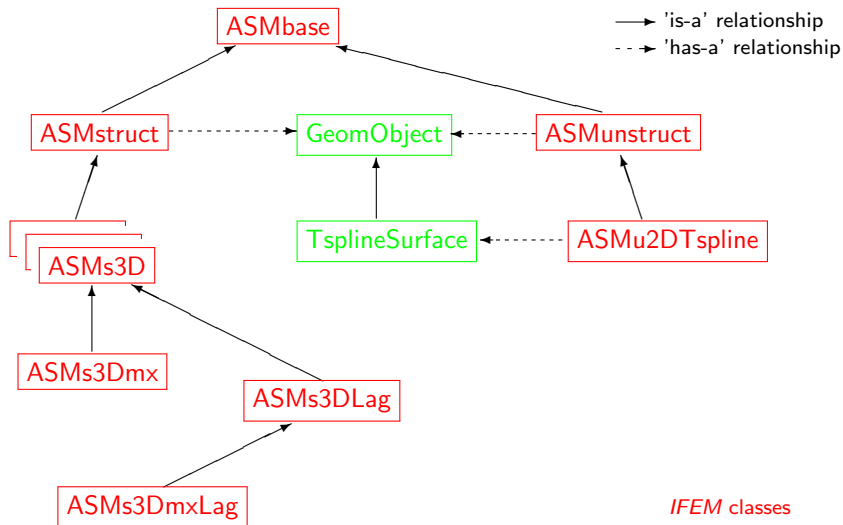
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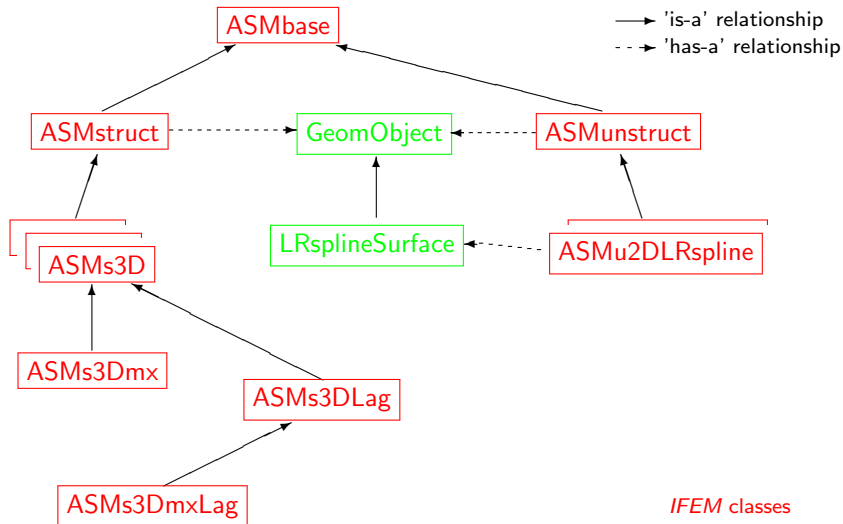


