

# *IFEM* - getting started

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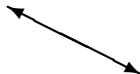
# IFEM module overview

## GEOM — Geometry Modeller

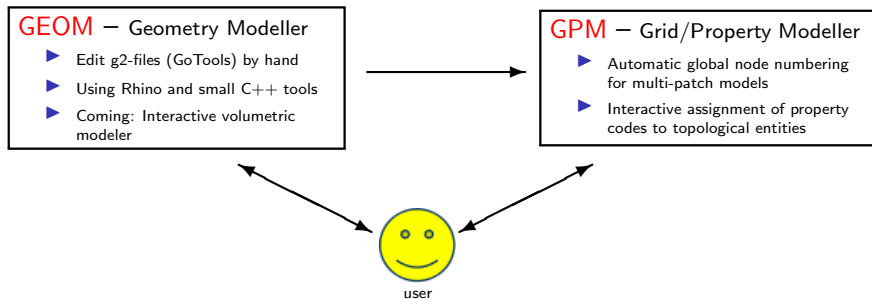
- ▶ Edit g2-files (GoTools) by hand
- ▶ Using Rhino and small C++ tools
- ▶ Coming: Interactive volumetric modeler



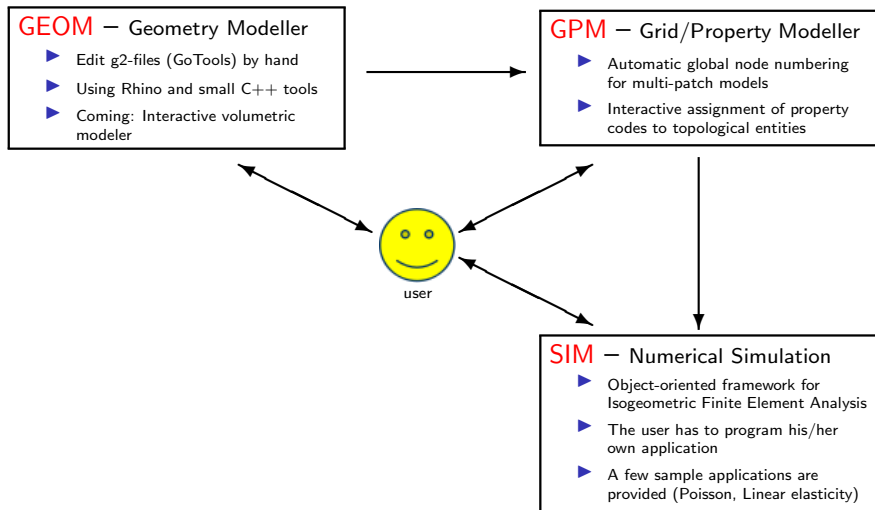
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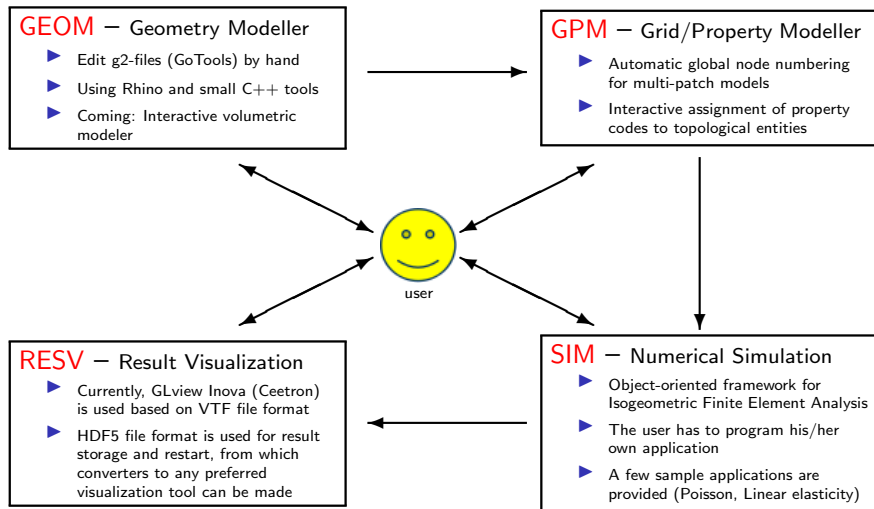
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# Major class hierarchies of the SIMulation environment

