ElmerSolver

Setup, execution

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Computational Environment & Application

CSC–Scientific Computing Ltd.

The Finnish IT center for science

Espoo, Finland

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Contents

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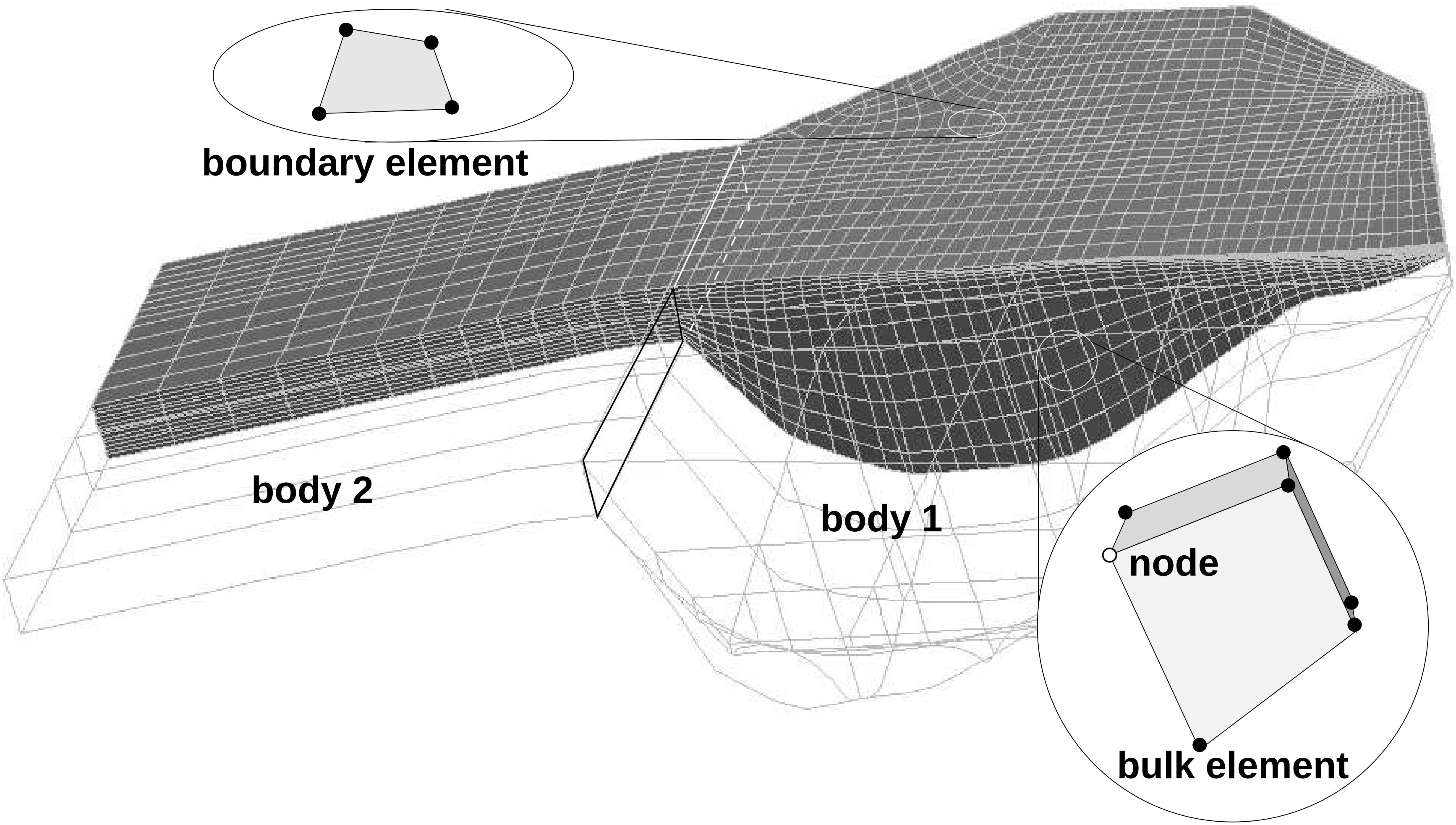
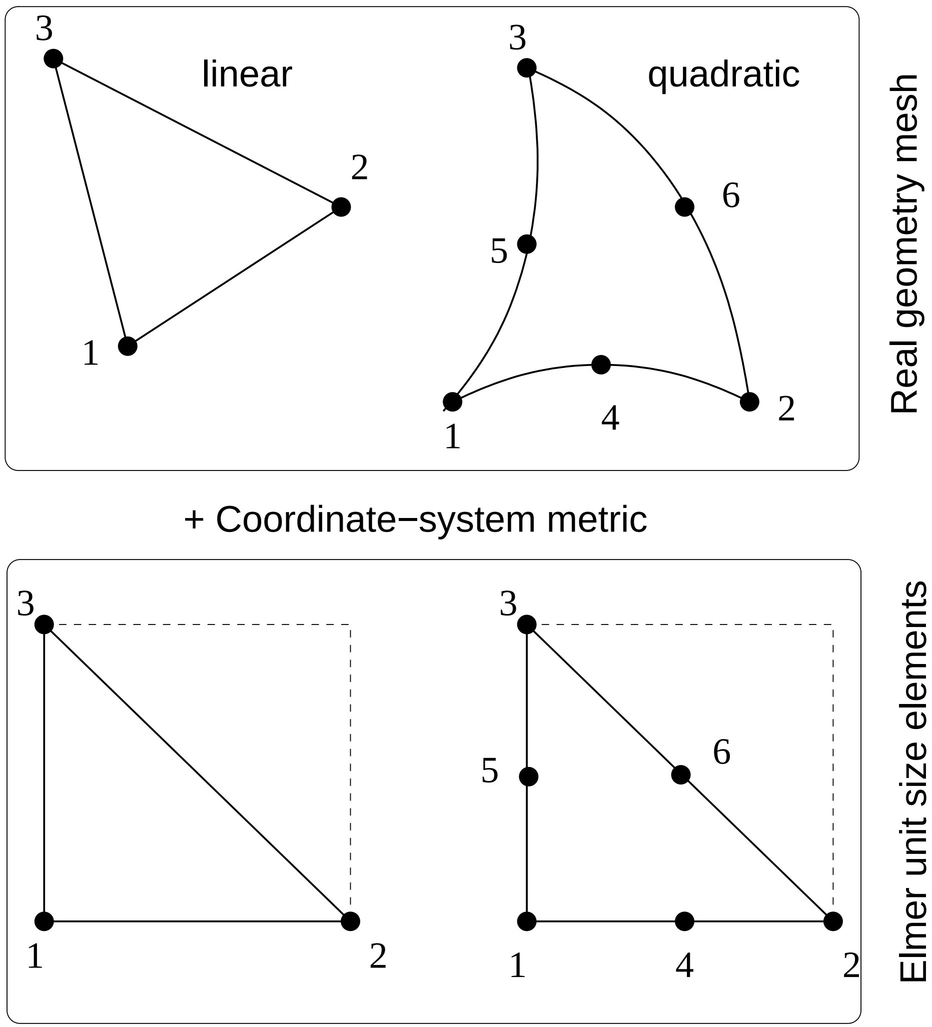
On Bodies and Boundaries