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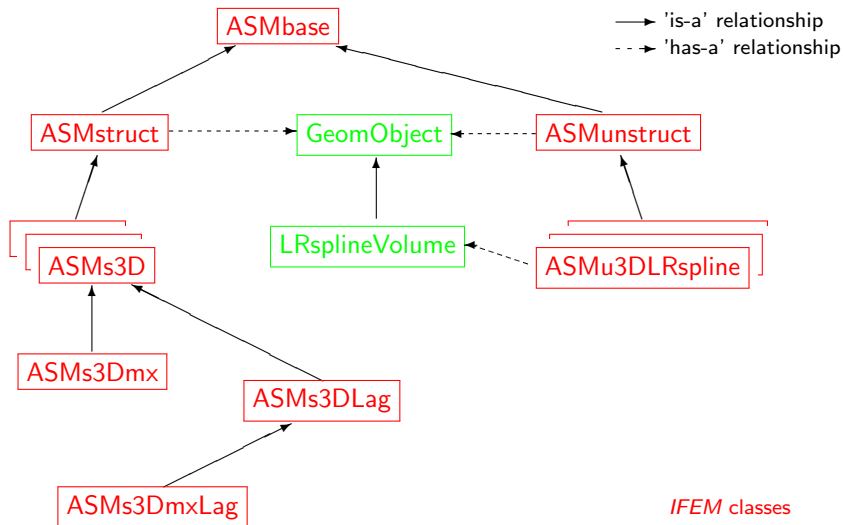
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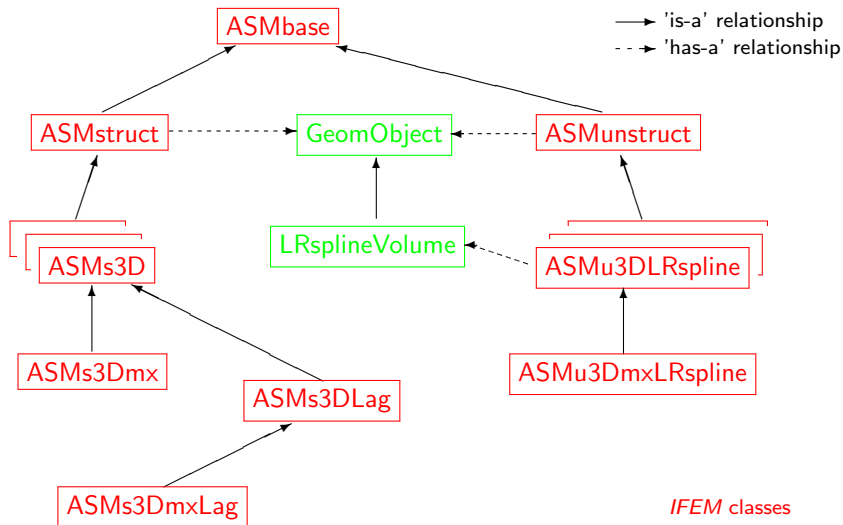
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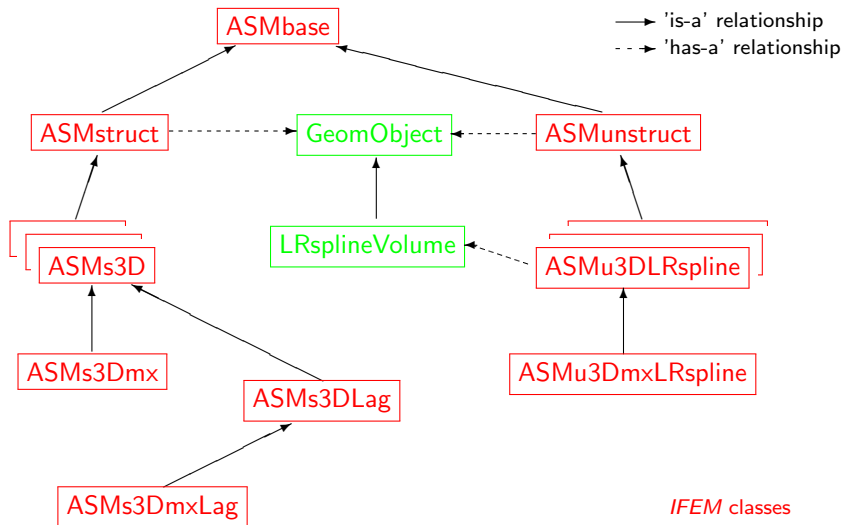
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ASM class hierarchy - the Isogeometry level



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ASM class hierarchy - the Isogeometry level



ASMbase is the interface between the isogeometric FE procedures, and the solution algorithms (from above) and the physical problem to be solved (from below).

The main ASM methods

```
class ASMbase
{
public:
    //! \brief Evaluates an integral over the interior patch domain.
    //! \param integrand Object with problem-specific data and methods
    //! \param glbInt The integrated quantity
    //! \param[in] time Parameters for nonlinear/time-dependent simulations
    virtual bool integrate(Integrand& integrand,
                          GlobalIntegral& glbInt, const TimeDomain& time) = 0;

    //! \brief Evaluates a boundary integral over a patch face/edge.
    //! \param integrand Object with problem-specific data and methods
    //! \param[in] lIndex Local index of the boundary face/edge
    //! \param glbInt The integrated quantity
    //! \param[in] time Parameters for nonlinear/time-dependent simulations
    virtual bool integrate(Integrand& integrand, int lIndex,
                          GlobalIntegral& glbInt, const TimeDomain& time) = 0;
};
```

LocalIntegral and **GlobalIntegral** are interfaces to the element-level and system-level matrices of the FE problem. **TimeDomain** contains the integration parameters needed for nonlinear and/or time-dependent simulations.

