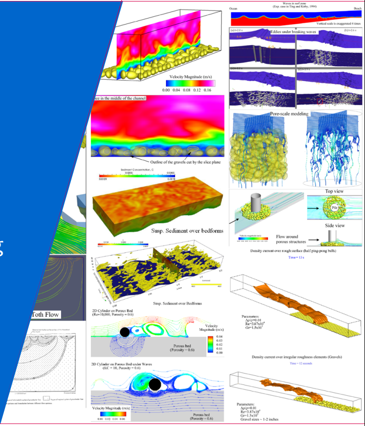
CE597D Special Topics, Fall, 2014

Chapter 1: Introduction

Xiaofeng Liu, Ph.D., P.E.
Assistant Professor
Department of Civil and Environmental Engineering
Pennsylvania State University
xliu@engr.psu.edu



Outline

All models are wrong, but some models are useful –George P. E. Box

All models are wrong, but some models are useful –George P. E. Box
The purpose of computing is insight not numbers. – C. Hastings, 1955

Aims and scope of this course

Aims

- Introduce the basics of computational hydraulics and CFD in general
  - Know what is running behind the scene
  - Theories about numerical methods and schemes
  - How to use computational tools to simulate the flow field you are interested in
  - Pre- and post-processing
  - How to interpret the simulation results
  - How to write computational code according to your own need
- Some exposure to independent research using computational tools
- Embedded in the term project
  - How to find the problem
  - Literature review: Critiques and new ideas
  - Research plan: scope, implementation, and schedule
  - Technical report writing and result presentation

Scope of this course

- This course is an advanced computational course

Scope of this course

- This course is an advanced computational course
- Assume you have already had some idea of
  - Fluid mechanics: governing equations (how they are derived and what physical laws they represent)
  - Numerical method:
    - general idea of how to descretize an equation: FDM, FEM, FVM
    - Implicit and explicit schemes
    - Order and accuracy of numerical schemes: 1st, 2nd order, etc.
    - Convergence
    - Stability of numerical schemes: stable and unstable, absolutely/conditional stable, etc.; region of stability

Introductions

What is Computational Fluid Dynamics?

- Fluid dynamics (a.k.a, hydraulics) usually studied using three different approaches
  - Experimental and field measurement
  - Analytical
  - Computational

What is Computational Fluid Dynamics?

- We use computational hydraulics interchangeably with CFD (computational fluid dynamics) in this course

What is Computational Fluid Dynamics?

- We use computational hydraulics interchangeably with CFD (computational fluid dynamics) in this course
- But we are more focused on the applications of CFD in environmental problems, hydraulics, as well as related areas such as hydrology, water resources, mechanical engineering

What is Computational Fluid Dynamics?

- We use computational hydraulics interchangeably with CFD (computational fluid dynamics) in this course
- But we are more focused on the applications of CFD in environmental problems, hydraulics, as well as related areas such as hydrology, water resources, mechanical engineering
- CFD is the analysis of systems involving fluid flow, heat and mass transfer, and associated phenomena such as chemical reactions by means of computer-based simulation.

What is Computational Fluid Dynamics?

- We use computational hydraulics interchangeably with CFD (computational fluid dynamics) in this course
- But we are more focused on the applications of CFD in environmental problems, hydraulics, as well as related areas such as hydrology, water resources, mechanical engineering
- CFD is the analysis of systems involving fluid flow, heat and mass transfer, and associated phenomena such as chemical reactions by means of computer-based simulation.
- Application areas
  - open channel flows in rivers
  - coastal flows
  - ocean flows
  - hydraulics in environmental processes
  - groundwater flows
  - turbomachinery
  - bio-fluids
  - micro-fluidics
  - ...

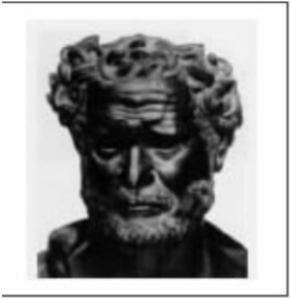
Brief history of CFD

A very brief history of computational fluid dynamics (CFD)

- Fluid (water, the most apparent example), has a long history in human civilization.
- People have notices the existence and uniqueness of fluid, comparing to solid, gas, and other forms of matters.
  - Flowing water in the river
  - Wind and weather change in the atmosphere
  - Ocean waves and currents
  - flow of blood
  - ...

