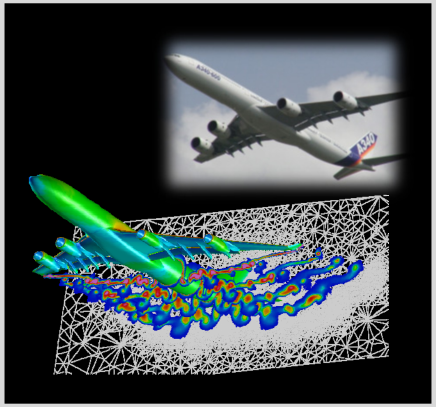


High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

Prof. Dr. – Ing. Morris Riedel
Adjunct Associated Professor
School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Iceland
Research Group Leader, Juelich Supercomputing Centre, Forschungszentrum Juelich, Germany

SHORT LECTURE 15

@Morris Riedel @MorrisRiedel @MorrisRiedel

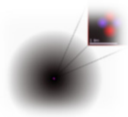
Computational Fluid Dynamics & Finite Elements

November 25, 2019
Room V02-156

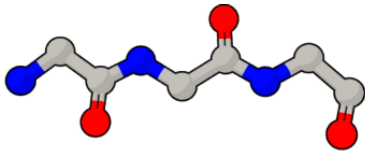
UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE
DEEP Projects
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES
HAICU HELMHOLTZ ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Review of Short Lecture 14 – Molecular Systems & Libraries

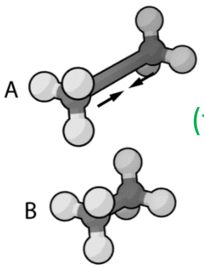
(atoms consists of 'electron cloud' & nucleus of protons and neutrons)



(molecules are a group of two or more atoms held together by chemical bonds)

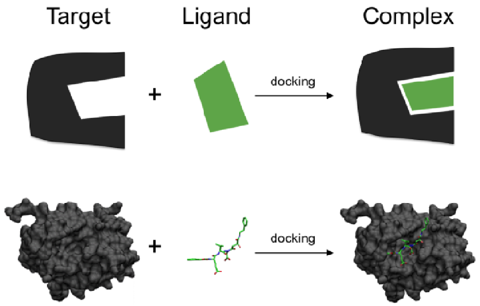


(example: molecular model of a protein)



(force field)

(example: drug design with molecular docking + dynamics)



(once docked a simulation of time is useful to apply)

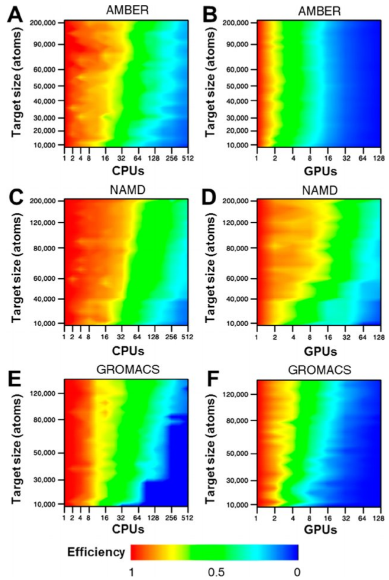
Give atoms initial positions $\boldsymbol{r}^{(t=0)}$, choose short Δt

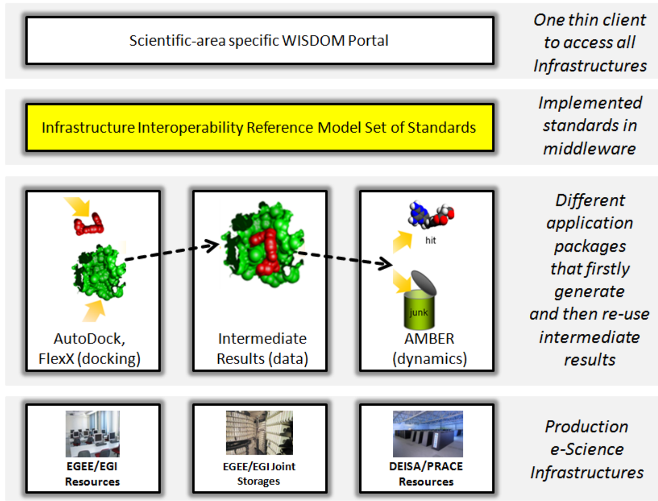
Get forces $\boldsymbol{F} = - \nabla V(\boldsymbol{r}^{(i)})$ and $\boldsymbol{a} = \boldsymbol{F}/m$