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    - ▶ Administers the element loop and numerical integration loop within a block (spline patch)
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  - ▶ Provides the integration point data

# ASM class hierarchy - *the Isogeometry level*

ASMbase

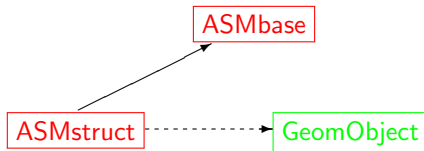
→ 'is-a' relationship

--> 'has-a' relationship

*IFEM* classes

*GoTools* classes

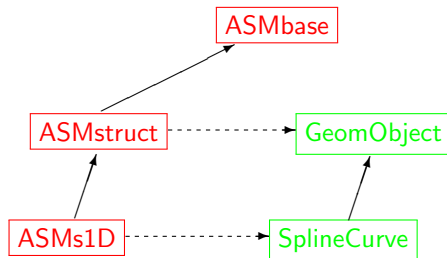
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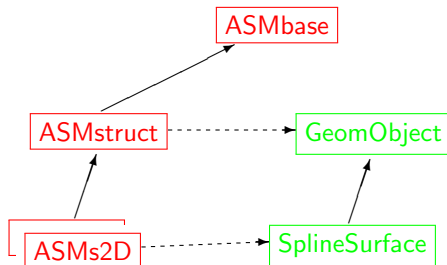
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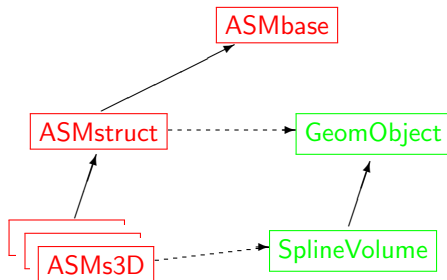


