Open-source CFD software: FeatFlow

The FEA(S)T groups

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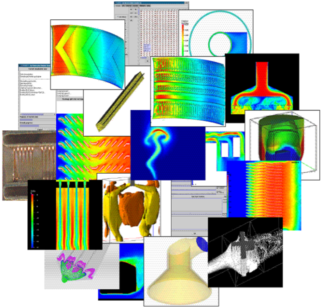
Lake Tahoe, January 7, 2009

Overview

1. FeatFlow
   - FeatFlow 1.x
   - FeatFlow 2.0
2. Preprocessing
   - DeViSoR Grid3D
3. Example application
   - Poisson equation
4. Postprocessing
   - General Mesh Viewer
5. UnConventional HPC
   - FEAST



FeatFlow 1.x

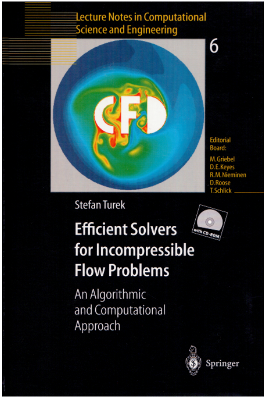
Finite **E**lement **A**nalysis **T**oolbox + Flow solver

High performance unstructured finite element package for the numerical solution of the incompressible Navier-Stokes equations

- based on the finite element packages Feat2D and Feat3D
- written in Fortran 77 (and some C routines) by Stefan Turek
- designed for education, scientific research and industrial applications
- full source-code and user manuals are available online
- many extensions are not included in the official release ☹

Visit the FeatFlow homepage

http://www.featflow.de



http://www.featflow.de/album

Theoretical background

Discretization techniques

Incompressible Navier-Stokes equations

$$\mathbf{u}_t - \nu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{f}, \quad \nabla\cdot\mathbf{u} = 0, \qquad \text{in } \Omega\times(0,T]$$

- Spatial discretization techniques
  - nonconforming rotated multilinear finite elements for $\mathbf{u}$
  - piecewise constant pressure approximation for p
  - Samarskij upwind or streamline diffusion stabilization
- Temporal discretization techniques
  - implicit one-step-θ-scheme (Backward Euler, Crank-Nicolson)
  - implicit fractional-step-θ scheme (second-order accurate)
  - adaptive time-stepping based on local discretization error

Solution techniques

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Discretized incompressible Navier-Stokes equations

Given $\mathbf{u}^n$, $\mathbf{g}$ and k, solve for $\mathbf{u} = \mathbf{u}^{n+1}$ and $p = p^{n+1}$

$$[M + \theta k N(\mathbf{u})]\mathbf{u} + kBp = \mathbf{g}, \qquad B^T\mathbf{u} = 0$$

where $\mathbf{g} = [M - \theta_1 k N(\mathbf{u}^n)]\mathbf{u}^n + \theta_2 k \mathbf{f}^{n+1} + \theta_3 k \mathbf{f}^n$

- Nonlinear/linear solution strategies
  - coupled fixed point defect correction method `CC2D/CC3D`
  - nonlinear discrete projection scheme `PP2D/PP3D`
  - linear multigrid techniques with adaptive step-length control
  - ILU/SOR or Vanka-like block Gauß-Seidel smoother/solver

Finite **E**lement **A**nalysis **T**oolbox + Flow solver

The modern successor of FeatFlow 1.x for the numerical solution of flow problems by the finite element method

- modular object-oriented design by Michael Köster et al.
- written in Fortran 95 (kernel + applications)
- external libraries in F77/C (BLAS, UMFPACK, LAPACK)
- designed for education of students and scientific research
- detailed in-place documentation of the source-code

Official release not yet available; get the ALPHA snapshot

`http://www.featflow.de/download/Featflow2_2.0ALPHA.tar.gz`

Prerequisites

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Unix/Linux and Mac OS X

- compatible `C` and `F95` compiler
  - `GCC` and `G95` version 0.91
  - Intel® C++/Fortran Compilers for Linux
  - Sun Studio C, C++ and Fortran Compilers
- GNU `make` utility
  - Makefiles are provided for all applications

