#### ICADA - Note 2011-001:

# IFEM - getting started

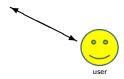
Knut Morten Okstad

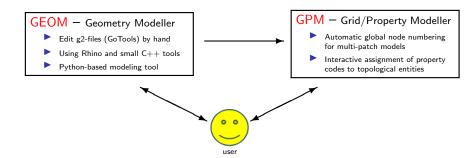
SINTEF ICT, Department of Applied Mathematics

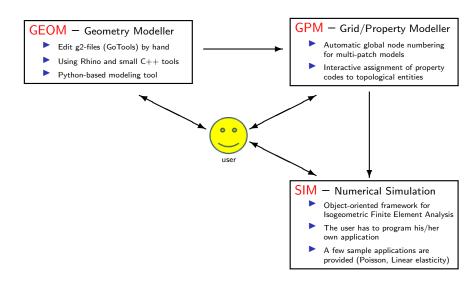
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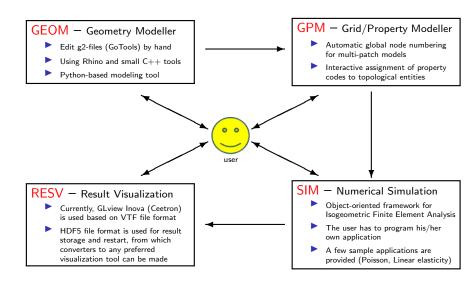
#### **GEOM** — Geometry Modeller

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









- 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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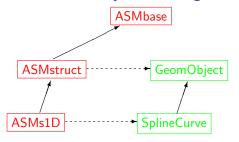
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  - User/Application level

ASMbase

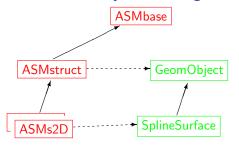
→ 'is-a' relationship- → 'has-a' relationship

IFEM classes

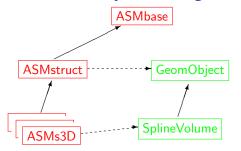




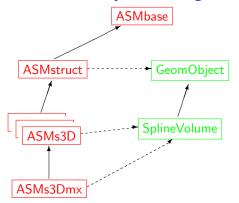
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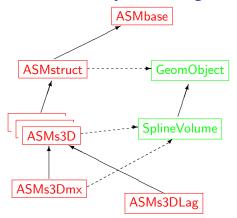
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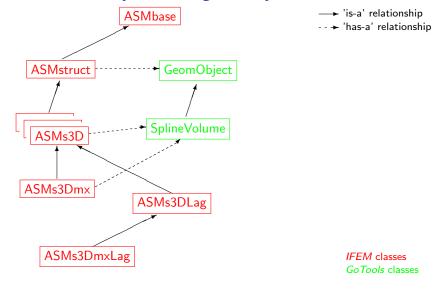
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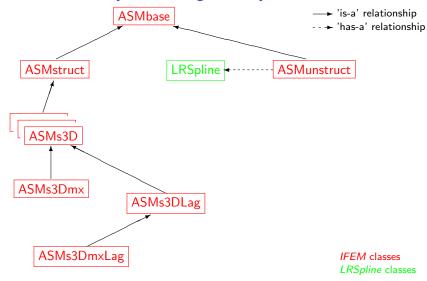


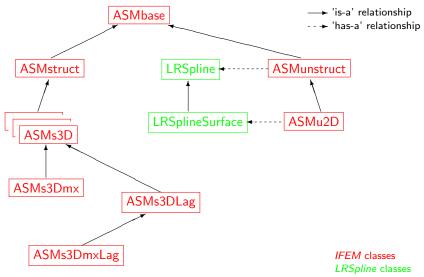
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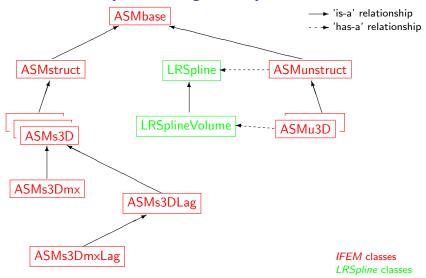