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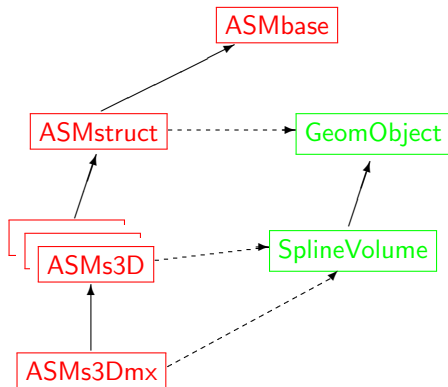
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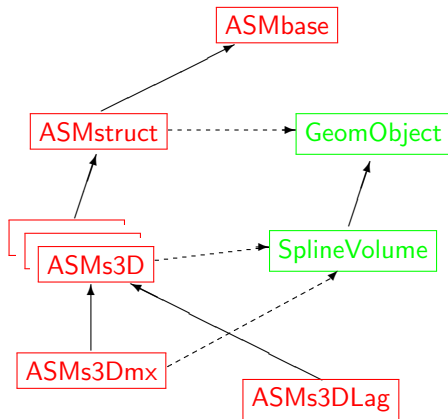
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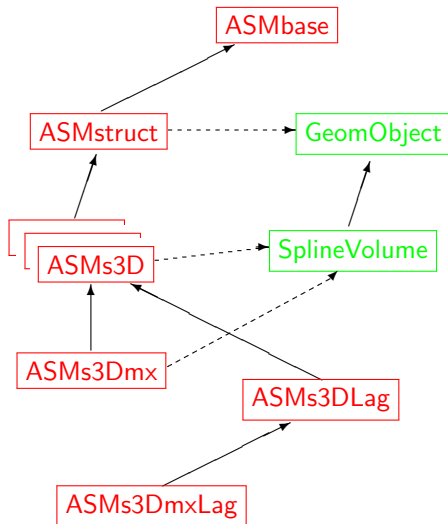
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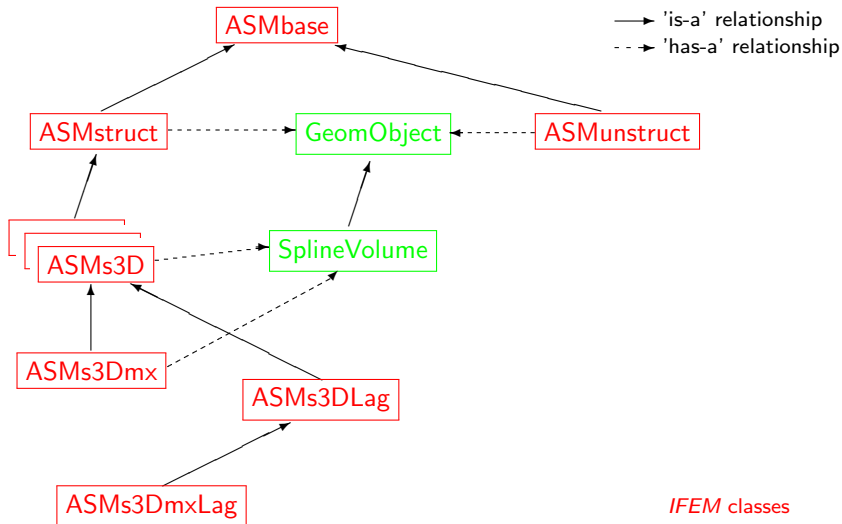
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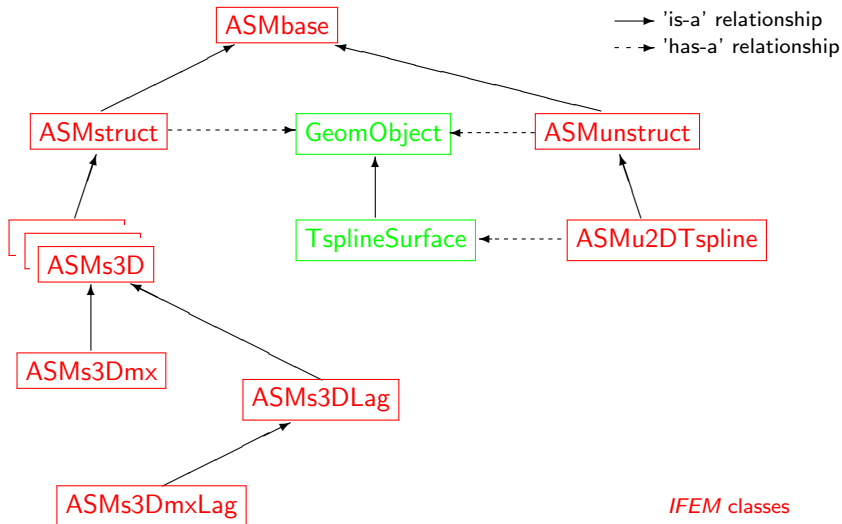
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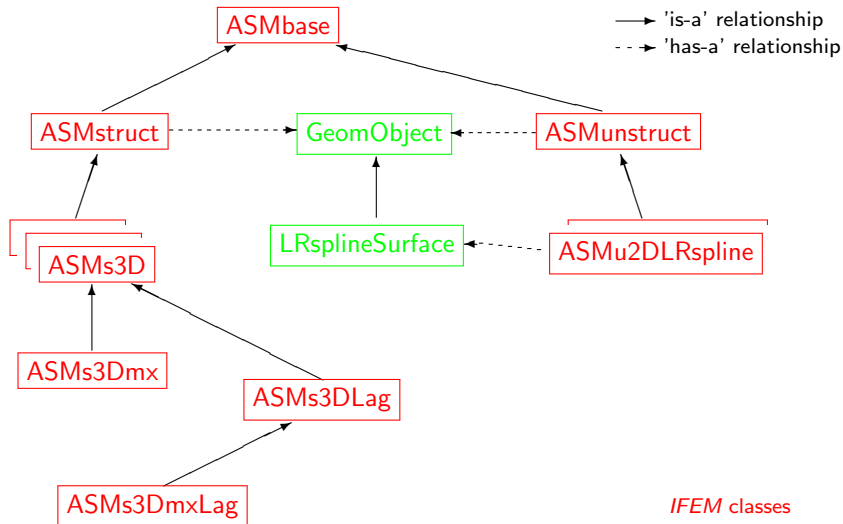