Finite Elements



Finite Elements contd.

General advection-diffusion:

$$\partial\Psi/\partial t + \mathbf{u}\cdot\nabla\Psi = \nabla\cdot\left(\kappa\nabla\Psi\right) + \sigma$$

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Partial integration of diffusion term:

$$\int_\Omega \partial\Psi/\partial t\,\phi_\alpha d\Omega + \int_\Omega \mathbf{u}\cdot\nabla\Psi\phi_\alpha d\Omega + \int_\Omega \kappa\nabla\Psi\cdot\nabla\phi_\alpha d\Omega =$$

$$\oint_{\partial\Omega} (\kappa\nabla\Psi\phi_\alpha)\cdot\mathbf{n}d\Omega + \int_\Omega \sigma\phi_\alpha d\Omega$$

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$$\underbrace{\Psi_\beta\, a(\Delta t) \int\limits_\Omega \phi_\beta \phi_\alpha d\Omega}_{\mathbf{M}} + \underbrace{\Psi_\beta \int\limits_\Omega \left[\mathbf{u} \cdot \nabla \phi_\beta \phi_\alpha + \kappa \nabla \phi_\beta \cdot \nabla \phi_\alpha\right] d\Omega}_{\mathbf{S}} =$$

$$\underbrace{\oint\limits_{\partial\Omega} (\kappa \nabla \Psi \phi_\alpha) \cdot \mathbf{n} d\Omega}_{\text{nat. BC}} + \underbrace{b(\Delta t)\Psi_\beta^{t-\Delta t} \int\limits_\Omega \phi_\beta \phi_\alpha d\Omega}_{\text{timeforce}} + \underbrace{\int\limits_\Omega \sigma \phi_\alpha d\Omega}_{\mathbf{f}}$$

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$$(\mathbf{M} + \mathbf{S}) \cdot \mathbf{\Psi} = \mathbf{f}$$

$\mathbf{M}$... Mass matrix, $\mathbf{S}$... Stiffness matrix, $\mathbf{f}$... force vector

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- Three solution methods for $\mathbf{A} \cdot \Psi = \mathbf{f}$
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  - standard LAPACK (`banded`)
  - alternatively UMFPACK - Unsymmetrical Multi Frontal (`UMFPACK`)

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  `Linear System Iterative Method =`

  Conjugate Gradient (`CG`), Conjugate Gradient Squared (`CGS`), BiConjugate Gradient Stabilized (`BiCGStab`), Transpose-Free Quasi-Minimal Residual (`TFQMR`), Generalized Minimal Residual (`GMRES`)

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- Multilevel (Keyword: `Multigrid`) Geometric (GMG) and Algebraic (AMG) Multigrid

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Precondition strategies

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solving instead:

$$\mathbf{A}\mathbf{M}^{-1} \cdot \mathbf{\Phi} = \mathbf{f}\text{, with } \Phi = \mathbf{M} \cdot \mathbf{\Psi}$$

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Why?: $\mathbf{AM}^{-1}$ shall have a towards convergence of iterative methods improved spectrum

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Why?: $\mathbf{AM}^{-1}$ shall have a towards convergence of iterative methods improved spectrum `Linear System Preconditioning =`