Brief history of CFD

- Famous notes from the history books
  - Heraclitus (636-470 BC): “Everything Flows”
  - Archimedes (287-212 BC): fluid statics

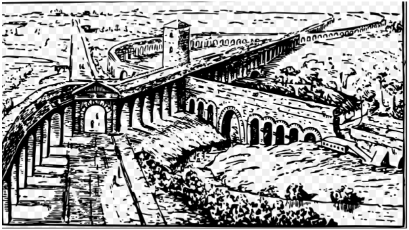


Heraclitus
536 - 470BC

Archimedes
287 - 212BC

Brief history of CFD

- Famous notes from the history books
  - Ancient Rome: starting from early 8th century BC, located along the Mediterranean see and centered in the city of Rome. Roman aqueducts, canals, harbors, and bathhouses.



Brief history of CFD

- Famous notes from the history books
  - Leonardo Da Vinci: Renaissance age; Describing fluid phenomenon covering water surfaces, waves, eddies, falling water, etc.
  - Issac Newton: 17th century: quantify and predict fluid flow through equations; Newton's second law; Newtonian fluid concept; etc.

Leonardo Da Vinci's sketches of objects and free surface effects in water

Sir Isaac Newton 1643 - 1727

Brief history of CFD

- Famous notes from the history books
  - Daniel Bernoulli (1700-1782): Bernoulli's equation
  - Leonhard Euler (1707-1783): Euler equation for inviscid fluid

Bernoulli

Euler

Brief history of CFD

- Famous notes from the history books
  - Claude Louis Marie Henry Navier (1785-1836, Frenchman) and George Gabriel Stokes (1819-1903, Irishman) : added viscous effect to the Euler equations, which resulting in the famous Navier-Stokes equations. These equations, proposed about 200 years ago, are the foundation of today's CFD field. NS equations are nonlinear, coupled PDEs. Very hard to solve.

Claude Navier

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=S_m$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j)= -\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\rho g_i+F_i$$

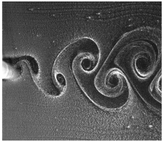
A simplified form of the Navier-Stokes equations

George Stokes

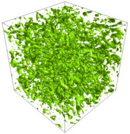
  - ...

Brief history of CFD

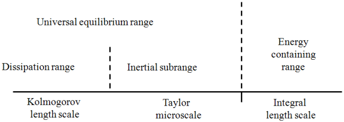
- Famous notes from the history books
  - Early 20th century:
    - Ludwig Prandtl (1875-1953): Boundary layer theories, mixing length concept, Prandtl number, etc.
    - Theodore von Karman (1881-1963): von Karman vortex street
    - Geoffrey Ingram Taylor (1886-1975): statistical theory of turbulence and the Taylor microscale
    - Andrey Nikolaevich Kolmogorov (1903-1987): the concept of Kolmogorov scales; the universal energy spectrum for turbulence
    - George Keith Batchelor (1920-2000): the theory of homogeneous turbulence



Vortex street behind a cylinder



Homogeneous turbulence



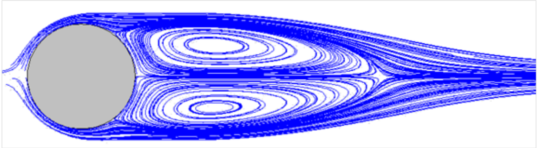
Turbulence length scales

Brief history of CFD

- Who did the first CFD? It is debatable (source: http://www.amwel.com/history.html).
  - Lewis Fry Richardson in England (1881-1953) developed the first numerical weather prediction system when he divided physical space into grid cells and used the finite difference approximations for weather prediction. It was not successful.
  - Richardson proposed a solution he called the "forecast-factory". The "factory" would have involved filling a vast stadium with 64,000 people. Each one, armed with a mechanical calculator, would perform part of the flow calculation. A leader in the center, using colored signal lights and telegraph communication, would coordinate the forecast.
  - It is probably the prototype of modern CFD though no electronic computer existed yet.