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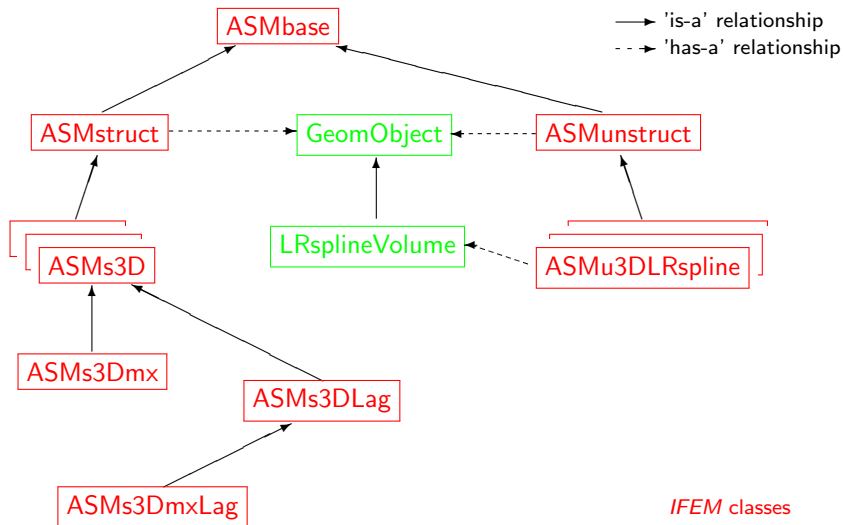
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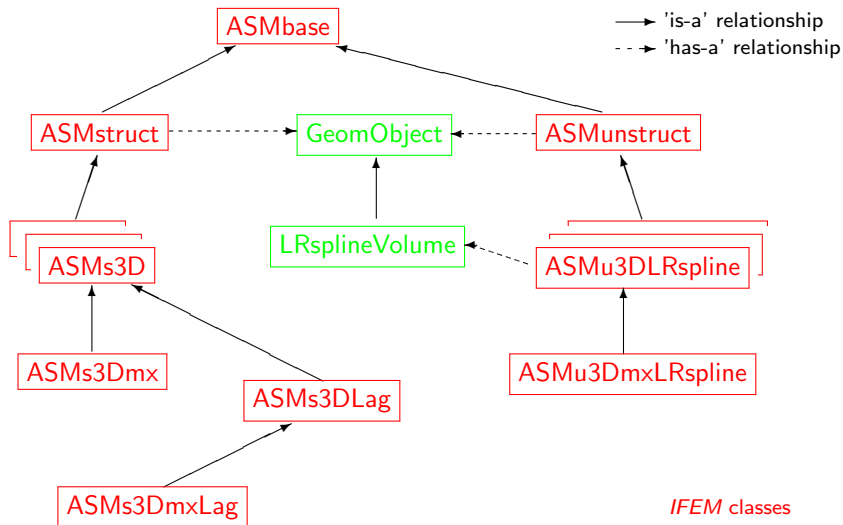
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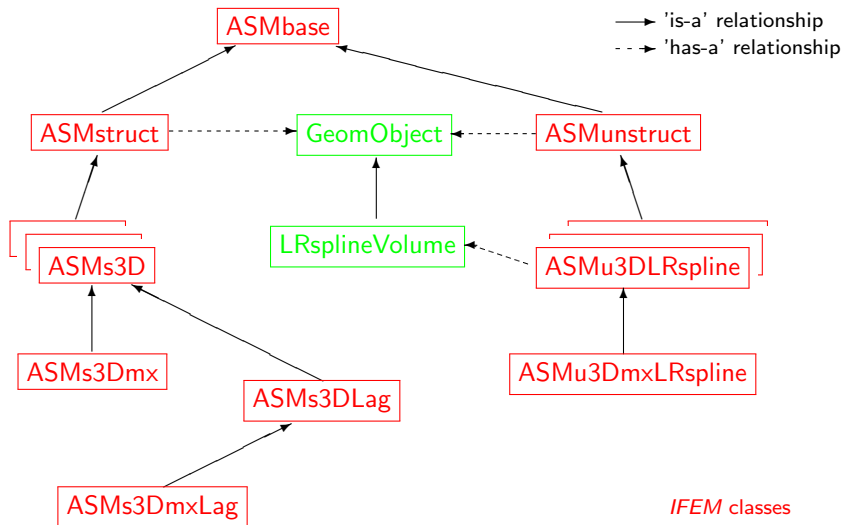