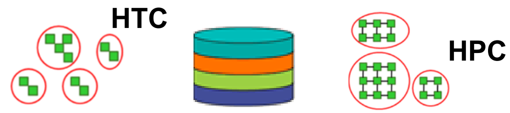
Move atoms: $\boldsymbol{r}^{(i+1)} = \boldsymbol{r}^{(i)} + \boldsymbol{v}^{(i)} \Delta t + {}^{1}/_{2}\, \boldsymbol{a}\, \Delta t^2 + \ldots$

Move time forward: $t = t + \Delta t$

Repeat as long as you need







[7] M. Riedel et al., 'Research Advances by using interoperable e-Science Infrastructures', 2009

modified from [5] Wikipedia on 'Molecular Dynamics'

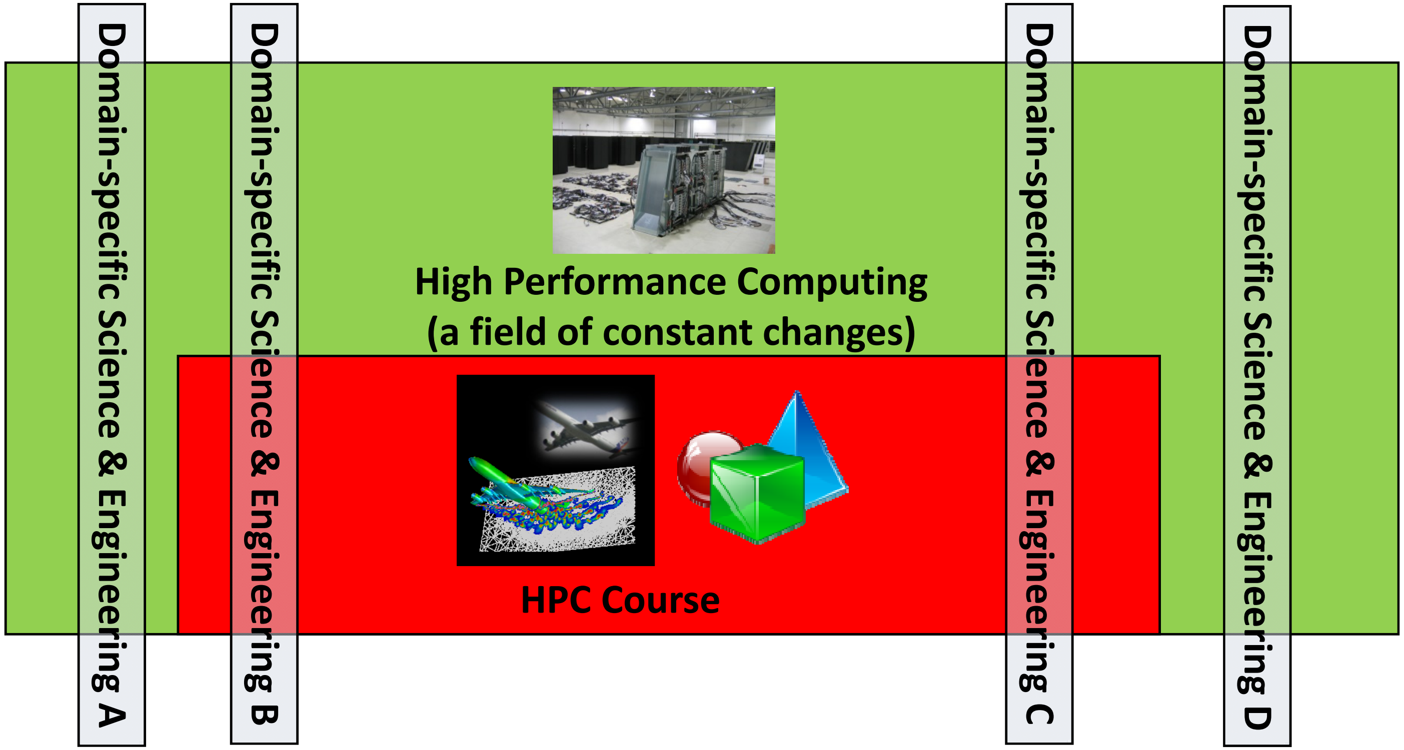
[6] Hu Ge et al.

modified from [4] Wikipedia on 'Molecular Docking'

[3] Wikipedia on 'Molecular Mechanics' *[2] Wikipedia on 'Atoms'* *[1] Wikipedia on 'Molecule'*