Windows XP, Vista

- Microsoft® VisualStudio 2003, 2005 or 2008
  - Project files are provided for all applications
- Intel® C++/Fortran Compilers for Windows
- Cygwin™ environment
  - General Mesh Viewer (GMV)

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Linux is used for this workshop

Getting FEATFLOW 2.0

- Unpack the downloaded archive file

```
$ tar xvzf Featflow2_2.0ALPHA.tar.gz
```

- Change into the base directory

```
$ cd Featflow2 ; ls
```

```
applications    Globals.power   object
bin             Globals.sparc   readme.txt
codefragments   Globals.x86     Rules_apps_f90.mk
feat2win.txt    Globals.x86_64  Rules_apps.mk
Globals.alpha   kernel          Rules_libs.mk
Globals.ia64    libraries       VERSIONS
Globals.mac     Makefile
Globals.mk      matlab
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Globals.ia64    libraries        VERSIONS
Globals.mac     Makefile
Globals.mk      matlab
```

Top-level build options

```
$ make [ALT=xxx] [ID=yyy] <target>
```

- Some values for `target`

`help`	- print additional help and further option
`id`	- print out settings for current ID
`all`	- compile all libraries and application modules
`apps`	- compile all application modules
`libs`	- compile all libraries

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`all`	- compile all libraries and application modules
`apps`	- compile all application modules
`libs`	- compile all libraries

- Some available make modifiers

`ALT=xxx`	- specify alternative ID-xxx to use
`ID=yyy`	- override the autodetected architecture ID by yyy

Building FEATFLOW 2.0, cont'd.

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Understanding the ALT/ID concept

$ make id   run on x86_64 GNU/Linux

```
Machine-ID (Barracuda) : pc64-core2-linux

Compilers to be used:
  C compiler:         /usr/bin/gcc
  C++ compiler:       /usr/bin/g++
  Fortran compiler:   /usr/local/g95/32bit_integers/0.91/bin/g95
  F-Library archiver: /usr/bin/ar
  C-Library archiver: /usr/bin/ar

Flags to be used:
  OPTFLAGS        = -O3 -m64 -ffast-math -fexpensive-optimizations -fprefetch-loop-arrays -mmmx -msse -msse2 -msse3
  OPTFLAGSC       =
  OPTFLAGSCPP     =
  OPTFLAGSF       =
  OPTFLAGSDEBUG   = -g
  OPTFLAGSCDEBUG  =
  OPTFLAGSCPPDEBUG=
  OPTFLAGSFDEBUG  = -O0 -g -Wall -fbounds-check -ftrace=full
  FCFLAGS         = -pipe -fmod= -march=nocona
  CCFLAGS         = -pipe -march=nocona
  CPPFLAGS        = -pipe -march=nocona
  BUILDLIB        = feat3d feat2d sysutils umfpack2 amd umfpack4 minisplib lapack blas
  BLASLIB         = (standard BLAS, included in installation package)
  LAPACKLIB       = (standard LAPACK, included in installation package)
  LDLIBS          =
  LDFLAGS         =
```

Building FEATFLOW 2.0, cont'd.

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Understanding the ALT/ID concept