# ASM class hierarchy - the Isogeometry level



*IFEM* classes  
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# ASM class hierarchy - the Isogeometry level



IFEM classes  
GoTools classes

**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

```
typedef std::vector<LocalIntegral*> LintegralVec; //!< Local integral container

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
    //!< \param locInt Vector of element-wise contributions to \a glbInt
    virtual bool integrate(Integrand& integrand,
                          GlobalIntegral& glbInt, const TimeDomain& time,
                          const LintegralVec& locInt = LintegralVec()) = 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
    //!< \param locInt Vector of element-wise contributions to \a glbInt
    virtual bool integrate(Integrand& integrand, int lIndex,
                          GlobalIntegral& glbInt, const TimeDomain& time,
                          const LintegralVec& locInt = LintegralVec()) = 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, const LintegralVec& locInt)  
{  
    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

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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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                integrand.evalInt(locInt[iel], time, detJ*weight, N, dN/dX, X);
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            glInt.assemble(locInt[iel], MGEL[iel]);
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    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
    double   u;        //!< First parameter of current point
    double   v;        //!< Second parameter of current point
    double   w;        //!< Third parameter of current 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
    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.

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- ▶ Current solution: Establish the first basis by order-elevating the second basis once
  - ▶ The knot-span elements become the same for the two bases,  $\Rightarrow$  simplifies the finite element topology management.
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- ▶ TODO: Manage bases with  $C^{p-1}$  continuity in both fields.





# Numerical integration for the two-field mixed method

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

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

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                and the gradients;  $dN_1/dX = dN_1/du * J^{-1}$ ,  $dN_2/dX = dN_2/du * J^{-1}$ ,

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                and the gradients;  $dN_1/dX = dN_1/du * J^{-1}$ ,  $dN_2/dX = dN_2/du * J^{-1}$ ,
                integrand.evalInt(locInt[iel], time, detJ*weight,
                                 $N_1$ ,  $dN_1/dX$ ,  $N_2$ ,  $dN_2/dX$ ,  $X$ );
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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(locInt[iel], time, detJ*weight,
                                N1, dN1/dX, N2, dN2/dX, X);
            end do i, j, k
            integrand.finalizeElement(locInt[iel]);
            glInt.assemble(locInt[iel], MGEL[iel]);
        end if
    end do iel
}
```

# Current Applications - **Integrand** sub-classes

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- ▶ Projection-based, decoupled Navier–Stokes solvers (Chorin method)
  - ▶ Mixed formulation (work in progress)

# Implementational issues (integration point level)

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- ▶ Using splines as basis function, especially the higher-order ones, the “elements” become large (in terms of nodal connectivities)  $\Rightarrow$  large, dense element matrices
- ▶ 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



# 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 in progress (based on PETSc and MPI)

# Detailed source code documentation

See the doxygen-generated html-pages [../html/index.html](http://../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  $\kappa_{ij}$  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)
    VecFunc*  fluxFld;  //!< Boundary heat flux field
    RealFunc* heatSrc;  //!< Interior heat source field

    // Finite element quantities
    Matrix* eM; //!< Element coefficient matrix
    Vector* eS; //!< Element right-hand-side vector
    Vector* eV; //!< Element solution vector

    mutable ElmMats myMats; //!< Local element matrices
```

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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    Matrix* eM; //!< Element coefficient matrix
    Vector* eS; //!< Element right-hand-side vector
    Vector* eV; //!< Element solution vector

    mutable ElmMats myMats; //!< Local element matrices

public:
    Poisson() : kappa(1.0), fluxFld(0), heatSrc(0)
    {
        primsol.resize(1);
        myMats.A.resize(1);
        myMats.b.resize(2);
        eM = &myMats.A[0];
        eS = &myMats.b[0];
        eV = &myMats.b[1];
    }
    virtual ~Poisson() {}
};
```

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

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

# Tutorial: Poisson equation

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

Initialization of physical properties.