HPC-A[dvanced] Scientific Computing (cf. Prologue) – Second Part

- Consists of techniques for programming & using large-scale HPC Systems
  - Approach: Get a broad understanding what HPC is and what can be done
  - Goal: Train general HPC techniques and systems and selected details of domain-specific applications



Outline of the Course

1. High Performance Computing
2. Parallel Programming with MPI
3. Parallelization Fundamentals
4. Advanced MPI Techniques
5. Parallel Algorithms & Data Structures
6. Parallel Programming with OpenMP
7. Graphical Processing Units (GPUs)
8. Parallel & Scalable Machine & Deep Learning
9. Debugging & Profiling & Performance Toolsets
10. Hybrid Programming & Patterns
11. Scientific Visualization & Scalable Infrastructures
12. Terrestrial Systems & Climate
13. Systems Biology & Bioinformatics
14. Molecular Systems & Libraries
15. Computational Fluid Dynamics & Finite Elements
16. Epilogue

+ additional practical lectures & Webinars for our hands-on assignments in context

- Practical Topics
- Theoretical / Conceptual Topics

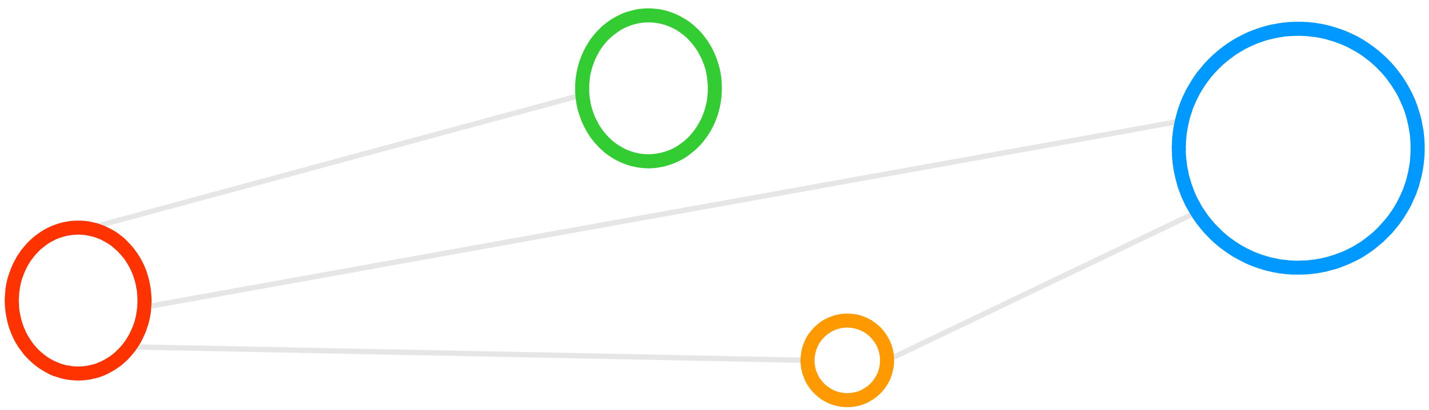
Outline

- Computational Fluid Dynamics (CFD)
  - Terminology & Motivation for CFD Applications
  - Naviar-Stokes & Lattice-Boltzmann Method
  - Large Eddy Turbulence Model
  - Modelling Methodology & Application Examples
  - Library Examples with OpenFOAM & iFluids
- Finite Elements Methods (FEM)
  - Terminology & Motivation for FEM Applications
  - Boundary Value Problems & Mesh Generation Techniques
  - Adaptive Mesh Refinement & Fire Dynamics Applications
  - Library Examples with OpenFOAM & Code_Aster & Ansys Suite
  - Library Elmer Dynamic Ice Simulation Application Example

- **Promises from previous lecture(s):**
- ***Lecture 2:*** **Lecture 12 – 15 will offer more insights into a wide variety of physics & engineering applications that take advantage of HPC with MPI**
- ***Lecture 3:*** **Lecture 15 will offer more details on HPC applications that perform computational fluid dynamics (CFD) on domain decompositions**
- ***Lecture 14:*** **Lecture 15 will give further details on computational fluid dynamics (CFD) techniques & codes including Finite Elements Method (FEM)**

- **Note that this lecture is only a short lecture that usually needs a full course**
- **The goal is to understand selected HPC application fields & provide a few pointers to other advanced related university courses/topics/tutorials**

Computational Fluid Dynamics (CFD)