$ make ID=pc-core2-linux id   run on x86_64 GNU/Linux

```
Machine-ID (Barracuda) : pc-core2-linux

Compilers to be used:
  C compiler:         /usr/bin/gcc
  C++ compiler:       /usr/bin/g++
  Fortran compiler:   /usr/local/g95/32bit_integers/0.91/bin/g95
  F-Library archiver: /usr/bin/ar
  C-Library archiver: /usr/bin/ar

Flags to be used:
  OPTFLAGS         = -O3 -m32 -ffast-math -fexpensive-optimizations -fprefetch-loop-arrays -mmmx -msse -msse2 -msse3
  OPTFLAGSC        =
  OPTFLAGSCPP      =
  OPTFLAGSF        =
  OPTFLAGSDEBUG    = -g
  OPTFLAGSCDEBUG   =
  OPTFLAGSCPPDEBUG=
  OPTFLAGSFDEBUG   = -O0 -g -Wall -fbounds-check -ftrace=full
  FCFLAGS          = -pipe -fmod= -march=nocona
  CCFLAGS          = -pipe -march=nocona
  CPPFLAGS         = -pipe -march=nocona
  BUILDLIB         = feat3d feat2d sysutils umfpack2 amd umfpack4 minisplib lapack blas
  BLASLIB          = (standard BLAS, included in installation package)
  LAPACKLIB        = (standard LAPACK, included in installation package)
  LDLIBS           =
  LDFLAGS          =
```

Building FeatFlow 2.0, cont'd.

Understanding the ALT/ID concept

`$ make ALT=ifc id` run on x86_64 GNU/Linux

```
Machine-ID (Barracuda) : pc64-core2-linux-ifc

Compilers to be used:
  C compiler:         /usr/local/intel/cce/10.1.021/bin/icc
  C++ compiler:       /usr/local/intel/cce/10.1.021/bin/icpc
  Fortran compiler:   /usr/local/intel/fce/10.1.021/bin/ifort
  F-Library archiver: /usr/local/intel/fce/10.1.021/bin/xiar
  C-Library archiver: /usr/local/intel/fce/10.1.021/bin/xiar

Flags to be used:
  OPTFLAGS         = -O3 -ipo -xT
  OPTFLAGSC        =
  OPTFLAGSCPP      =
  OPTFLAGSF        =
  OPTFLAGSDEBUG    = -g
  OPTFLAGSCDEBUG   = -traceback
  OPTFLAGSCPPDEBUG= -traceback
  OPTFLAGSFDEBUG   = -warn all -check all -traceback
  FCFLAGS          = -cm -fpe0 -vec-report0 -module
  CCFLAGS          = -vec-report0
  CPPFLAGS         = -vec-report0
  BUILDLIB         = feat3d feat2d sysutils umfpack2 amd umfpack4 minisplib lapack blas
  BLASLIB          = (standard BLAS, included in installation package)
  LAPACKLIB        = (standard LAPACK, included in installation package)
  LDLIBS           =
  LDFLAGS          = -lsvml
```

Building FeatFlow 2.0, cont'd.

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Understanding the ALT/ID concept

```
$ make [ALT=xxx] [ID=yyy] <target>
```

- compiler settings are defined in the global configuration files `Global.[alpha,ia64,mac,power,sparc,x86,x86_64]`
- new compilers and/or architectures can be easily included
- special purpose settings, e.g. `pc64-opteron-linux-ifclarge`

Building FeatFlow 2.0, cont'd.

Understanding the `ALT/ID` concept

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Building the Poisson example application

```
$ cd applications/poisson
$ make
```

... after some time ...

```
Done, poisson-pc64-core2-linux is ready.
```

Building FeatFlow 2.0, cont'd.

Understanding the ALT/ID concept

```
$ make [ALT=xxx] [ID=yyy] <target>
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Building the Poisson example application

```
$ cd applications/poisson
$ make debug
```

turn on debugging facilities of the compiler

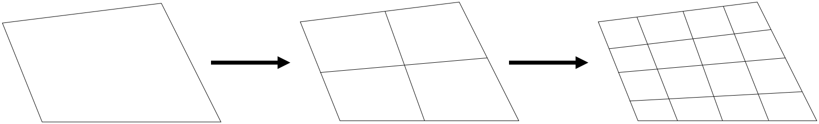
... after some time ...