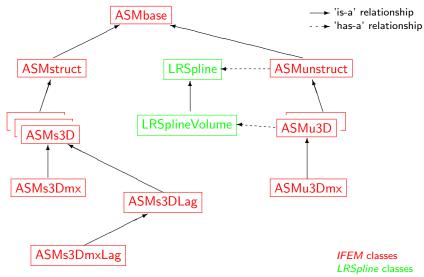
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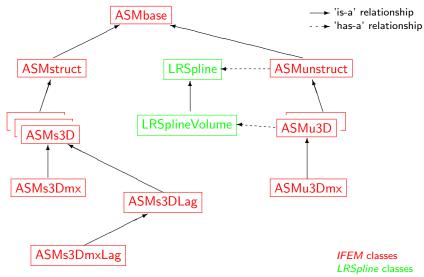


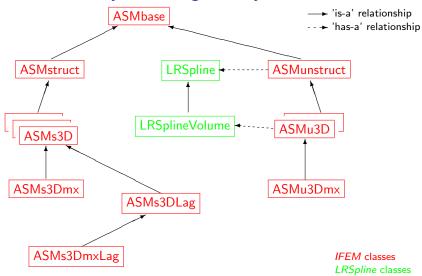












ASMbase is the interface between the isogeometric FE procedures, and the solution algorithms (from above) and the physical problem to be solved (from below).

#### 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.

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

```
end if
end do iel
}
```

```
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
```

```
end if
end do iel
}
```

end do i, j, k

```
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
```

```
end if
end do iel
```

end do i, j, k



```
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);
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      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}
      end do i, j, k
```

```
end if
end do iel
```



```
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);
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      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
```

# 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
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  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);
    end if
  end do iel
```

## Numerical integration method for a 3D spline patch

```
bool ASMs3D::integrate (Integrand& integrand, GlobalIntegral& glInt,
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  Compute parameter values (u,v,w) of all integration points within the patch
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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
                                                    4D > 4B > 4B > 4B > 900
```

# 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
                                                   4 D > 4 A > 4 B > 4 B > B 9 Q P
```

#### 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;
ጉ:
```

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.

► Two sets of basis functions — the first basis should be of one order higher than the second

- ➤ 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 posess C<sup>p-1</sup> continuity but will have separate control point locations).

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  - Second approach: Add one extra control point for the first basis in each parameter direction, and then reparameterize (both bases will posess  $\mathcal{C}^{p-1}$  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.
- ► Since the geometry represented by the two bases will be identical, it suffice 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.

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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).
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- ► The knot-span elements become the same for the two bases,
  ⇒ simplifies the finite element topology management.
- ➤ Since the geometry represented by the two bases will be identical, it suffice 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.

```
end if
end do iel
}
```

```
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);

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 for current element, Xnod (Note: for basis2 only)
    Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
```

```
end if
end do iel
```

end do i, j, k

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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)

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

Fetch data from splineData[12]; N1, dN1/du, N2, dN2/du
```

```
end if
end do iel
```

end do i, j, k

```
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);
  Loop over elements (knot-spans); do iel=0,nel-1
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      Initialize for numerical integration over the element
       Fetch nodal coordinates for current element, Xnod (Note: for basis2 only)
      Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
         Fetch data from splineData[12]; N<sub>1</sub>, dN<sub>1</sub>/du, N<sub>2</sub>, dN<sub>2</sub>/du
         Compute Cartesian coordinates and Jacobian; X = N2*Xnod, J = dN2/du*Xnod
         and the gradients; dN_1/dX = dN_1/du * J^{-1}, dN_2/dX = dN_2/du * J^{-1},
      end do i, j, k
```

```
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);
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      LocalIntegral* A = integrand.getLocalIntegral(iel);
      Initialize for numerical integration over the element
       Fetch nodal coordinates for current element, Xnod (Note: for basis2 only)
      Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
         Fetch data from splineData[12]; N<sub>1</sub>, dN<sub>1</sub>/du, N<sub>2</sub>, dN<sub>2</sub>/du
         Compute Cartesian coordinates and Jacobian; X = N2*Xnod, J = dN2/du*Xnod
         and the gradients; dN_1/dX = dN_1/du * J^{-1}, dN_2/dX = dN_2/du * J^{-1},
         integrand.evalInt(*A, time, detJ*weight,
                             N_1, dN_1/dX, N_2, dN_2/dX, X);
      end do i, j, k
```

```
end if
end do iel
```

```
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);
  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 for current element, Xnod (Note: for basis2 only)
      Loop over integration points; do i=1,nGauss, j=1,nGauss, k=1,nGauss
         Fetch data from splineData[12]; N<sub>1</sub>, dN<sub>1</sub>/du, N<sub>2</sub>, dN<sub>2</sub>/du
        Compute Cartesian coordinates and Jacobian; X = N2*Xnod, J = dN2/du*Xnod
        and the gradients; dN_1/dX = dN_1/du * J^{-1}, dN_2/dX = dN_2/du * J^{-1},
        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
                                                      4 D > 4 A > 4 B > 4 B > B 9 Q P
```