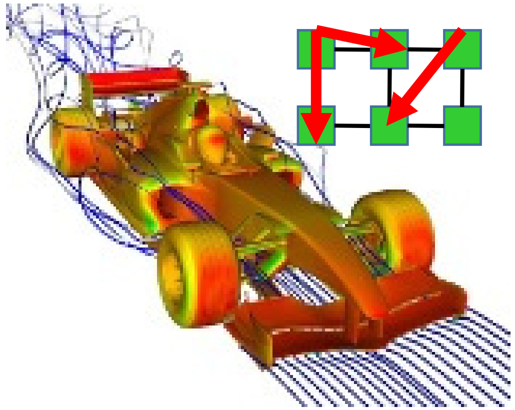


Computational Fluid Dynamics (CFD) – Terminology & Motivation

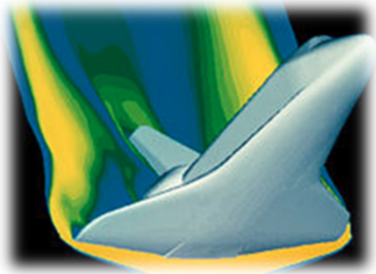
- ‘Fluid Dynamics‘ as branch of ‘Fluid Mechanics‘
  - Alternative to Experimental fluid dynamics & Theoretical Fluid Dynamics
  - Computational Fluid Dynamics (CFD) use numerical methods (cf. Lecture 12)
  - Interaction of fluids with surfaces defined by certain boundary conditions & equations
- Usage
  - Detailed product development (e.g. cars, aircraft)
  - Conceptual studies of new designs
  - Troubleshooting & Redesign
- Various Approaches
  - E.g. Naviar-Stokes equations, Lattice-Boltzmann method, Large-Eddy, etc.

> - **Fluid dynamics stands for the science of fluid motion in order to understand liquids, gases, etc.**
> - **Computational Fluid Dynamics (CFD) use numerical methods to analyze fluid flows**

[8] Wikipedia on CFD



Modified from [9] Caterham F1 team



Computational Fluid Dynamics – Methods Overview – Revisited (cf. Lecture 14)

Real Fluid
Free molecules in continous space

Continuum Kinetic Theory
Microscopic particles (Boltzmann Equation)

Conventional CFD Methods

Construction of fluid equations
Navier-Stokes equations (PDE)

Discrete approximation of PDE
Finite difference, finite element, etc

Numerical integration
Solve the equations on a given mesh and apply PDE boundary conditions

Lattice Based Method

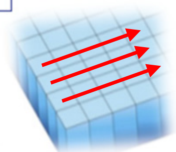
Discrete formulation of kinetic theory
Lattice Boltzmann equations

No further approximation
The equations are already in discrete form

Numerical integration
Solve on lattices and apply kinetic based BC

Simple conversion to fluid variables
These are theoretically shown to obey the required fluid equations

Results
Fluid dynamic quantities at discrete points in space and time



[10] S. Orszag et al.

CFD – Navier-Stokes Method

- Origin of unique name
  - Named after Claude-Louis Navier and George Gabriel Stokes
- Solving equations
  - Solution is a velocity (not a position)
  - Result is a 'velocity/flow field'
  - Description of the velocity of the fluid at a given point in space and time
- Modeling CFD examples
  - Ocean currents (cf. assignments)
  - Water flow in a pipe
  - Air flow around a wing

- **Navier-Stokes equations are used in CFD simulations to describe the motion of fluid substances**
- **Equations describe the physics of a wide variety of elements in scientific and engineering domains**

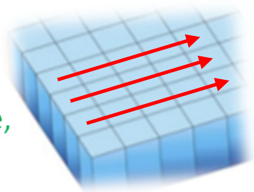
modified from [11] Wikipedia on Navier-Stokes

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \nabla\cdot\mathbf{T} + \mathbf{f}$$

(equations are nonlinear partial differential equations - PDEs, cf. Lecture 12)

$\mathbf{v}$ is the flow velocity,
ρ is the fluid density,
p is the pressure,
$\mathbf{T}$ is the (deviatoric) component of the total stress tensor, which has order two,
$\mathbf{f}$ represents body forces (per unit volume) acting on the fluid,
∇ is the del operator.