Numerical integration method for a 3D spline patch

```
bool ASMs3D::integrate (Integrand& integrand, GlobalIntegral& glInt,  
                        const TimeDomain& time)  
{
```

```
}
```

Numerical integration method for a 3D spline patch

```
bool ASMs3D::integrate (Integrand& integrand, GlobalIntegral& glInt,  
                        const TimeDomain& time)  
{  
    Compute parameter values (u,v,w) of all integration points within the patch  
    basis->SplineVolume::computeBasisGrid(u,v,w,splineData);  
    splineData contains derivatives w.r.t. u,v,w of all basis functions  
    at all integration points and the function values themselves  
  
}
```

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    Loop over elements (knot-spans); do iel=0,nel-1  
  
    end do iel  
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            end if
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            LocalIntegral* A = integrand.getLocalIntegral(iel);
            Initialize for numerical integration over the element
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                Fetch data from splineData belonging to current integration point; N, dN/du

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                Fetch data from splineData belonging to current integration point; N, dN/du
                Compute Cartesian coordinates and Jacobian; X = N*Xnod, J = dN/du*Xnod
                and the gradient; dN/dX = dN/du * J-1

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                Compute Cartesian coordinates and Jacobian; X = N*Xnod, J = dN/du*Xnod
                and the gradient; dN/dX = dN/du * J-1
                integrand.evalInt(*A, time, detJ*weight, N, dN/dX, X);
            end do i, j, k

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Numerical integration method for a 3D spline patch

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                and the gradient; dN/dX = dN/du * J-1
                integrand.evalInt(*A, time, detJ*weight, N, dN/dX, X);
            end do i, j, k
            integrand.finalizeElement(*A);

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            Initialize for numerical integration over the element
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                Fetch data from splineData belonging to current integration point; N, dN/du
                Compute Cartesian coordinates and Jacobian;  $X = N * Xnod$ ,  $J = dN/du * Xnod$ 
                and the gradient;  $dN/dX = dN/du * J^{-1}$ 
                integrand.evalInt(*A, time, detJ*weight, N, dN/dX, X);
            end do i, j, k
            integrand.finalizeElement(*A);
            glInt.assemble(A->ref(), MGEL[iel]);
            A->destruct();
        end if
    end do iel
}
```

Numerical integration method for a 3D spline patch

```
bool ASMs3D::integrate (Integrand& integrand, GlobalIntegral& glInt,  
                        const TimeDomain& time)
```

```
{
```

Compute parameter values (u,v,w) of all integration points within the patch

```
basis->SplineVolume::computeBasisGrid(u,v,w,splineData);
```

splineData contains derivatives w.r.t. u,v,w of all basis functions
at all integration points and the function values themselves

```
Loop over elements (knot-spans); do iel=0,nel-1
```

```
If current knot span is non-zero in all three directions then
```

```
LocalIntegral* A = integrand.getLocalIntegral(iel);
```

```
Initialize for numerical integration over the element
```

```
Fetch nodal coordinates (control points) for current element, Xnod
```

```
Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
```

```
Fetch data from splineData belonging to current integration point; N, dN/du
```

```
Compute Cartesian coordinates and Jacobian; X = N*Xnod, J = dN/du*Xnod
```

```
and the gradient; dN/dX = dN/du * J-1
```

```
integrand.evalInt(*A, time, detJ*weight, N, dN/dX, X);
```

```
end do i, j, k
```

```
integrand.finalizeElement(*A);
```

```
glInt.assemble(A->ref(), MGEL[iel]);
```

```
A->destruct();
```

```
end if
```

```
end do iel
```

```
}
```

The “user” interface ...

```
class Integrand
{
    //! \brief Evaluates the integrand at an interior point.
    //! \param elmInt The local integral object to receive the contributions
    //! \param[in] fe Finite element data of current integration point
    //! \param[in] time Parameters for nonlinear and time-dependent simulations
    //! \param[in] X Cartesian coordinates of current integration point
    //!
    //! \details The default implementation forwards to the stationary version.
    //! Reimplement this method for time-dependent or non-linear problems.
    virtual bool evalInt(LocalIntegral*& elmInt, const FiniteElement& fe,
                        const TimeDomain& time, const Vec3& X) const;

    //! \brief Evaluates the integrand at a boundary point.
    //! \param elmInt The local integral object to receive the contributions
    //! \param[in] fe Finite element data of current integration point
    //! \param[in] time Parameters for nonlinear and time-dependent simulations
    //! \param[in] X Cartesian coordinates of current integration point
    //! \param[in] normal Boundary normal vector at current integration point
    //!
    //! \details The default implementation forwards to the stationary version.
    //! Reimplement this method for time-dependent or non-linear problems.
    virtual bool evalBou(LocalIntegral*& elmInt, const FiniteElement& fe,
                        const TimeDomain& time,
                        const Vec3& X, const Vec3& normal) const;