```
Done, poisson-pc64-core2-linux is ready.
```

Preprocessing: *Grid generation*

Geometric multigrid approach

1. Construct initial coarse grid in the external preprocessing step
2. Generate hierarchy of regularly refined meshes in the application



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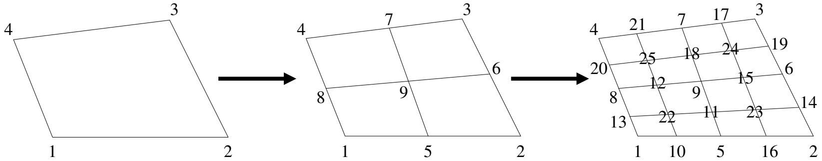

Two-level ordering strategy

- adopt all coordinates from coarser grid levels unchanged
- introduce new coordinates at edge/face/cell midpoints

Coarse grid description

- File format is described in the FEAT2D/FEAT3D manuals
- Supported element types: triangles, quads (2D) and hexahedra (3D)

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- Domain triangulation is specified in `TRI` file (2D/3D)
  - coordinate values of vertices in the interior
  - parameter values of vertices at the boundary
  - elements in terms of their corner nodes
  - first two lines are treated as header/comments!

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- Supported element types: triangles, quads (2D) and hexahedra (3D)
- Domain triangulation is specified in `TRI` file (2D/3D)
  - coordinate values of vertices in the interior
  - parameter values of vertices at the boundary
  - elements in terms of their corner nodes
  - first two lines are treated as header/comments!
- Boundary parametrization is specified in `PRM` file (only 2D)
  - each boundary component is described by $p \in [0, p_{\max}]$
  - the 'interior' is located left to the boundary
    $\rightarrow$ do not mix up (counter-)clockwise orientation
  - supported boundary types: lines, (arcs of) circles

DeViSoR Grid3D

Coarse grid generator for FEATFLOW and FEAST

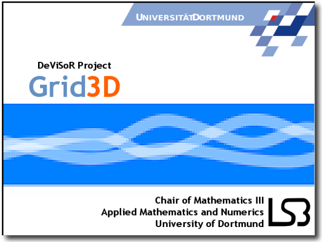
- written in Java + OpenGL and published under the GPL
- available at http://www.feast.uni-dortmund.de
- send requests, bug reports to devisor@featflow.de
- on-line help system and self-contained tutorial included

- Unpack the downloaded archive file

```
$ unzip grid-3.0.21.zip
```

- Start the application

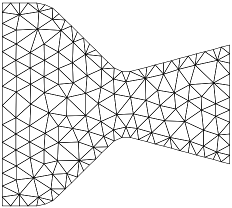
```
$ cd grid-3.0.21
$ java -jar grid3d.jar
```

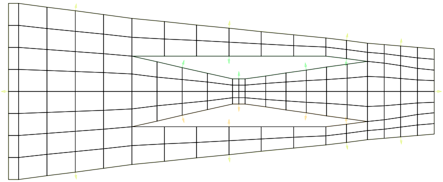


Alternative grid generators

- GiD – the personal pre- and post-processor
  - evaluation version is available at http://gid.cimne.upc.es
  - fully automatic structured and unstructured coarse grid generator
  - supports triangular, quadrilateral, tetrahedral, hexahedral elements
  - provides an effective easy-to-use and geometric user interface

- GiD2Feat – set of tools to convert GiD meshes to PRM/TRI files





Example application: *Poisson equation*

Possion equation

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- Change into the application source directory

```
$ cd applications/poisson/src; ls
```

```
poissonXd_callback.f90  poisson.f90
poissonXd_methodYYY.f90
```

- Open the application main source file

```
$ emacs poisson.f90
```

Possion equation

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  ```
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  ```
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  poissonXd_callback.f90  poisson.f90
  poissonXd_methodYYY.f90
  ```

- Open the application main source file
  ```
  $ emacs poisson.f90
  ```

Initialization and finalization

- `system_init()` initialize system-wide settings
- `storage_init(999, 100)` initialize storage management
- `storage_done()` finalize storage management

Possion equation, cont'd.