Brief history of CFD

- The first "modern sense" CFD is the flow past a cylinder simulation in 1933 by A. Thom. *A.Thom, The Flow Past Circular Cylinders at Low Speeds, Proc. Royal Society, A141, pp. 651-666, London, 1933*
- Kawaguti in Japan obtained a similar solution for flow around a cylinder in 1953 by using a mechanical desk calculator, working 20 hours per week for 18 months. *M. Kawaguti, Numerical Solution of the NS Equations for the Flow Around a Circular Cylinder at Reynolds Number 40, Journal of Phy. Soc. Japan, vol. 8, pp. 747-757, 1953.*



Brief history of CFD

- In the 1960s, NASA's contributions:
  - Particle-In-Cell (PIC) method
  - Marker-And-Cell (MAC) method (Harlow and Welch, 1965)
  - Vorticity-Stream function method
  - Arbitrary Lagrangian-Eulerian (ALE) method
  - Original k-ϵ turbulence model
  - ...
- In the 1970s, Imperial College, London (Spalding group):
  - SIMPLE algorithm for NS equations
  - k-ϵ turbulence model still used today (Spalding and Launder, 1972)
  - ...
- In the 1980s:
  - S. V. Patankar classic book: *"Numerical Heat Transfer and Fluid Flow"*
  - Commercial CFD codes came to market
  - ...

Brief history of CFD

To recap, a few milestones in the history of CFD (source: cfd-online):

- 1910 - Richardson, 50 page paper to Royal Society, hand calculations with human computers, 2000 operations per week...
- Around 1960 - Scientific American articles on CFD
- 1965 - Marker and Cell methods - Harlow and Welch
- 1965 - Use in research and "grand challenges" (NASA, Los Alamos...)
- 1970 - Finite difference methods for Navier-Stokes
- 1970 - Finite element methods for stress analysis
- 1980 - Finite volume methods
- 1985 - Use in "aero" industries (Boeing, General Electric, ...)
- 1995 - Use in "non-aero" industries
- 2004 - OpenFOAM released under GPL license (free and open-source)

Basic elements of a CFD package

Three basic elements of a CFD package

- Pre-processing
- Solver
- Post-processing

Basic elements of a CFD package

Three basic elements of a CFD package

- Pre-processing
- Solver
- Post-processing

A CFD package does not necessary have pre- or post-processing part. But the trend is that most commercial and open source CFD packages have certain level of these functionalities.

Basic elements of a CFD package

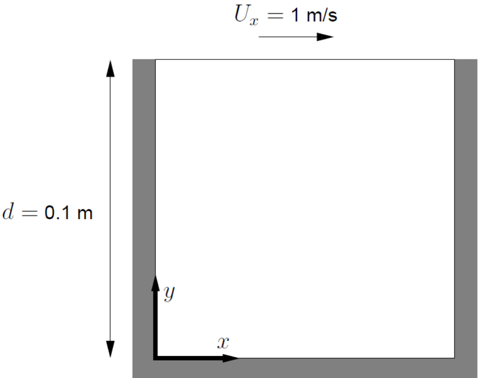
Typical cycle of a CFD Simulation

- Pre-Processing
  - Choice of mathematical model: what kind of fluid, what equations are of interest: compressible or incompressible, steady-state or transient, energy equation, turbulence, buoyancy effects, chemical reactions, etc.
  - Initial and boundary condition setup
- Flow Solution
  - Setting up solution and solver parameters: discretisation schemes, relaxation parameters, choice of models, linear equation solver etc
  - Running the solver
- Post-Processing and Data Analysis
  - Extracting global flow parameters, e.g., lift and drag, pressure drop
  - Flow visualisation: vectors, contours, iso-surfaces, streamlines or stream ribbons. Used to help understand the flow behaviour
  - Using simulation results in the design process
    - Geometry or flow condition variations; parametric studies or sensitivity analysis; error estimation and mesh refinement studies

Basic elements of a CFD package

Mesh generation and pre-processing softwares

- Activities in the pre-processing stage of CFD
  - Definition of the geometry of the region of interest: computational domain
  - Grid (mesh) generation: the sub-division of the domain into pieces.
  - Selection of the physical laws: compressible or incompressible; laminar or turbulent; ec.
  - Definition of fluid properties
  - Specification of boundary condition (B.C.) and initial condition (I.C.)



Basic elements of a CFD package

Mesh generation and pre-processing softwares

- Commercial packages:
    - Pointwise and Gridgen
    - GridPro
    - ANSA
    - ICEM
    - HyperMesh: http://www.altair.com/, more popular in structural engineering.
    - ...