    ...
};
```

Overloaded versions of these method interfaces exist without the TimeDomain argument, for stationary/linear problems.

Finite element data at integration point level

```
class FiniteElement
{
public:
    int      iel;      //!< Element identifier
    size_t   iGP;      //!< Global integration point counter
    double   u;        //!< First parameter of current point
    double   v;        //!< Second parameter of current point
    double   w;        //!< Third parameter of current point
    double   xi;       //!< First local coordinate of current integration point
    double   eta;      //!< Second local coordinate of current integration point
    double   zeta;     //!< Third local coordinate of current integration point
    double   h;        //!< Characteristic element size
    Vector   N;        //!< Basis function values
    Vector   Navg;     //!< Volume-averaged basis function values
    Matrix   dNdX;     //!< First derivatives (gradient) of the basis functions
    Matrix3D d2NdX2;   //!< Second derivatives of the basis functions
    Matrix   G;        //!< Matrix used for stabilized methods
    double   detJxW;   //!< Weighted determinant of the coordinate mapping
};
```

An object of this class is used to transport all integration point quantities to the application-dependent integrands.

Framework for two-field mixed formulations

- ▶ Two sets of basis functions – the first basis should be of one order higher than the second

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 - ▶ First approach: Establish the first basis by order-elevating the second basis (yields only C^{p-2} continuity for the first basis).
 - ▶ Second approach: Add one extra control point for the first basis in each parameter direction, and then reparameterize (both bases will possess C^{p-1} continuity but will have separate control point locations).

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 - ▶ First approach: Establish the first basis by order-elevating the second basis (yields only \mathcal{C}^{p-2} continuity for the first basis).
 - ▶ Second approach: Add one extra control point for the first basis in each parameter direction, and then reparameterize (both bases will possess \mathcal{C}^{p-1} continuity but will have separate control point locations).
- ▶ The knot-span elements become the same for the two bases,
⇒ simplifies the finite element topology management.

Framework for two-field mixed formulations

- ▶ Two sets of basis functions – the first basis should be of one order higher than the second
 - ▶ First approach: Establish the first basis by order-elevating the second basis (yields only C^{p-2} continuity for the first basis).
 - ▶ Second approach: Add one extra control point for the first basis in each parameter direction, and then reparameterize (both bases will possess C^{p-1} continuity but will have separate control point locations).
- ▶ The knot-span elements become the same for the two bases, \Rightarrow simplifies the finite element topology management.
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- ▶ Since the geometry represented by the two bases will be identical, it suffices to use the second (lowest order) basis only, when evaluating the Jacobian of the geometry mapping and the basis function gradients w.r.t. Cartesian coordinates.
- ▶ The user only needs to relate to the lowest-order grid/basis, the higher order basis is established internally automatically.

Numerical integration for the two-field mixed method

```
bool ASMs3Dmx::integrate (Integrand& integrand, GlobalIntegral& glInt,  
                           const TimeDomain& time)  
{
```

```
}
```

Numerical integration for the two-field mixed method

```
bool ASMs3Dmx::integrate (Integrand& integrand, GlobalIntegral& glInt,  
                           const TimeDomain& time)  
{  
    Compute parameter values (u,v,w) of all integration points within the patch  
    basis1->SplineVolume::computeBasisGrid(u,v,w,splineData1);  
    basis2->SplineVolume::computeBasisGrid(u,v,w,splineData2);  
  
}
```


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        If current knot span is non-zero in all three directions then  
  
        end if  
    end do iel  
}
```

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        If current knot span is non-zero in all three directions then
            LocalIntegral* A = integrand.getLocalIntegral(iel);
            Initialize for numerical integration over the element
            Fetch nodal coordinates for current element, Xnod (Note: for basis2 only)

            end if
        end do iel
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```