# Tutorial: Poisson equation

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```

```
virtual bool initElement(const std::vector<int>& MNPC);  
virtual bool initElementBou(const std::vector<int>& MNPC);
```

Initialization of physical properties.

Virtual methods for element initialization during the numerical integration.

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virtual bool initElementBou(const std::vector<int>& MNPC);
```

```
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;
```

Initialization of physical properties.

Virtual methods for element initialization during the numerical integration.

Virtual methods for integrand and solution field evaluation.



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

Initialization of physical properties.

Virtual methods for element initialization during the numerical integration.

Virtual methods for integrand and solution field evaluation.

Methods for solution norm integration.

# Tutorial: Poisson equation

```
bool Poisson::initElement (const std::vector<int>& MNPC)
{
    const size_t nen = MNPC.size();

    eM->resize(nen,nen,true);
    eS->resize(nen,true);

    int ierr = 0;
    if (!primsol.front().empty())
        if ((ierr = utl::gather(MNPC,1,primsol.front(),*eV)))
            std::cerr << " *** Poisson::initElement: Detected "
                << ierr << " node numbers out of range."
                << std::endl;

    myMats.withLHS = true;
    return ierr == 0;
}

bool Poisson::initElementBou (const std::vector<int>& MNPC)
{
    eS->resize(MNPC.size(),true);

    myMats.withLHS = false;
    return true;
}
```

Element initialization:

Set the size of the element matrices based on the number of element nodes.

Extract the element solution vector from the global (patch-level) vector.

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
{
    elmInt = &myMats;

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

    Matrix CB;
    CB.multiply(C,fe.dNdX,false,true).multiply(fe.detJxW);
    eM->multiply(fe.dNdX,CB,false,false,true);

    if (heatSrc)
        eS->add(fe.N,(*heatSrc)(X)*fe.detJxW);

    return true;
}
```

```
bool Poisson::evalBou (LocalIntegral*& elmInt,
                      const FiniteElement& fe,
                      const Vec3& X, const Vec3& normal) const
{
    elmInt = &myMats;
    if (!fluxFld) return false;

    Vec3 q = (*fluxFld)(X); // heat flux at point X

    double flux = -(q*normal);
    eS->add(fe.N,flux*fe.detJxW);

    return true;
}
```

Integrand evaluations:

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

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

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

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

$$\{eS\} = \sum (-(\mathbf{q} \cdot \mathbf{n}) \{N\} |J|_w)$$

# 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;

    Matrix C;
    this->formCmatrix(C,X);

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

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

    return true;
}
```

Secondary solution evaluation:

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

```
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

```
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));
}
```

```
class PoissonNorm : public NormBase
{
    Poisson& problem; //!< The problem-specific data
    VecFunc* anasol;  //!< Analytical heat flux

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

    virtual bool initElement(const std::vector<int>& MNPC)
    {
        return problem.initElement(MNPC);
    }

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

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
{
    ElmNorm* eNorm = dynamic_cast<ElmNorm*>(elmInt);
    if (!eNorm) return false;

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

    // Evaluate the finite element heat flux field
    Vector sigmah;
    if (!problem.evalSol(sigmah,fe.dNdX,X)) return false;

    // Integrate the energy norm  $a(u^h,u^h)$ 
    ElmNorm& pnorm = *eNorm;
    pnorm[0] += sigmah.dot(Cinv*sigmah)*fe.detJxW;
    if (anasol)
    {
        // Evaluate the analytical heat flux
        Vector sigma((*anasol)(X).ptr(),sigmah.size());
        // Integrate the energy norm  $a(u,u)$ 
        pnorm[1] += sigma.dot(Cinv*sigma)*fe.detJxW;
        // Integrate the error in energy norm  $a(u-u^h,u-u^h)$ 
        sigma -= sigmah;
        pnorm[2] += sigma.dot(Cinv*sigma)*fe.detJxW;
    }

    return true;
}
```