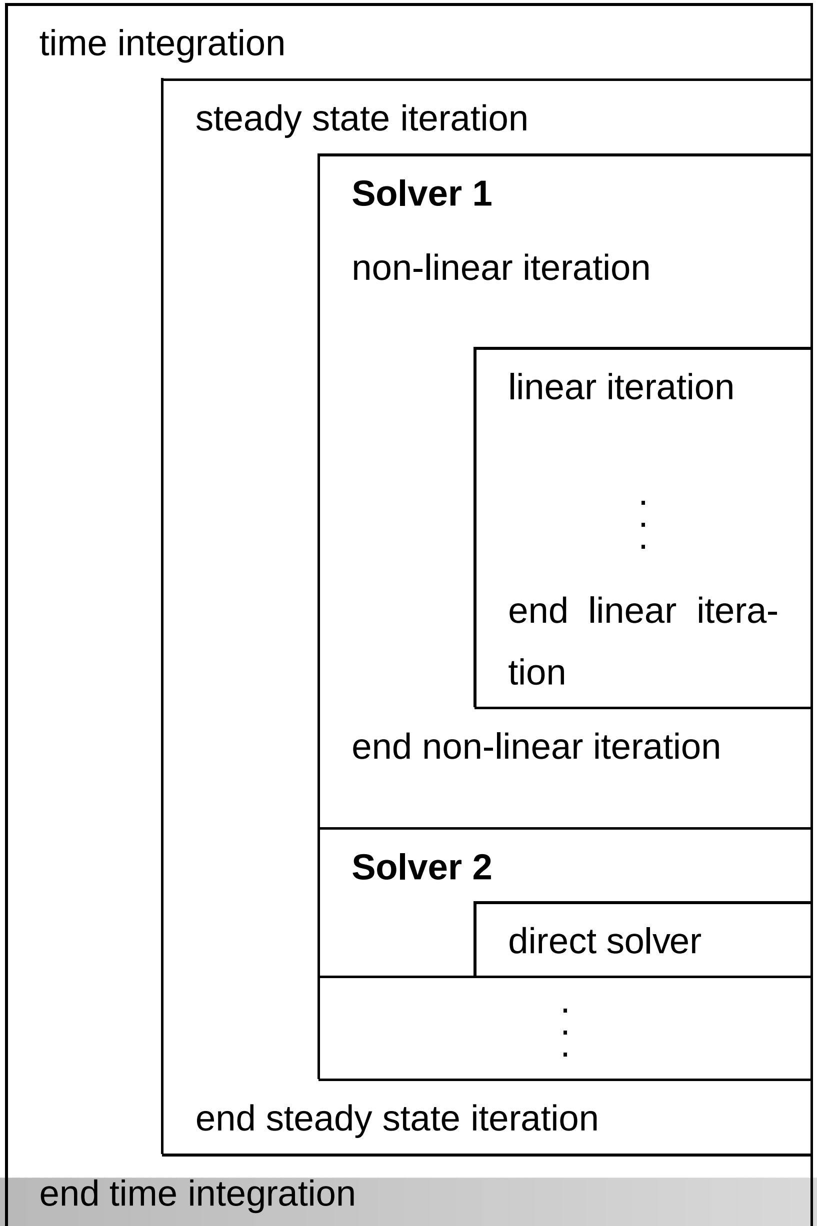
- `None`
- `Diagonal`
- `ILU`*n* $n = 0,1,2,\ldots$
- `ILUT`
- `Multigrid`

Solution Levels

- time integration
  - steady state iteration
    - **Solver 1**
      - non-linear iteration
        - linear iteration
          - ⋮
        - end linear iteration
      - end non-linear iteration
    - **Solver 2**
      - direct solver
    - ⋮
  - end steady state iteration
- end time integration

`Time Steps`

Solution Levels



`Time Steps`

`Steady State Max Iterations`

`Steady State Convergence Tolerance`

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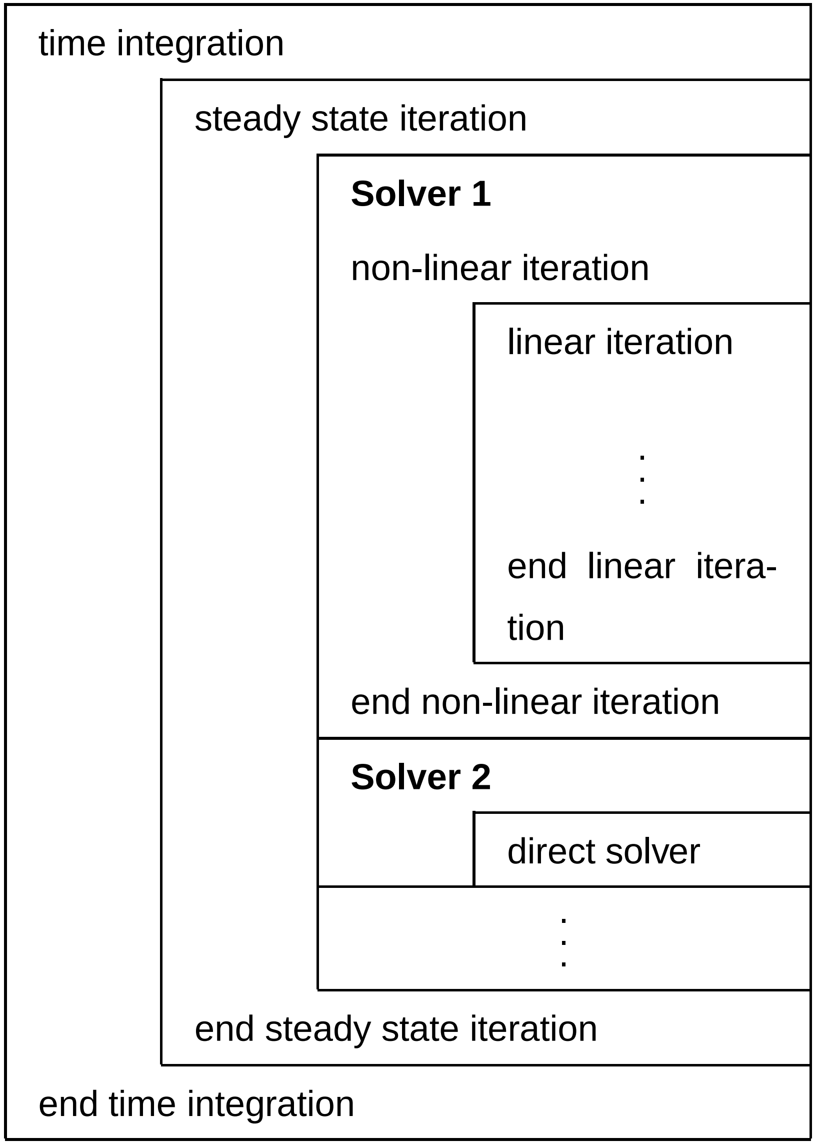