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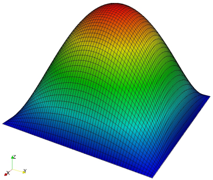
Sample problem: $-\Delta u = f$ in $\Omega = (0,1)^2$, $u = 0$ on $\partial\Omega$

- right hand side $f(x,y) = 32(x(1-x) + y(1-y))$
- analytical solution $u(x,y) = 16x(1-x)y(1-y)$

- Open the demonstration module file
  `$ emacs poisson2d_method0_simple.f90`
  - contains the corresponding subroutine
  - includes all required kernel modules
  - provides detailed step-by-step tutorial
- Open the callback function module file
  `$ emacs poisson2d_callback.f90`



Possion equation, cont'd.

Grid generation

- `boundary_read_prm` read boundary parametrization
- `tria_readTriFile2D` read domain triangulation
- `tria_quickRefine2LevelOrdering` perform regular refinement
- `tria_initStandardMeshFromRaw` generate data structures

Spatial discretization

- `spdiscr_initBlockDiscr2D` prepare block discretization
- `spdiscr_initDiscr_simple` initialize spatial discretization
- `bilf_createMatrixStructure` create scalar matrix structure
- `bilf_buildMatrixScalar` discretize the bilinear form
- `linf_buildVectorScalar` discretize the linear form/r.h.s.

Possion equation, cont'd.

Dirichlet boundary conditions

- `boundary_createRegion` specify boundary segment
- `bcasm_newDirichletBConRealBD` calculate discrete b.c.'s
- `matfil_discreteBC` set b.c.'s in system matrix
- `vecfil_discreteBCrhs` set b.c.'s in right hand side
- `vecfil_discreteBCsol` set b.c.'s in solution vector

Linear BiCGStab solver

- `linsol_initBiCGStab` initialize linear solver
- `linsol_setMatrices` attach system matrix
- `linsol_initStructure`, `linsol_initData`
- `linsol_solveAdaptively` solve linear system

Possion equation, cont'd.

Solution output

- `ucd_startGMV` start export on GMV format
- `ucd_addVariableVertexBased` add vertex-based solution data
- `ucd_addVariableElementBased` add cell-based solution data
- `ucd_write` write solution data to file

Clean-up and finalization

- `XXX_release`, `XXX_releaseYYY` free allocated memory
- `XXX_done` stop sub-system

General naming convention of subroutines

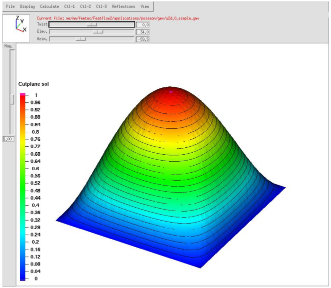
- `abbreviatedModulefile_NameOfSubroutine`

Postprocessing: *Visualization of the solution*

3D scientific visualization tool

- developed at Los Alamos National Lab by Frank Ortega
- available at http://www-xdiv.lanl.gov/XCM/gmv/
- supported OS: UNIX/Linux, Mac OS X, Windows (Cygwin)

- unstructured meshes in 2D/3D
- cutlines, cutplanes, cutspheres
- vertex-based, cell-based data sets
- contour, vector plots



Alternative: importer for ParaView based on development CVS-version

Advanced topics: *Multigrid, Mesh Adaptation, ...*

Possion equation, revisited

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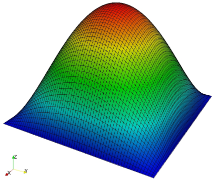
- Open the demonstration module file
  $ emacs poisson2d_method1_mg.f90
  - linear geometric multigrid solver
  - Jacobi or ILU(0) smoother
  - direct coarse grid solver (UMFPACK)



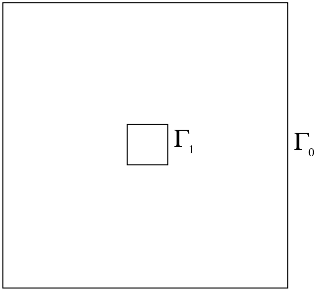
Anisotropic diffusion

Example: `applications/anisotropicdiffusion.f90`

$$\mathcal{D} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$\begin{cases} -\nabla \cdot (\mathcal{D}\nabla u) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_0 \\ u = 2 & \text{on } \Gamma_1 \end{cases}$$