Basic elements of a CFD package

Mesh generation and pre-processing softwares

- Open source and free-ware packages:
    - *blockMesh* and *snappyHexMesh* in OpenFOAM®
    - Gmsh: http://geuz.org/gmsh/, 3D FEM mesh generator with built-in pre- and post-processing facilities
    - Netgen: http://www.hpfem.jku.at/netgen/, an automatic 3D tetrahedral mesh generator. Input from constructive solid geometry (CSG) or boundary representation from STL file format.
    - Salome: http://www.salome-platform.org/, a generic platform for pre- and post-processing for numerical simulation. It has a module for mesh generation.
    - enGrid: http://engits.eu/en/engrid, native export to OpenFOAM®
    - CGNS: http://cgns.sourceforge.net. It is not a software, but a "Standard". CFD General Notation System (CGNS) provides a general, portable, and extensible standard for the storage and retrieval of computational fluid dynamics (CFD) analysis data. It consists of a collection of conventions, and free and open software implementing those conventions.
    - ...

Basic elements of a CFD package

Solvers: All solvers are different. But generally, they should have all or part of the following:

- Dimensionality of the computational domain: 2D planar, 2D axisymmetric, or 3D
- Unstructured mesh (triangle and quadrilateral elements for 2D; tetrahedral, hexahedral, prism and pyramid elements for 3D) or structured mesh
- Steady-state or transient flows or both
- Compressibility: incompressible or compressible
- Viscosity effect: Inviscid or viscid (laminar and turbulent flows)
- Selection of turbulence models: RANS (k-ϵ, k-ω), DES, and LES
- Rheology: Newtonian or non-Newtonian flows
- Free surface and multiphase models, including heat transfer and reactions
- Lagrangian tracking of dispersed phase such as particles

Basic elements of a CFD package

Solvers: All solvers are different. But generally, they should have all or part of the following:

- Porous media flow model
- Dynamic mesh capability for modelling flow around moving objects
- Inertial (stationary) or non-inertial (rotating or accelerating) reference frames
- Multiple reference frame (MRF) and sliding mesh options
- Volumetric sources of mass, momentum, heat, and chemical species
- Material property database
- Extensive customization capability via user-defined functions (UDF, a nomenclature used in Fluent)
- ...

Basic elements of a CFD package

Solvers:

- solve the governing equations using numerical methods, including finite volume method (FVM), finite difference method (FDM), finite element method (FEM), spectral method, etc.
- There are other methods to solve governing equations, such as particle method, meshless method. In hydrodynamics, popular examples are SPH (smoothed-particle hydrodynamics) and Lattice-Boltzmann method.
- In this course, we will only focus on the finite volume method (using OpenFOAM®).

Basic elements of a CFD package

- The essence of a fluid solver using FVM
  - Integration of the governing equations over each of the grid cells in the domain
  - Discretization-conversion of the resulting integral equations into a system of algebraic equations
  - Solution of the algebraic equations by an iterative method

$$\underbrace{\frac{\partial \rho\phi}{\partial t}}_{Transient\ \ term} + \underbrace{\nabla\cdot(\rho\vec{u}\phi)}_{Convection\ \ term} = \underbrace{\nabla\cdot(\Gamma\nabla\phi)}_{Diffusion\ \ term} + \underbrace{S_\phi}_{Source\ \ term} \tag{1}$$

Basic elements of a CFD package

Brief demonstration of OpenFOAM® package

Available CFD solvers

- Commercial CFD packages
  - Ansys CFX
  - Ansys Fluent
  - Ansys CFD-Flo
  - Phoenix
  - StarCD
  - Flow3D: good at free surface, very easy to use
  - NUMECA
  - ...

Available CFD solvers

- Commercial CFD packages
  - Ansys CFX
  - Ansys Fluent
  - Ansys CFD-Flo
  - Phoenix
  - StarCD
  - Flow3D: good at free surface, very easy to use
  - NUMECA
  - ...

- Open Source CFD packages
  - OpenFOAM
  - Gerris
  - CFL3D: NASA, only available to a "U.S. person" within the United States.
  - OVERFLOW: NASA
  - TetrUSS: NASA, (TETRahedral Unstructured Software System)
  - Delft3D: more specialized in hydraulics, coastal flow, etc.
  - Telemac: also specialized in hydraulis
  - ...