`Time Steps`

`Steady State Max Iterations`

`Nonlinear Max Iterations`

`Nonlinear System Convergence Tolerance`

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Solution Levels

- time integration — `Time Steps`
  - steady state iteration — `Steady State Max Iterations`
    - **Solver 1**
      - non-linear iteration — `Nonlinear Max Iterations`
        - linear iteration — `Linear System Max Iterations`
        - ⋮
        - end linear iteration — `Linear System Convergence Tolerance`
      - end non-linear iteration — `Nonlinear System Convergence Tolerance`
    - **Solver 2**
      - direct solver
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  - end steady state iteration — `Steady State Convergence Tolerance`
- end time integration

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- `Parametername(n,m)` indicates a $n \times m$ array

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Header

The header declares where to search for the mesh database

```
Header
   Mesh DB "." "dirname"
End
```

preceding path + directory name of mesh database

Constants

Declaration of constant values that can be obtained from within **every** solver and boundary condition **subroutine** or **function**, can be declared.

```
Constants
   Gas Constant = Real 8.314E00
   Gravity (4) = 0 -1 0 9.81
End
```

a scalar constant

Gravity vector, an array with a registered name

Simulation

Principle declarations for simulation

```
Simulation
   Coordinate System = "Cartesian 2D"
   Coordinate Mapping(3) = Integer 1 2 3
   Simulation Type ="Steady"
   Output Intervals = 1
   Steady State Max Iterations = 10
   Steady State Min Iterations = 2
   Output File = "name.result"
   Post File = "name.ep"
   max output level = n
End
```

- Coordinate System — choices: `Cartesian {1D,2D,3D}`, `Polar {2D,3D}`, `Cylindric`, `Cylindric Symmetric`, `Axi Symmetric`
- Coordinate Mapping — permute, if you want to interchange directions
- Simulation Type — either `Steady` or `Transient`
- Output Intervals — how often you want to have results
- Steady State Max Iterations — maximum rounds on one time level
- Steady State Min Iterations — minimum rounds on one Timestep
- Output File — contains data to restart run
- Post File — `ElmerPost`-file
- max output level — n=1 talkative like a Finnish lumberjack, n=42 all and everything

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Solver

Example: (Navier) Stokes solver

```
Solver 1
   Equation = "Navier-Stokes"
   Linear System Solver = "Direct"
   Linear System Direct Method = "UMFPack"
   Linear System Convergence Tolerance = 1.0E-06
   Linear System Abort Not Converged = True
   Linear System Preconditioning = "ILU2"
   Steady State Convergence Tolerance = 1.0E-03
   Stabilization Method = Stabilized
   Nonlinear System Convergence Tolerance = 1.0E-05
   Nonlinear System Max Iterations = 1
   Nonlinear System Min Iterations = 1
   Nonlinear System Newton After Iterations = 30
   Nonlinear System Newton After Tolerance = 1.0E-05
End
```

name of the solver

alt. `Iterative`

a linear problem

Body

Here the different bodies (there can be more than one) get their `Equation`, `Material`, `Body Force` and `Initial Condition` assigned

```
Body 1
   Name = "identifier"
   Equation = 1
   Material = 1
   Body Force = 1
   Initial Condition = 1
End
```

give the body a name

Equation

- set active solvers
- give keywords for the behaviour of different solvers

```
Equation 1
   Active Solvers(2) = 1 2
   Convection = Computed
   Flow Solution Name = String "Flow Solution"
   NS Convect = False
End
```

Bodyforce

- declares the solver-specific $\mathbf{f}$ from $\mathbf{A} \cdot \mathbf{\Psi} = \mathbf{f}$ for the body
- body force can also be a dependent function (see later).

Here for the (Navier) Stokes solver

```
Body Force 1
   Flow BodyForce 1 = 0.0
   Flow BodyForce 2 = -9.81 !  good old gravity
End
```

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Material

- sets material properties for the body.
- material properties can be scalars or tensors and also
- can be given as dependent functions

```
Material 1
   Viscosity = 1.0E13
   Density = 918.0
   My Heat Capacity = Real 1002.0
End
```

not in keyword DB!

Initial Conditions

- initializes variable values
- sets initial guess for steady state simulation
- sets initial value for transient simulation
- variable values can be functions

```
Initial Condition 1
   Velocity 1 = 0.0
   Velocity 2 = 1.0
   Pressure = 0.0
   My Variable = Real 0.0
End
```

not in keyword DB

Boundary Conditions

- Dirichlet: `variablename` = *value*
- Neumann: often enabled with keyword (e.g., HTEqu. `Heat Flux BC = True`) followed by the flux value
- No BC $\equiv$ Natural BC!
- values can be given as functions

Example: (Navier) Stokes with no penetration (normal) and free slip (tangential)

```
Boundary Condition 1
    Name = "slip"
    Target Boundaries = 4
    Normal-Tangential Velocity = Logical True
    Velocity 1 = Real 0.0
End
```

name

refers to boundary no. 4 in mesh

components with respect to surface nor

normal component

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Bodies on Boundaries

- need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)

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- define `Body Force`, `Material`, `Equation` and `Initial Condition` for that body
- full dimensional metric is still valid on the BC body $\Rightarrow$ has to be taken into account in user supplied subroutines