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            Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss

                end do i, j, k

            end if
        end do iel
    }
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            Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
                Fetch data from splineData[12];  $N_1$ ,  $dN_1/du$ ,  $N_2$ ,  $dN_2/du$ 

                end do i, j, k

            end if
        end do iel
    }
```

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                Fetch data from splineData[12];  $N_1$ ,  $dN_1/du$ ,  $N_2$ ,  $dN_2/du$ 
                Compute Cartesian coordinates and Jacobian;  $X = N_2 * Xnod$ ,  $J = dN_2/du * Xnod$ 
                and the gradients;  $dN_1/dX = dN_1/du * J^{-1}$ ,  $dN_2/dX = dN_2/du * J^{-1}$ ,

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                Fetch data from splineData[12]; N1, dN1/du, N2, dN2/du
                Compute Cartesian coordinates and Jacobian; X = N2*Xnod, J = dN2/du*Xnod
                and the gradients; dN1/dX = dN1/du * J-1, dN2/dX = dN2/du * J-1,
                integrand.evalInt(*A, time, detJ*weight,
                                N1, dN1/dX, N2, dN2/dX, X);
            end do i, j, k
        end if
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                integrand.evalInt(*A, time, detJ*weight,
                                 $N_1$ ,  $dN_1/dX$ ,  $N_2$ ,  $dN_2/dX$ ,  $X$ );
            end do i, j, k
            integrand.finalizeElement(*A);
            glInt.assemble(A->ref(), MGEL[iel]);
            A->destruct();
        end if
    end do iel
}
```

Current Applications - **Integrand** sub-classes

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- ▶ Navier–Stokes CFD solvers (not part of the *ICADA* project)

Implementational issues (integration point level)

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- ▶ Element-level linear algebra: Use machine-optimized **BLAS** rather than inline C++ code
- ▶ Important to express the nonlinear FE formulation on *matrix* form (Voigt notation) — not *tensor* form
- ▶ In addition: Integration and assembly of element-level matrices is done in parallel using multi-threading (OpenMP)

System-level linear algebra – equation solving

- ▶ Interfaced through classes **SystemMatrix** and **SystemVector** with sub-classes for particular solvers.
- ▶ Current available linear equation solvers:
 - ▶ LAPACK DGESV (dense matrices, small problems only)
 - ▶ SuperLU (direct methods) <http://crd.lbl.gov/~xiaoye/SuperLU>
 - ▶ PETSc (iterative methods) <http://www.mcs.anl.gov/petsc>
 - ▶ Parallelization on distributed memory based on PETSc/MPI

Detailed source code documentation

See the doxygen-generated html-pages ../html/index.html

Tutorial: Poisson equation in R^2

Given a heat source function $f(x, y)$ defined over a domain $\Omega \in R^2$, a flux function $h(x, y)$ defined over the boundary $\partial\Omega_h$, and a function $g(x, y)$ defined over the boundary $\partial\Omega_g = \partial\Omega \setminus \partial\Omega_h$, find the scalar function $u(x, y)$ satisfying

$$\left. \begin{aligned} q_{i,i} &= f \\ q_i &= -\kappa_{ij} u_{,j} \end{aligned} \right\} \quad \forall \quad \{x, y\} \in \bar{\Omega} \quad (1)$$

$$q_i n_i = h \quad \forall \quad \{x, y\} \in \partial\Omega_h \quad (2)$$

$$u = g \quad \forall \quad \{x, y\} \in \partial\Omega_g \quad (3)$$

where κ_{ij} is the conductivity tensor and n_i defines the outward-directed unit normal vector on $\partial\Omega_h$.

Tutorial: Poisson equation

```
class Poisson : public Integrand
{
protected:
    // Physical properties
    double    kappa;    //!< Conductivity (constant)
    RealFunc* fluxFld;  //!< Boundary normal flux field
    RealFunc* heatSrc;  //!< Interior heat source field
```

Define the class Poisson as an Integrand subclass, containing data and methods that are specific to the 2D Poisson problem (assuming constant conductivity).

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public:
    Poisson() : kappa(1.0), fluxFld(0), heatSrc(0)
    {
        primsol.resize(1);
    }
    virtual ~Poisson() {}
}
```

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Class constructor and destructor. The constructor Poisson() initializes the data members.

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public:
    Poisson() : kappa(1.0), fluxFld(0), heatSrc(0)
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    }
    virtual ~Poisson() {}

    void setMaterial(double K) { kappa = K; }
    void setFlux(RealFunc* ff) { fluxFld = ff; }
    void setSource(RealFunc* src) { heatSrc = src; }
```

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    void setMaterial(double K) { kappa = K; }
    void setFlux(RealFunc* ff) { fluxFld = ff; }
    void setSource(RealFunc* src) { heatSrc = src; }

    virtual LocalIntegral* getLocalIntegral(size_t nen, size_t,
                                           bool neumann) const;
```

Define the class Poisson as an Integrand subclass, containing data and methods that are specific to the 2D Poisson problem (assuming constant conductivity).

Class constructor and destructor. The constructor Poisson() initializes the data members.

Initialization of physical properties.

Virtual method returning an element matrix object for the Poisson integrand.

Tutorial: Poisson equation