- $k_1 = 100, \quad k_2 = 1, \quad \theta = -\frac{\pi}{6}$
- linear finite elements, $h = 1/36$
- Galerkin fails: $u^{\min} = -0.0553$
- h-adaptation: $u^{\min} = -0.0068$



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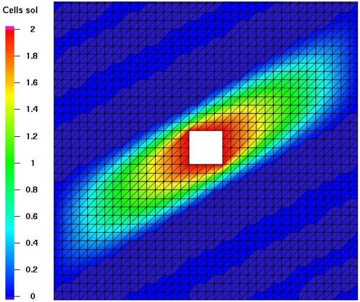

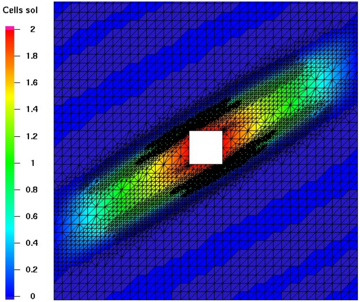

Mesh adaptation

- conformal mesh refinement based on red-green strategy
- vertex-locking algorithm for mesh re-coarsening procedure
- nodal generation function stores birth certificates
  - provides complete characterization of elements
  - youngest node corresponds to refinement level
  - is required for the vertex-locking algorithm
- state function for element characterization
- local two-level ordering strategy

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This has been addressed in the talk on Monday

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Mesh genealogy, revisited

Triangulation $\mathcal{T}_m(\mathcal{E}_m, \mathcal{V}_m)$, $m = 0, 1, 2, \ldots$ consists of

$$\mathcal{E}_m = \{\Omega_k \,:\, k = 1, \ldots, N_{\mathrm{E}}\} \quad \text{and} \quad \mathcal{V}_m = \{\mathrm{v}_i \,:\, i = 1, \ldots, N_{\mathrm{V}}\}$$

- nodal **generation function** $g : \mathcal{V}_m \rightarrow \mathbb{N}_0$ is defined recursively

$$g(\mathrm{v}_i) := \begin{cases} 0 & \text{if} \quad \mathrm{v}_i \in \mathcal{V}_0 \\ \max\limits_{\mathrm{v}_j \in \Gamma_{kl}} g(\mathrm{v}_j) + 1 & \text{if} \quad \mathrm{v}_i \in \Gamma_{kl} := \bar{\Omega}_k \cap \bar{\Omega}_l \\ \max\limits_{\mathrm{v}_j \in \partial\Omega_k} g(\mathrm{v}_j) + 1 & \text{if} \quad \mathrm{v}_i \in \Omega_k \setminus \partial\Omega_k \end{cases}$$

Characterization of elements

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Idea I: State function $s : \mathcal{E}_m \to \mathbb{Z}$ (in MSB representation)

- Set `Bit[0]` to 1 for quadrilateral, otherwise set it to zero
- Set `Bit[k=1..4]` to 1 if both endpoints of edge k have same age
- If no two endpoints have same age, then find local position k of the youngest vertex, set `Bit[k]` to 1 and negate the state

Idea II: Define local ordering strategy within each element *a priori*

element characterization	element state
triangle/quadrilateral from $\mathcal{T}_0$	0/1
green quadrilateral	3, 5, 9, 11,17, 21
red quadrilateral	7, 13, 19, 25
inner red triangle	14
'other' triangle	2, 4, 8
green triangle	-8, -4, -2

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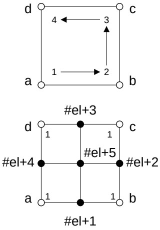

Storage management

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Concept of dynamically allocatable arrays in Fortran 9x

- `integer, dimension(:), allocatable :: Iarray`
- `allocate(Iarray(n))` allocate array of size `n` dynamically
- `deallocate(Iarray)` deallocate dynamically allocated array

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Concept of dynamically allocatable arrays in FeatFlow

- `storage_init`, `storage_done` — initialize/finalize storage
- `storage_new` — allocate new memory storage
- `storage_realloc` — re-allocate memory storage
- `storage_free` — deallocate memory storage
- `storage_getbase_XXX` — access memory storage

Storage management, cont'd.