Available CFD solvers

So there are TOO many choices. What we should consider when making a choice?

http://www.whandassociates.com/too-many-choices-can-affect-the-client-experience-and-revenue/

Available CFD solvers

So there are TOO many choices. What we should consider when making a choice?

- Functionalities:
  - Any particular module that you want? Specialties of each package
  - Do you just need a off-the-shelf package or you want to do more secondary development
  - All-in-one or pieces?
  - Pre-processing, solver, postprocessing together?

Available CFD solvers

So there are TOO many choices. What we should consider when making a choice?

- Functionalities:
  - Any particular module that you want? Specialties of each package
  - Do you just need a off-the-shelf package or you want to do more secondary development
  - All-in-one or pieces?
  - Pre-processing, solver, postprocessing together?
- Popularity and public acceptance
  - Look around and see what other people are using in your field
  - It is easy to compare notes if you use the same (or similar) as others
  - How long the package has been around? Does it have a long and credible history?

Available CFD solvers

So there are TOO many choices. What we should consider when making a choice?

- Functionalities:
  - Any particular module that you want? Specialties of each package
  - Do you just need a off-the-shelf package or you want to do more secondary development
  - All-in-one or pieces?
  - Pre-processing, solver, postprocessing together?
- Popularity and public acceptance
  - Look around and see what other people are using in your field
  - It is easy to compare notes if you use the same (or similar) as others
  - How long the package has been around? Does it have a long and credible history?
- Availability of technical support
  - Much better for commercial packages since you forked out $$$
  - For open source packages, the price you pay for the freedom is less support. However, when the user base getting bigger, there are always active online community support.

Available CFD solvers

So there are TOO many choices. What we should consider when making a choice?

- Functionalities:
  - Any particular module that you want? Specialties of each package
  - Do you just need a off-the-shelf package or you want to do more secondary development
  - All-in-one or pieces?
  - Pre-processing, solver, postprocessing together?
- Popularity and public acceptance
  - Look around and see what other people are using in your field
  - It is easy to compare notes if you use the same (or similar) as others
  - How long the package has been around? Does it have a long and credible history?
- Availability of technical support
  - Much better for commercial packages since you forked out $$$
  - For open source packages, the price you pay for the freedom is less support. However, when the user base getting bigger, there are always active online community support.
- Availability of training

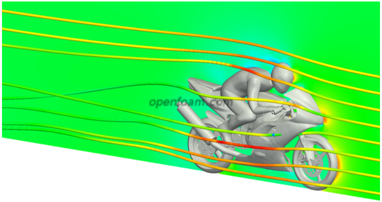
Available CFD solvers

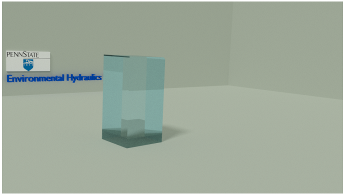
So there are TOO many choices. What we should consider when making a choice?

- Functionalities:
  - Any particular module that you want? Specialties of each package
  - Do you just need a off-the-shelf package or you want to do more secondary development
  - All-in-one or pieces?
  - Pre-processing, solver, postprocessing together?
- Popularity and public acceptance
  - Look around and see what other people are using in your field
  - It is easy to compare notes if you use the same (or similar) as others
  - How long the package has been around? Does it have a long and credible history?
- Availability of technical support
  - Much better for commercial packages since you forked out $$$
  - For open source packages, the price you pay for the freedom is less support. However, when the user base getting bigger, there are always active online community support.
- Availability of training
- Last but not least, your personal preference

Post-processing

- Activities in the post-processing stage of CFD
  - Model verification, validation, and sensitivity analysis
  - Display domain geometry and grid
  - Plot scalars, vectors, and tensors
  - Plot forms: line or shaded contour plot, 2D and 3D surface plot
  - Particle tracking (position of particles as a function of time)
  - Figure and animation output
  - ...





Post-processing

Model verification, validation, and sensitivity analysis

- Validation: Are we solving the correct equations?
- Verification: Are we solving the equations correctly?

Model sensitivity and uncertainty

- Sensitivity: parameter
- Uncertainty: propagation of uncertainties, quantifications, etc.

Post-processing

Post-processing and visualization softwares

- Commercial packages:
  - Tecplot:
  - EnSight
  - FieldView
  - Avizo: http://www.vsg3d.com/avizo, package with different editions, such as material science and industrial inspection, geoscience and oil & gas, environment and climate, ...
  - ...