```
virtual bool evalInt(LocalIntegral*& elmInt,  
                    const FiniteElement& fe,  
                    const Vec3& X) const;  
virtual bool evalBou(LocalIntegral*& elmInt,  
                    const FiniteElement& fe,  
                    const Vec3& X,  
                    const Vec3& normal) const;  
virtual bool evalSol(Vector& s,  
                    const Vector& N,  
                    const Matrix& dNdX,  
                    const Vec3& X,  
                    const std::vector<int>& MNPC) const;  
virtual bool evalSol(Vector& s,  
                    const VecFunc& asol,  
                    const Vec3& X) const;
```

Virtual methods for
integrand and solution field
evaluation.

Tutorial: Poisson equation

```
virtual bool evalInt(LocalIntegral*& elmInt,
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                    const Vec3& X) const;

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virtual bool evalSol(Vector& s,
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                    const Matrix& dNdX,
                    const Vec3& X,
                    const std::vector<int>& MNPC) const;

virtual bool evalSol(Vector& s,
                    const VecFunc& asol,
                    const Vec3& X) const;

virtual NormBase* getNormIntegrand(AnaSol* asol = 0) const;

bool evalSol(Vector& s,
            const Vector& eV,
            const Matrix& dNdX,
            const Vec3& X) const;

bool formCmatrix(Matrix& C, const Vec3& X,
                bool invers = false) const;
};
```

Virtual methods for
integrand and solution field
evaluation.

Methods for solution norm
integration.

Tutorial: Poisson equation

```
LocalIntegral* Poisson::getLocalIntegral (size_t nen, size_t,  
                                           bool neumann) const  
{  
    ElmMats* result = new ElmMats;  
    result->rhsOnly = neumann;  
    result->withLHS = !neumann;  
    result->resize(neumann ? 0 : 1, 1);  
  
    if (!result->A.empty())  
        result->A.front().resize(nen,nen);  
  
    if (!result->b.empty())  
        result->b.front().resize(nen);  
  
    return result;  
}
```

Element initialization:

Allocate an element matrix object and set the size of the matrices based on the number of element nodes. Indicate whether the left-hand-side matrices are to be integrated or not.

Tutorial: Poisson equation

```
bool Poisson::evalInt (LocalIntegral& elmInt,
                      const FiniteElement& fe,
                      const Vec3& X) const
{
    ElmMats& elMat = static_cast<ElmMats&>(elmInt);

    if (!elMat.A.empty())
    {
        Matrix C; C.diag(kappa,2); // Diagonal constitutive matrix

        Matrix CB;
        CB.multiply(C,fe.dNdX,false,true).multiply(fe.detJxW);
        elMat.A.front().multiply(fe.dNdX,CB,false,false,true);
    }

    if (heatSrc && !elMat.b.empty())
        elMat.b.front().add(fe.N,(*heatSrc)(X)*fe.detJxW);

    return true;
}

bool Poisson::evalBou (LocalIntegral*& elmInt,
                      const FiniteElement& fe,
                      const Vec3& X, const Vec3& normal) const
{
    ElmMats& elMat = static_cast<ElmMats&>(elmInt);
    if (!fluxFld || elMat.b.empty()) return false;

    double h = -(*fluxFld)(X); // normal flux at point X

    elMat.b.front().add(fe.N,h*fe.detJxW);

    return true;
}
```

Integrand evaluations:

Assuming here $\kappa_{ij} = \kappa \delta_{ij}$

$$[CB] = [C] \cdot [\partial N / \partial \mathbf{X}]^T |J|_w$$

$$[eM] = \sum ([\partial N / \partial \mathbf{X}] \cdot [CB])$$

$$\{eS\} = \sum (f\{N\} |J|_w)$$

$$\{eS\} = \sum (-h\{N\} |J|_w)$$

Tutorial: Poisson equation

```
bool Poisson::evalSol (Vector& q, const Vector&,
                      const Matrix& dNdX, const Vec3& X,
                      const std::vector<int>& MNPC) const
{
    if (primsol.front().empty()) return false;

    Vector eV;
    int ierr = utl::gather(MNPC,1,primsol.front(),eV);
    if (ierr > 0) return false;

    Matrix C; C.diag(kappa,2); // Diagonal constitutive matrix

    // Evaluate the heat flux vector
    Matrix CB;
    CB.multiply(C,dNdX,false,true).multiply(eV,q);
    q *= -1.0;

    return true;
}
```

Secondary solution evaluation:

$$\mathbf{q} = [C] \cdot [\partial N / \partial \mathbf{X}]^T \cdot \{eV\}$$