► Poisson - Simple scalar equation

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  - LinearElasticity Linear elasticity, isotropic material
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- ► Navier–Stokes CFD solvers (not part of the *ICADA* project)
- ► Many others (coupled simulators, etc.)



# Implementational issues (integration point level)

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- ► Important to express the nonlinear FE formulation on *matrix* form (Voigt notation) not *tensor* form

# Implementational issues (integration point level)

- ► Using splines as basis function, especially the higher-order ones, the "elements" become large (in terms of nodal connectivities) ⇒ 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
- 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

$$\left.\begin{array}{l}
q_{i,i} = f \\
q_i = -\kappa_{ij} u_{,j}
\end{array}\right\} \quad \forall \quad \{x, y\} \in \overline{\Omega} \tag{1}$$

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

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

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

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

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

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

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

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

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

```
class Poisson : public IntegrandBase
protected:
  // Physical properties
  double kappa; //! < Conductivity (constant)
  RealFunc* fluxFld: //! Boundary normal flux field
  RealFunc* heatSrc: //! Interior heat source field
public:
  Poisson(): kappa(1.0), fluxFld(0), heatSrc(0)
    primsol.resize(1):
  virtual "Poisson() {}
  void setMaterial(double K) { kappa = K; }
  void setFlux(RealFunc* ff) { fluxFld = ff: }
  void setSource(RealFunc* src) { heatSrc = src: }
```

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Initialization of physical properties.

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    primsol.resize(1):
  virtual "Poisson() {}
  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 IntegrandBase subclass (the class IntegrandBase inherits Integrand), containing data and methods 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.

Virtual methods for integrand and solution field evaluation.

```
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 FiniteElement& fe.
                       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.

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.

return true;

```
bool Poisson::evalInt (LocalIntegral& elmInt.
                        const FiniteElement& fe.
                        const Vec3& X) const
  ElmMats& elMat = static cast<ElmMats&>(elmInt):
                                                                   Integrand evaluations:
                                                                   Assuming here \kappa_{ii} = \kappa \delta_{ii}
  if (!elMat.A.emptv())
    Matrix C; C.diag(kappa,2); // Diagonal constitutive matrix
                                                                    [CB] = [C] \cdot [\partial N/\partial \mathbf{X}]^T |J|w
    Matrix CB:
    CB.multiply(C,fe.dNdX,false,true).multiply(fe.detJxW);
    elMat.A.front().multiply(fe.dNdX,CB,false,false,true);
                                                                   [eM] = \sum ([\partial N/\partial \mathbf{X}] \cdot [CB])
  if (heatSrc && !elMat.b.empty())
                                                                      \{eS\} = \sum (f\{N\}|J|w)
    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.emptv()) return false:
                                                                     \{eS\} = \sum (-h\{N\}|J|w)
  double h = -(*fluxFld)(X); // normal flux at point X
  elMat.b.front().add(fe.N.h*fe.detJxW):
```

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```
bool Poisson::evalSol (Vector& q,
                        const FiniteElement& fe, const Vec3& X,
                        const std::vector<int>& MNPC) const
                                                              Secondary solution evaluation:
  if (primsol.front().empty()) return false;
  Vector eV:
                                                                 \mathbf{q} = [C] \cdot [\partial N/\partial \mathbf{X}]^T \cdot \{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,fe.dNdX,false,true).multiply(eV,q);
  a *= -1.0:
  return true:
bool Poisson::evalSol (Vector& s. const VecFunc& asol.
                                                              Analytical solution
                        const Vec3& X) const
  s = Vector(asol(X).ptr(),2);
  return true:
```

```
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.