Post-processing

Post-processing and visualization softwares

- Commercial packages:
  - Tecplot:
  - EnSight
  - FieldView
  - Avizo: http://www.vsg3d.com/avizo, package with different editions, such as material science and industrial inspection, geoscience and oil & gas, environment and climate, ...
  - ...
- Open source and free-ware packages:
  - ParaView: http://www.paraview.org/, is an open-source, multi-platform data analysis and visualization application. Developed for extremely large dataset using distributed memory computers.
  - VisIt: https://wci.llnl.gov/codes/visit/
  - OpenDX: http://www.opendx.org/, open source software project based on IBM's visualization data explorer. Not actively developed and used.
  - ...

Post-processing

Comparing to experimental and analytical methods, what are the advantages of CFD?

- Low cost
  - Laboratory experiments and field campaigns are expensive and time consuming. Lab experiment is not flexible to change.
  - Analytical solutions are not easy, if not totally impossible. A lot of simplifications and assumptions to make analytical solutions possible.
  - CFD simulations are relatively inexpensive, easy to change configurations and conditions, fast to see the results.
- Some conditions can not (or very dangerous) be replicated in the lab. CFD can simulate these conditions *virtually*.
- CFD can produce detailed information, whilst experiments can only provide very limited data, such as point measurement of velocity using ADV and LDV.

Post-processing

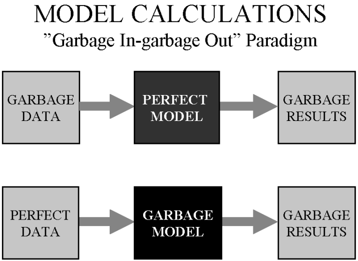
Comparing to experimental and analytical methods, what are the disadvantages (limitations) of CFD?

- Limited by the mathematical abstraction of real world physical processes. Examples are:
  - Turbulence: How valid is your turbulence model?
  - Computational domain might not represent the real space the fluid flows through. Example, rivers, coastal, blood veins, etc.
  - Compressibility: All fluids are compressible to some extend. Incompressibility is only a simplification.
  -
- Limited by the discrete and numerical nature of the solution.
  - Solutions are given in discrete locations at discrete time instances.
  - Subject to numerical errors: round-off errors due to the way numbers are represented in digital computers and truncation errors due the approximations in the numerical discretization. Round-off errors are inevitable. Truncation errors depends on the order of the numerical scheme and are functions of the grid size. They diminish when the grid is refined. So CFD usually requires grid independence study.

Post-processing

Comparing to experimental and analytical methods, what are the disadvantages (limitations) of CFD?

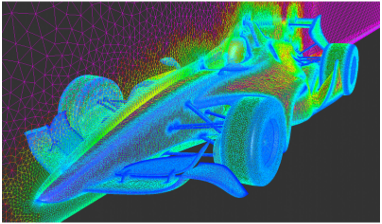
- Limited by boundary conditions and initial conditions
  - The accuracy of the CFD solutions is only as good as the B.C. and I.C. provided to the solver. Remember "*Garbage in, Garbage out*".
  - Ideally, you want model the whole world. But you can only model a domain of limited size. You have to cutoff at some point. Where you cut it off might affect your solution.
  - For nonlinear problems, different I.C. could evolve the system status to different solutions.



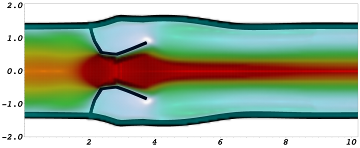
http://101proofsforgod.blogspot.com/2014/02/52-garbage-in-garbage-out-gigo.html

Current challenges in the field of CFD

- Mesh generation. Labor intensive. Needs experiences. The new direction is automatic and parallel mesh generation.
- HPC with massively parallel simulations
- Integration into the CAD-based design process
- Multiphysics, multiscales, multicomponents, multidomain: Example, turbulence, fluid-structure interaction (FSI)
- ...



http://blog.pointwise.com/2012/03/23/this-week-in-cfd-44/



http://numerik.iwr.uni-heidelberg.de/Research/research.html

Student feedback

- Discussion items
  - What is your goal of taking this course?
  - What are the specific problems you want to solve for your work and research?
  - What items you are specifically interested?

Questions?