```
bool Poisson::evalSol (Vector& s, const VecFunc& asol,
                      const Vec3& X) const
{
    s = Vector(asol(X).ptr(),2);
    return true;
}
```

Analytical solution

Tutorial: Poisson equation

```
class PoissonNorm : public NormBase
{
    VecFunc* anasol;  //!< Analytical heat flux

public:
    PoissonNorm(Poisson& p, VecFunc* a = 0)
        : NormBase(p), anasol(a) {}
    virtual ~PoissonNorm() {}

    virtual bool hasBoundaryTerms() const { return true; }

    virtual bool evalInt(LocalIntegral& elmInt,
                        const FiniteElement& fe,
                        const Vec3& X) const;
    virtual bool evalBou(LocalIntegral& elmInt,
                        const FiniteElement& fe,
                        const Vec3& X,
                        const Vec3& normal) const;
};
```

```
NormBase* Poisson::getNormIntegrand (AnaSol* asol) const
{
    if (asol)
        return new PoissonNorm(*const_cast<Poisson*>(this),
                                asol->getScalarSecSol());
    else
        return new PoissonNorm(*const_cast<Poisson*>(this));
}
```

Accompanying class for solution norm integration

NormBase is a sub-class of Integrand with a couple of added methods common to all norm classes.

Tutorial: Poisson equation

```
bool PoissonNorm::evalInt (LocalIntegral& elmInt,
                           const FiniteElement& fe,
                           const Vec3& X) const
{
    Poisson& problem = static_cast<Poisson&>(myProblem);
    ElmNorm& pnorm = static_cast<ElmNorm&>(elmInt);

    // Evaluate the inverse constitutive matrix at this point
    Matrix Cinv;
    problem.formCmatrix(Cinv,X,true);

    // Evaluate the finite element heat flux field
    Vector sigmah;
    problem.evalSol(sigmah,pnorm.vec.front(),fe.dNdX,X);

    // Integrate the energy norm  $a(u^h,u^h)$ 
    pnorm[0] += sigmah.dot(Cinv*sigmah)*fe.detJxW;
    // Integrate the external energy  $(h,u^h)$ 
    double u = pnorm.vec.front().dot(fe.N);
    pnorm[1] += problem.getHeat(X)*u*fe.detJxW;

    if (anasol) {
        // Evaluate the analytical heat flux
        Vector sigma((*anasol)(X).ptr(),sigmah.size());
        // Integrate the energy norm  $a(u,u)$ 
        pnorm[2] += sigma.dot(Cinv*sigma)*fe.detJxW;
        // Integrate the error in energy norm  $a(u-u^h,u-u^h)$ 
        sigma -= sigmah;
        pnorm[3] += sigma.dot(Cinv*sigma)*fe.detJxW;
    }

    return true;
}
```

Norm integrand evaluation

Tutorial: Poisson equation

```
bool PoissonNorm::evalBou (LocalIntegral& elmInt,
                           const FiniteElement& fe,
                           const Vec3& X,
                           const Vec3& normal) const
{
    Poisson& problem = static_cast<Poisson&>(myProblem);
    ElmNorm& pnorm = static_cast<ElmNorm&>(elmInt);

    // Evaluate the surface heat flux
    double t = problem.getTraction(X,normal);
    // Evaluate the temperature field
    double u = pnorm.vec.front().dot(fe.N);

    // Integrate the external energy (t,u^h)
    pnorm[1] += t*u*fe.detJxW;

    return true;
}
```

Integration of external energy
due to boundary flux.

Tutorial: Poisson equation

```
class SIMPoisson2D : public SIM2D
{
    Poisson    prob; //!< Poisson data and methods
    RealArray mVec; //!< Material data

public:
    SIMPoisson2D() : SIM2D(1), prob(2)
    { myProblem = &prob; }

    virtual ~SIMPoisson2D()
    { myProblem = NULL; }

protected:
    virtual bool parse(char* keyWord, std::istream& is);
    virtual bool initMaterial(size_t propInd);
    virtual bool initNeumann(size_t propInd);
};

bool SIMPoisson2D::initMaterial (size_t propInd)
{
    if (propInd >= mVec.size()) return false;
    prob.setMaterial(mVec[propInd]);
    return true;
}

bool SIMPoisson2D::initNeumann (size_t propInd)
{
    SclFuncMap::const_iterator sit = myScalars.find(propInd);
    if (sit == myVectors.end()) return false;
    prob.setFlux(sit->second);
    return true;
}
```

Simulation driver class

Tutorial: Poisson equation