```
bool PoissonNorm::evalInt (LocalIntegral& elmInt.
                           const FiniteElement& fe.
                           const Vec3& X) const
  Poisson& problem = static cast<Poisson&>(mvProblem):
  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

```
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.

```
class SIMPoisson2D : public SIM2D
            prob: //!< Poisson data and methods
  RealArray mVec: //!< Material data
public:
  SIMPoisson2D() : SIM2D(1) { myProblem = &prob; }
  virtual ~SIMPoisson2D() { myProblem = 0; }
protected:
  virtual bool parse(const TiXmlElement* elem);
  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 = mvScalars.find(propInd):
  if (sit == mvVectors.end()) return false:
  prob.setFlux(tit->second);
  return true:
```

Simulation driver for 2D problems.

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}:
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  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 == mvVectors.end()) return false:
  prob.setFlux(tit->second);
  return true:
```

Simulation driver for 2D problems.

Alternative, use templates to support multiple dimensions:

where Dim can be either SIM1D, SIM2D or SIM3D.

```
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 = this->parseMaterialSet(child, mVec.size());
     double kappa = 1000.0;
     utl::getAttribute(child, "kappa", kappa);
     if (code == 0)
        prob.setMaterial(kappa);
        mVec.push_back(kappa);
}
```

```
else if (!strcasecmp(child->Value(), "source")) {
    int code = -1: // Reserve negative code(s) for the source term function
    while (mvScalars.find(code) != mvScalars.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;
      mvScalars[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 (!mvSol) mvSol = new AnaSol(child):
    else
      std::cerr <<" ** SIMPoisson2D::parse: Invalid analytical solution "<< type << std::endl:
7
return true:
```

```
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(): // (or new SIMPoisson<SIM2D>:)
  if (!model->read(infile))
    return 1:
  if (!model->preprocess(ignoredPatches.fixDup))
    return 1:
  model->setQuadratureRule(nGauss):
  Matrix eNorm:
  Vector gNorm, sol:
                                                              Core parts of the main program
  model->initSystem(solver,1,1);
  model->setAssociatedRHS(0,0);
  if (!model->assembleSvstem())
    return 2:
  // Solve the linear system of equations
  if (!model->solveSvstem(sol.1))
    return 3:
  // Evaluate solution norms
  if (!model->solutionNorms(Vectors(1,sol),eNorm,gNorm))
    return 4:
  // Print output to terminal and VTF, etc.
```

### Tutorial: Poisson equation, sample input files

<simulation>

</simulation>

```
<!-- General - geometry definitions !-->
<geometry>
                                                                        square2d.g2:
  <patchfile>square2D.g2</patchfile>
  <raiseorder patch="1" u="2" v="2"/>
                                                                         200 1 0 0
  <refine type="uniform" patch="1" u="7" v="7"/>
                                                                         3 0
  <topologysets>
                                                                        2 2
    <set name="Dirichlet" type="edge">
                                                                        0 0 1 1
      <item patch="1">4</item>
                                                                         22
    </set>
                                                                        0 0 1 1
    <set name="Neumann" type="edge">
                                                                        0.0 0.0 0.0
      <item patch="1">3</item>
                                                                        2 0 0 0 0 0
    </set>
                                                                        0.0 2.0 0.0
  </topologysets>
                                                                        2.0 2.0 0.0
</geometry>
<!-- General - boundary conditions !-->
<box>
<br/>boundaryconditions></br>
  <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">
    cos(PI*x)*(2-v)
    <secondary>PI*sin(PI*x)*(2-y)|cos(PI*x)</secondary>
  </anasol>
</poisson>
```

### Tutorial: Poisson equation, sample input files

```
<!-- 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>
<!-- General - boundary conditions !-->
<box>
<br/>boundaryconditions></br>
 <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">
   cos(PI*x)*(2-y)
   <secondary>PI*sin(PI*x)*(2-y)|cos(PI*x)</secondary>
 </anasol>
</poisson>
```

<simulation>

</simulation>

```
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
2.0 2.0 0.0
```

This is equivalent to both of the following:

```
<geometry scale="2.0"/>
<geometry Lx="2.0" Ly="2.0"/>
```