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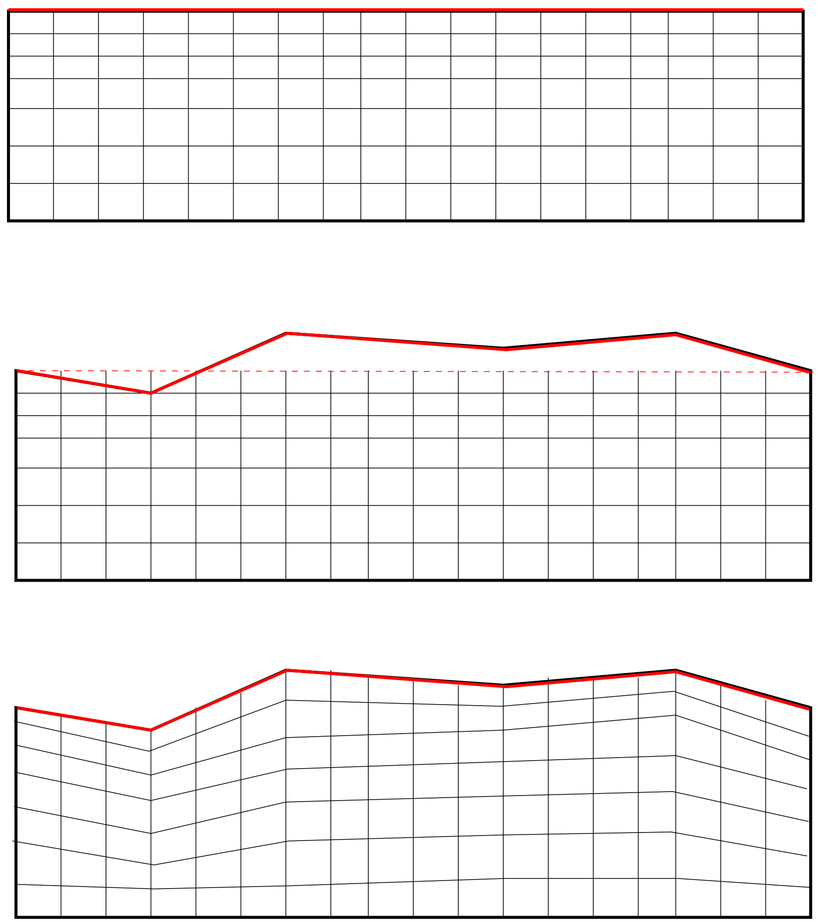
Deforming Meshes

- solving the free surface on body 2:

  solving

  $$\partial s/\partial t + u\partial s/\partial x + v\partial s/\partial y = a_\perp$$



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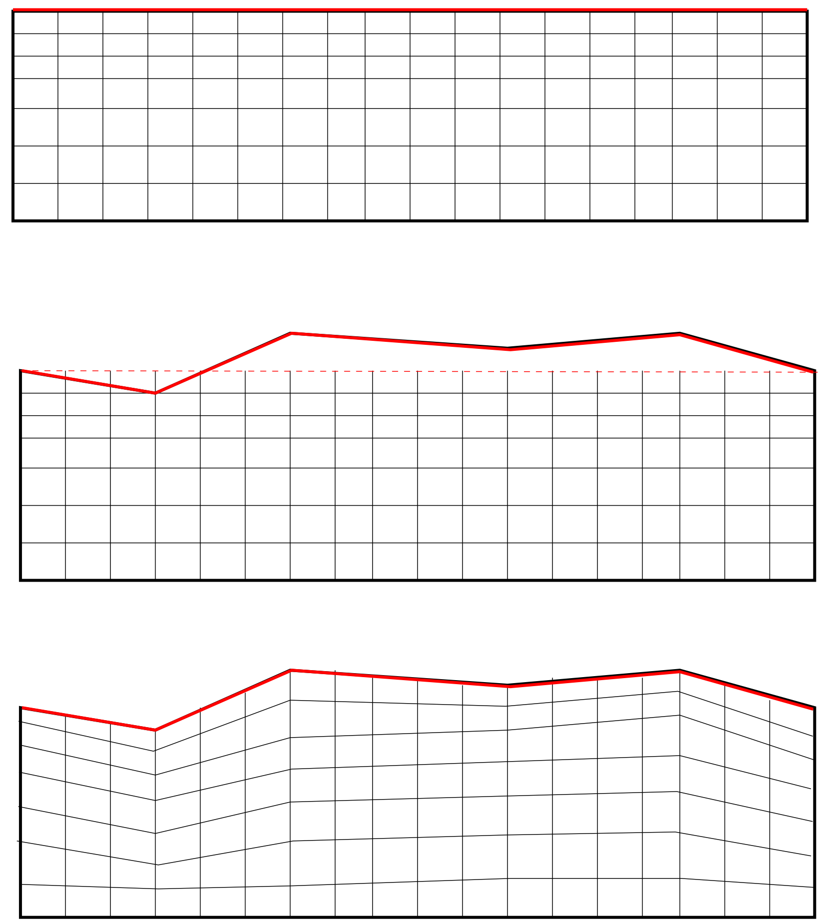

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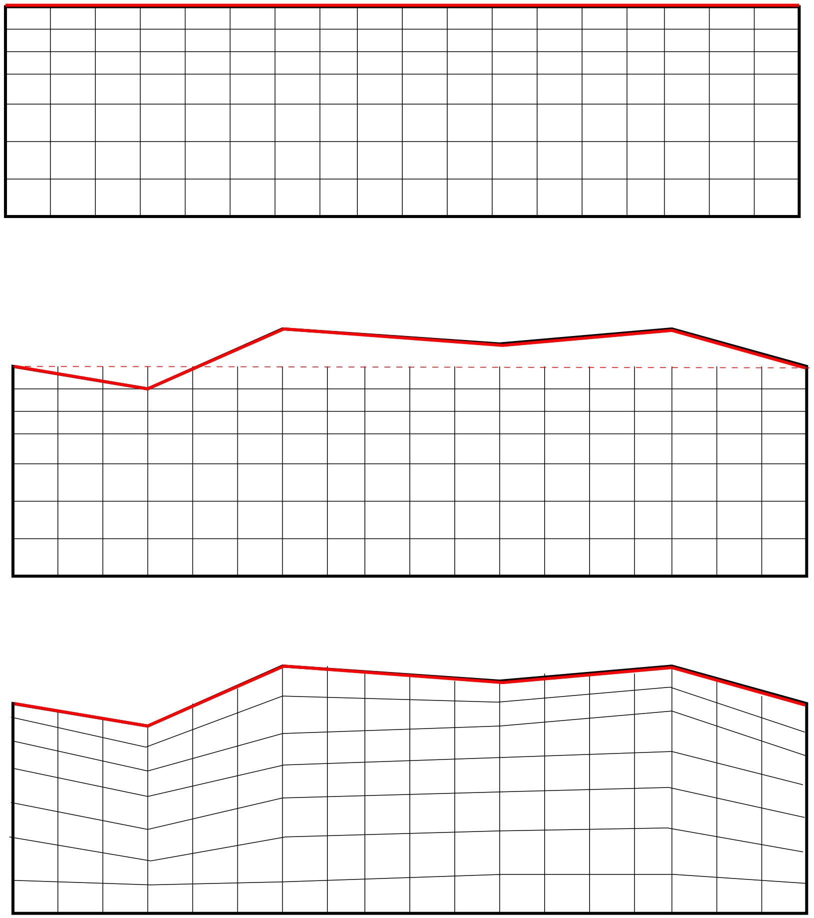
- run MeshUpdate solver:

  re-distributing the mesh nodes



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  launch with `mpirun -np 4 --hostfile hostfilename ElmerSolver`

Tables and Arrays

- **Tables** may be used for piecewise linear dependency of a variable

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```
Density   = Variable Temperature
   Real
      0   900
    273   1000
    300   1020
    400   1000
    End
```

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- **Arrays** may be used to declare vector/tensor parameters

```
Target Boundaries(3) = 2 4 5
My Parameter Array(3,3) = Real 1 2 3 \
                               4 5 6 \
                                 7 8 9
```

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e.g. K $\longrightarrow$ $^\circ$C: `math Celsius = Temperature + 273.16`

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  also logical evaluations (if) and loops (for)
- documentation on Funet (MATC Manual)

MATC contd.

- simple numerical evaluation:

```
Viscosity Exponent = Real MATC "1.0/3.0"
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or

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- as a function dependent on a variable:

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```

- as a function of multiple variables:

```
Temp = Variable Latitude, Coordinate 3
Real MATC "49.13 + 273.16 - 0.7576 * tx(0) - 7.992E-03 * tx(1)"
```

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MATC contd.

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- as function defined before header:

```
$ function stemp(X) { _stemp = 49.13 + 273.16 - 0.7576*X(0)
                                            - 7.992E-03*X(1) }
```

```
Temp = Variable Latitude, Coordinate 3
Real MATC "stemp(tx)"
```

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Real MATC "2.1275D03 + 7.253D00*(tx - 273.16)"
```

- as a function of multiple variables:

```
Temp = Variable Latitude, Coordinate 3
Real MATC "49.13 + 273.16 - 0.7576 * tx(0) - 7.992E-03 * tx(1)"
```

- as function defined before header:

```
$ function stemp(X) { _stemp = 49.13 + 273.16 - 0.7576*X(0)
                                       - 7.992E-03*X(1) }
```

```
Temp = Variable Latitude, Coordinate 3
Real MATC "stemp(tx)"
```

CSC

User Defined Functions

Example: $\rho(T(^\circ C)) = 1000 \cdot [1 - 10^{-4} \cdot (T - 273.0)]$

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```
FUNCTION getdensity( Model, n, T ) RESULT(dens)
USE DefUtils
IMPLICIT None
 TYPE(Model_t) ::  Model
 INTEGER ::  n
 REAL(KIND=dp) ::  T, dens
 dens = 1000*(1-1.0d-4(T-273.0d0))
END FUNCTION getdensity
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SIF: `Density = Variable Temperature`

`Procedure "mydensity" "getdensity"`

CSC

User Defined Subroutines

```
RECURSIVE SUBROUTINE &
mysolver( Model,Solver,dt,TransientSimulation )
TYPE(Model_t) ::  Model
TYPE(Solver_t) ::  Solver
REAL(KIND=dp) ::  dt
LOGICAL ::  TransientSimulation
...
assembly, solution
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END SUBROUTINE mysolver
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`Model`	pointer to the whole Model (solvers, variables)
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CSC

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compile:

```
elmerf90 mysolverfile.f90 -o mysolverexe
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CSC

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```
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```
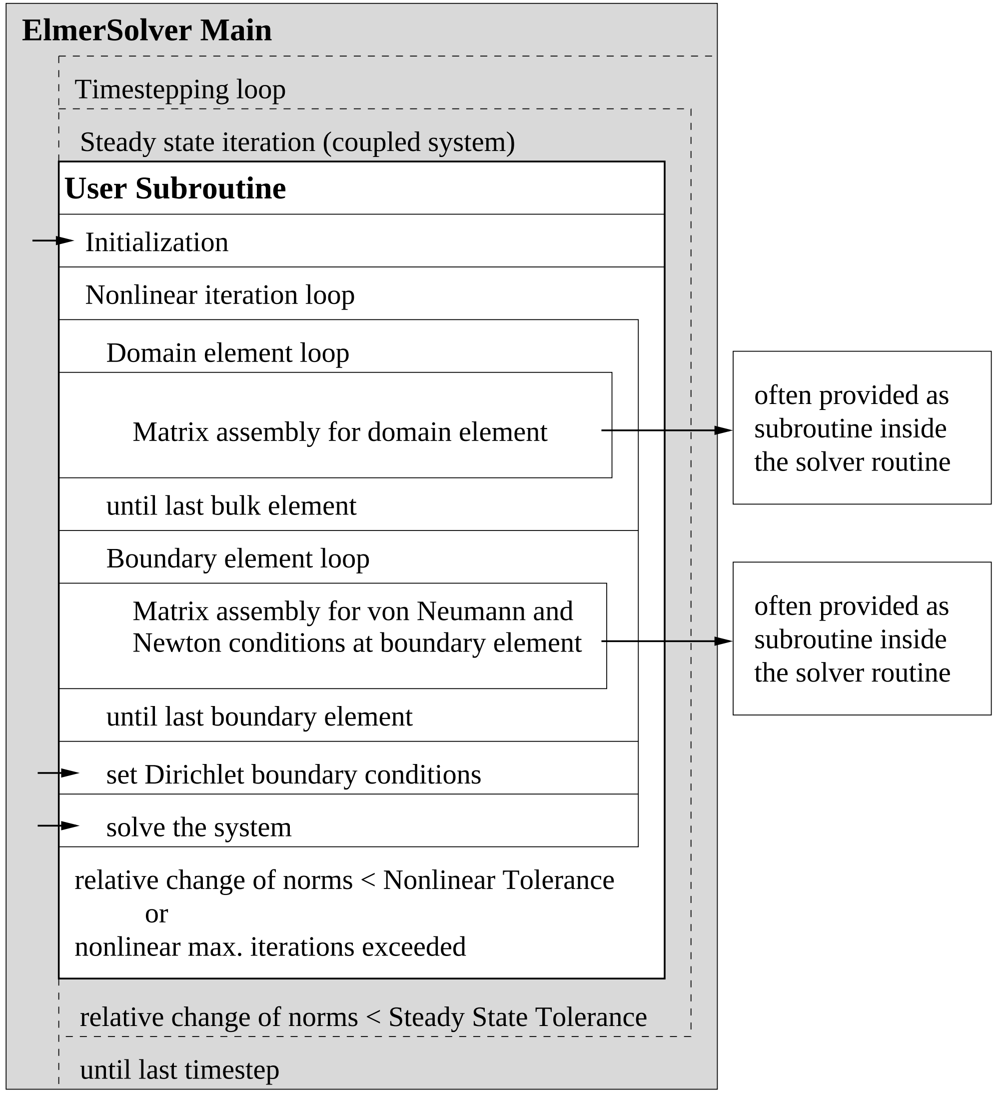

SIF:

```
Procedure = "/path/to/mysolverexe" "mysolver"
```

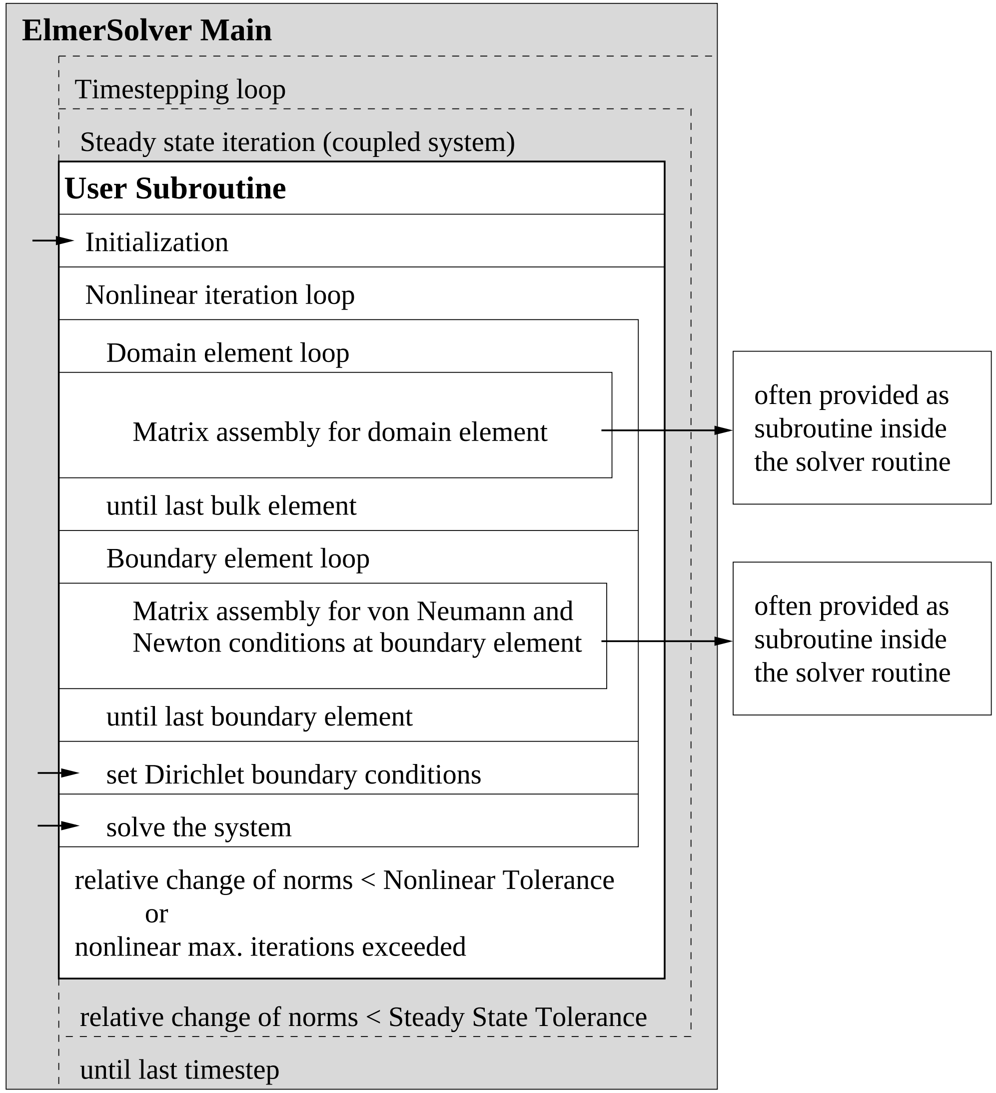
User Defined Subroutines contd.



User Defined Subroutines contd.

Pre-defined routines

- `CALL DefaultInitialize()`
- `CALL DefaultUpdateEquations( STIFF, FORCE )`
- `CALL DefaultFinishAssembly()`
- `CALL DefaultDirichletBCs()`
- `Norm = DefaultSolve()`



Multiple Meshes

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  ⚠ they will boldly be extrapolated, should your meshes not be congruent!

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CSC

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  selectively for each solver:

```
Element[1] = ...
Element[2] = ...
:
Element[n] = ...
```

CSC

Specialities

- given names for components of vector fields:

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Variable = var_name[cname 1:#dofs cname 2:#dofs ...  ]
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Procedure = "FlowSolve" "FlowSolver"
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- Solver execution:

```
Exec Solver = {Before Simulation, After Simulation, Never, Always}
```

Elmer Parallel Version

- Pre-processing: `ElmerGrid` with options:

Partition by direction:

`-partition 2 2 1 0`	First partition elements (default)
`-partition 2 2 1 1`	First partition nodes
$2 \times 2 \times = 4$	

Partition using METIS:

`-metis` *n* `0`	PartMeshNodal (default)
`-metis` *n* `1`	PartGraphRecursive
`-metis` *n* `2`	PartGraphKway
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`-metis` *n* `3`	PartGraphVKway

- Execution: `mpirun -np` *n* `ElmerSolver_mpi`
- Combining parallel results: in mesh-database directory

  `ElmerGrid 15 3` *name*

Elmer Parallel Version contd.

- need iterative method for linear solver!

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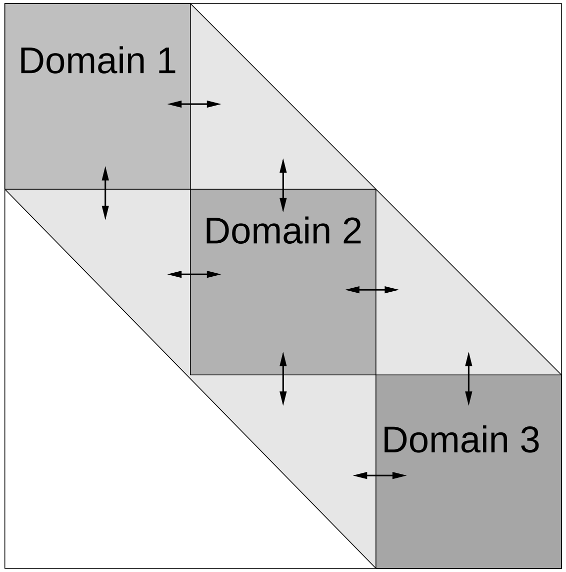

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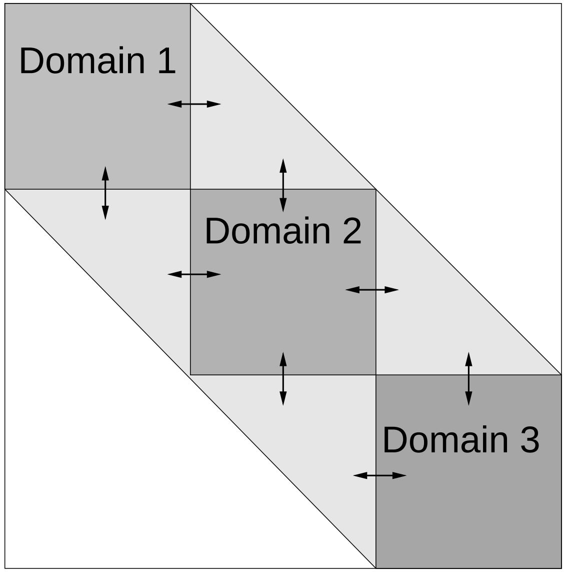

- `Linear System Use Hypre = Logical True`

Elmer Parallel Version contd.

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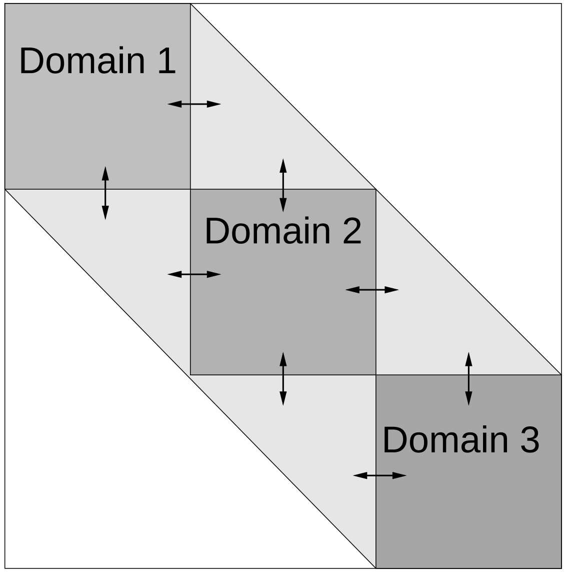

- `Linear System Use Hypre = Logical True`
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Elmer Parallel Version contd.

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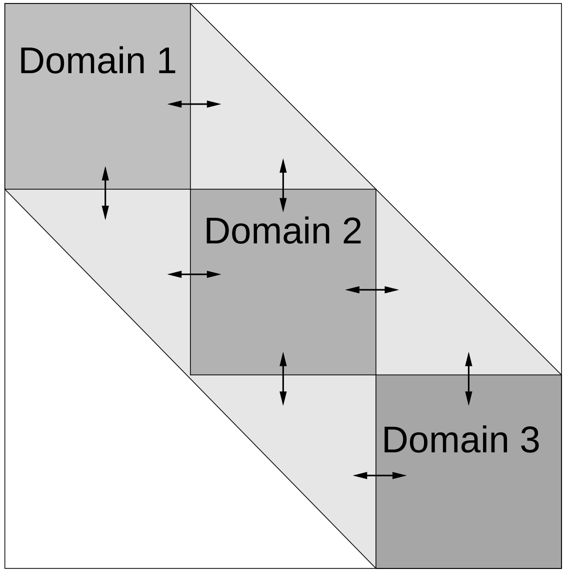

- `Linear System Use Hypre = Logical True`
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- `ParaSails Threshold, ParaSails Filter, ParaSails Maxlevel, ParaSails Symmetry`