```
bool SIMPoisson2D::parse (const TiXmlElement* elem)
{
    if (strcasecmp(elem->Value(),"poisson"))
        return this->SIM2D::parse(elem);

    const TiXmlElement* child = elem->FirstChildElement();
    for (; child; child = child->NextSiblingElement())

        if (!strcasecmp(child->Value(),"isotropic")) {
            int code = 0;
            double kappa = 1000.0;
            utl::getAttribute(child,"code",code);
            utl::getAttribute(child,"kappa",kappa);
            if (code == 0)
                prob.setMaterial(kappa);
            else
                this->setPropertyType(code,Property::MATERIAL,mVec.size());
            mVec.push_back(kappa);
        }
}
```

Tutorial: Poisson equation

```
else if (!strcasecmp(child->Value(),"source")) {
    int code = -1; // Reserve negative code(s) for the source term function
    while (myScalars.find(code) != myScalars.end()) --code;
    std::string type;
    utl::getAttribute(child,"type",type,true);
    if (type == "expression" && child->FirstChild()) {
        std::cout <<"\tHeat source function: "
                  << child->FirstChild()->Value() << std::endl;
        myScalars[code] = new EvalFunction(child->FirstChild()->Value());
    }
    else {
        std::cerr <<" ** SIMPoisson2D::parse: Invalid source function "<< type << std::endl;
        continue;
    }
    prob.setSource(myScalars[code]);
}

else if (!strcasecmp(child->Value(),"anasol")) {
    std::string type;
    utl::getAttribute(child,"type",type,true);
    if (type == "expression") {
        std::cout <<"\tAnalytical solution: Expression"<< std::endl;
        if (!mySol) mySol = new AnaSol(child);
    }
    else {
        std::cerr <<" ** SIMPoisson2D::parse: Invalid analytical solution "<< type << std::endl;
    }
}

return true;
}
```


Tutorial: Poisson equation

```
int main (int argc, char** argv)
{
    // (Lots of initialisations skipped here...)

    // Read in model definitions and establish the FE data structures
    SIMbase* model = new SIMPoisson2D();
    if (!model->read(infile))
        return 1;
    if (!model->preprocess(ignoredPatches,fixDup))
        return 1;

    model->setQuadratureRule(nGauss);

    Matrix eNorm;
    Vector gNorm, sol;

    model->initSystem(solver,1,1);
    model->setAssociatedRHS(0,0);
    if (!model->assembleSystem())
        return 2;

    // Solve the linear system of equations
    if (!model->solveSystem(sol,1))
        return 3;

    // Evaluate solution norms
    if (!model->solutionNorms(Vectors(1,sol),eNorm,gNorm))
        return 4;

    // Print output to terminal and VTF, etc.
}
```

Core parts of the main program

Tutorial: Poisson equation, sample input files

```
<simulation>
```

```
<!-- General - geometry definitions !-->
```

```
<geometry>
```

```
<patchfile>square2D.g2</patchfile>
```

```
<raiseorder patch="1" u="2" v="2"/>
```

```
<refine type="uniform" patch="1" u="7" v="7"/>
```

```
<topologysets>
```

```
<set name="Dirichlet" type="edge">
```

```
<item patch="1">4</item>
```

```
</set>
```

```
<set name="Neumann" type="edge">
```

```
<item patch="1">3</item>
```

```
</set>
```

```
</topologysets>
```

```
</geometry>
```

square2d.g2:

200 1 0 0

3 0

2 2

0 0 1 1

2 2

0 0 1 1

0.0 0.0 0.0

2.0 0.0 0.0

0.0 2.0 0.0

2.0 2.0 0.0

```
<!-- General - boundary conditions !-->
```

```
<boundaryconditions>
```

```
<dirichlet set="Dirichlet" comp="1"/>
```

```
<neumann type="anasol" set="Neumann" comp="1"/>
```

```
</boundaryconditions>
```

```
<!-- Problem-specific block !-->
```

```
<poisson>
```

```
<source type="expression">PI*PI*cos(PI*x)*(2-y)</source>
```

```
<anasol type="expression">
```

```
<primary>cos(PI*x)*(2-y)</primary>
```

```
<secondary>PI*sin(PI*x)*(2-y)|cos(PI*x)</secondary>
```

```
</anasol>
```

```
</poisson>
```

```
</simulation>
```