- Supported data: 8/16/32/64 integer, SP/DP real, logical, strings
- Memory storage is accessible via integer handle `ihandle`
- Pointer to the memory is assigned via `storage_getbase_XXX`

Implementation details

- memory storage handling is internally mapped to de/allocate
- different storage management can be implemented without changes
- handles can be easily passed to subroutines and functions
- derived types typically consist of a set of handles + scalar data

Storage management, cont'd.

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Impl

ges

Derived type for triangulation structure

```
type t_triangulation
   integer :: ndim = 0
   integer :: NVT = 0
   integer :: NMT = 0
   integer :: NAT = 0
   integer :: NEL = 0
   . . .
   integer :: h_DvertexCoords = ST_NOHANDLE
   integer :: h_IverticesAtElement = ST_NOHANDLE
   integer :: h_IneighboursAtElement = ST_NOHANDLE
end type
```

Example: *Using handles*

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Create new storage

- `storage_new (scall, sname, Isize, ctype, ihandle, &`
  `cinitNewBlock, <rheap>)`
- `ctype` ∈ {`ST_DOUBLE`,`ST_SINGLE`,`ST_INTx`,`ST_CHAR`,`ST_LOGICAL`}
- `cinitNewBlock` ∈ {`ST_NEWBLOCK_ZERO`,`ST_NEWBLOCK_NOINIT`}

Accessing storage, e.g. 2-dimensional double array

- `real(DP), dimension(:,:), pointer :: p_Darray`
- `storage_getbase_double2D (ihandle, p_Darray, <rheap>)`

Releasing storage

- `storage_free (ihandle)`

UnConventional High Performance Computing

Finite **E**lement **A**nalysis & **S**olution **T**ools

High performance finite element package for the efficient simulation of large scale problems on heterogeneous hardware

- written in Fortran 90 and C (MPI communication)
- CFD (Stokes, Navier-Stokes), CSM (Elasticity)
- macro-wise domain decomposition approach
- fast and robust parallel multigrid methods
- unconventional hardware as FEM co-processors

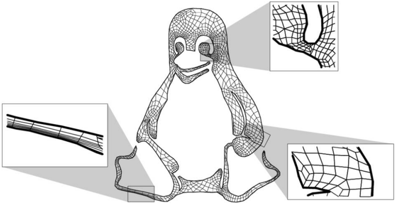
Visit the Feast homepage

http://www.feast.uni-dortmund.de

Scalable **R**ecursive **C**lustering (ScaRC) solver

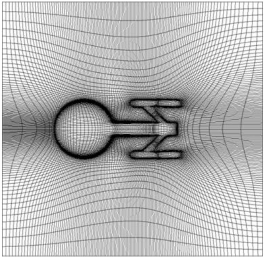
Combine domain decomposition and cascaded multigrid methods

Globally unstructured



hide anisotropies to improve robustness

Locally structured



UnConventional HPC

- Graphic processing unit (GPU)
  128 parallel scalar processors
  @ 1.35 GHz, $\approx$ 350 GFLOP/s
  GDDR3 memory @ 900 MHz

- Cell multi-core processor (PS3)
  7 synergistic processing units
  @ 3.2 GHz, 218 GFLOPS/s
  Memory @ 3.2 GHz

Future vision

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Unified FEAT+FEAST finite element package

- Decompose the domain into **globally** unstructured macro-cells
- Use generalized tensor product grid or unstructured mesh **locally**
- Reuse FEM co-processors in the FEATFLOW package
- Enable special features, (e.g. h-adaptation) per macro-cell

On-line resources and additional material

- FeatFlow project: `http://www.featflow.de`
- Feast project: `http://www.feast.uni-dortmund.de`