Norm integrand evaluation

# 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 = 0; }

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)
{
    VecFuncMap::const_iterator tit = myVectors.find(propInd);
    if (tit == myVectors.end()) return false;
    prob.setTraction(tit->second);
    return true;
}
```

Simulation driver class

# Tutorial: Poisson equation

```
bool SIMPoisson2D::parse (char* keyWord, std::istream& is)
{
    char* cline = 0;
    if (!strncasecmp(keyWord,"ISOTROPIC",9))
    {
        int nmat = atoi(keyWord+10);
        std::cout <<"\nNumber of isotropic materials: "<< nmat << std::endl;
        for (int i = 0; i < nmat && (cline = utl::readLine(is)); i++)
        {
            int code = atoi(strtok(cline," "));
            double kappa = atof(strtok(NULL," "));
            std::cout <<"\tMaterial code "<< code <<": "<< kappa << std::endl;
            if (code == 0)
                prob.setMaterial(kappa);
            else if (this->setPropertyType(code,Property::MATERIAL,mVec.size()))
                mVec.push_back(kappa);
        }
    }
    else if (!strncasecmp(keyWord,"SOURCE",6))
    {
        cline = strtok(keyWord+6," ");
        if (!strncasecmp(cline,"SQUARE",6))
        {
            double L = atof(strtok(NULL," "));
            std::cout <<"\nHeat source function: Square L="<< L << std::endl;
            prob.setSource(new Square2DHeat(L));
        }
        else
            std::cerr <<" ** SIMPoisson2D::parse: Unknown source function "
                << cline << std::endl;
    }
}
```



# Tutorial: Poisson equation

```
else if (!strncasecmp(keyWord,"ANASOL",6))
{
    cline = strtok(keyWord+6," ");
    if (!strncasecmp(cline,"SQUARE",6))
    {
        double L = atof(strtok(NULL," "));
        std::cout <<"\nAnalytical solution: Square L="<< L << std::endl;
        mySol = new AnaSol(NULL,new Square2D(L));
    }
    else if (!strncasecmp(cline,"LSHAPE",6))
    {
        mySol = new AnaSol(NULL,new LshapePoisson());
        std::cout <<"\nAnalytical solution: Lshape"<< std::endl;
    }
    else
    {
        std::cerr <<" ** SIMPoisson2D::parse: Unknown analytical solution "
        << cline <<" (ignored)"<< std::endl;
        return true;
    }
}

// Define the analytical boundary traction field
int code = (cline = strtok(NULL," ")) ? atoi(cline) : 0;
if (code > 0 && mySol->getScalarSecSol())
{
    this->setPropertyType(code,Property::NEUMANN);
    myVectors[code] = mySol->getScalarSecSol();
}
}
else
    return this->SIM2D::parse(keyWord,is);

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

```
PATCHFILE    lshape2d.g2
PROPERTYFILE  lshape2d.prc
```

```
RAISEORDER 1
# patch ru rv
  1      2  2
```

```
REFINE 1
# patch ru rv
  1      7  7
```

```
DIRICHLET 1
# code
  1
```

```
# Analytical solution
# Specifier   code
ANASOL Lshape 2
```

lshape2d.prc:

```
1 0 1 2
2 0 1 0
2 0 1 1
2 0 1 3
```

lshape2d.g2:

```
200 1 0 0
3 0
7 4
0 0 0 0 1 1 1 2 2 2 2
4 4
0 0 0 0 1 1 1 1
```

```
0.000000 -1.000000 0
0.000000 -0.666667 0
0.000000 -0.333333 0
0.000000 -0.000000 0
0.333333 -0.000000 0
0.666667 -0.000000 0
1.000000 -0.000000 0
-0.333333 -1.000000 0
-0.333333 -0.555556 0
-0.333333 -0.111111 0
-0.333333 0.333333 0
0.111111 0.333333 0
0.555556 0.333333 0
1.000000 0.333333 0
-0.666667 -1.000000 0
-0.666667 -0.444444 0
-0.666667 0.111111 0
-0.666667 0.666667 0
```

+ 10 more lines