(classical mechanics solutions are rather trajectories of positions of a certain particle, here fluid velocity is in focus)



CFD – Lattice Boltzmann Method

- Alternative to Navier-Stokes
  - Different set of equations
- Modeling approach
  - Fluid consisting of particles
  - Particles have a finite number of discrete velocity values
  - Particles perform consecutive propagation and collision processes
  - Performed over discrete lattice mesh
- Modeling complex CFD examples
  - Airflow around a vehicle
  - Blood flow in a brain

(traditional CFD methods solve the conversation equations of macroscopic properties like mass, momentum, and energy)

$$f_i^*(\vec{x}, t+\delta_t) = f_i(\vec{x}, t) + \frac{1}{\tau_f}(f_i^{eq} - f_i)$$

(Collision step)

$$f_i(\vec{x} + \vec{e}_i\delta_t, t+\delta_t) = f_i^*(\vec{x}, t+\delta_t)$$

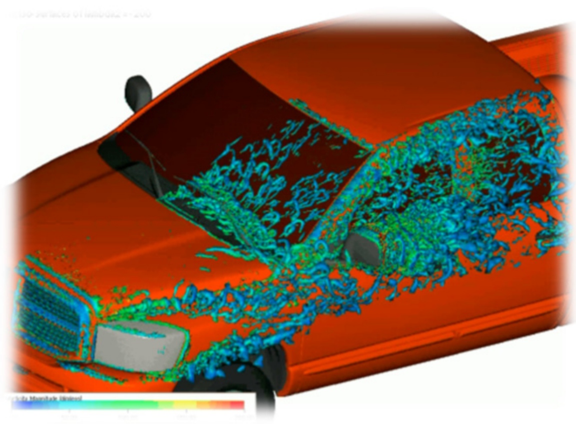
(Streaming step)

- **The Lattice Boltzmann Method (LBM) is used in CFD simulations to perform fluid simulations**
- **Discrete Boltzmann equations are solved to simulate the flow of fluids including collision models**

modified from [12] Wikipedia on LBM

(Research accoustic impact of headlights)

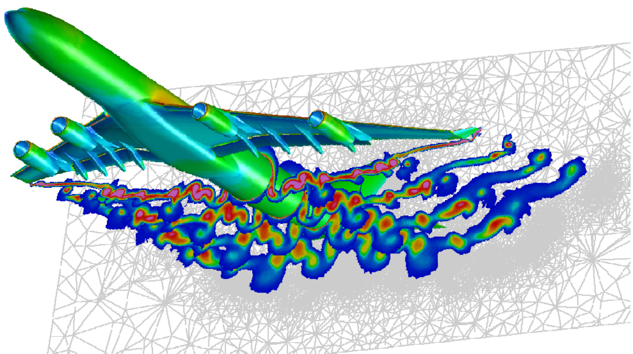
[10] S. Orszag et al.



CFD – Large Eddy Simulations (LES) for Turbulence

- Simulating ‘Turbulence‘
  - Flow characterized by ‘chaotic property changes‘ (chaotic from chaos theory)
  - Low momentum diffusion
  - High momentum convection
  - Rapid variation of pressure and velocity (in space and time)
- LES enables complex simulations
  - Solution is a filtered velocity field (filtered Naviar-Stokes equations)
  - Small length and time scales enable computational simulation

[14] Wikipedia on Turbulence

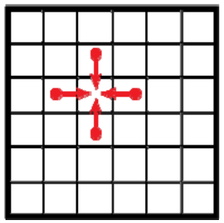


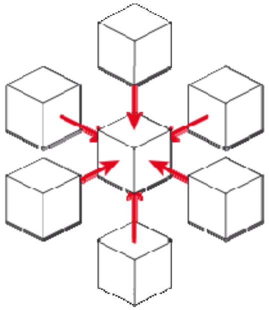
- **Large Eddy Simulation (LES) is a mathematical model for turbulence used in CFD simulations**
- **LES operates on the Navier-Stokes equations to reduce the range of length scales of the solution**

modified from [13] Wikipedia on LES

Stencil-based Iterative Methods – Revisited (cf. Lecture 10)

- Simulation sciences & numerical methods
  - Stencil-based iterative methods
  - Applicable with exceptions with other methods: Finite element method (selected codes on regular grids can use stencil codes)
- Selected application examples
  - Computational Fluid Dynamics (CFD) codes
  - Partial differential equations (PDE) solver
  - Jacobi method
  - Gauss-Seidel method
  - Image processing





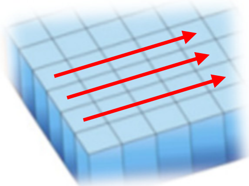
- **Stencil-based iterative methods update array elements according to a fixed pattern called 'stencil'**
- **The key of stencil methods is its regular structure mostly implemented using arrays in codes**
- **Method is often used in computational science as part of scientific and angineering applications**

[15] Wikipedia on 'stencil code'

CFD – Modeling Methodology

- Solve practical fluid flow problems
  - Modeling & simulating reality but with specific scientific detailed elements

[8] Wikipedia on CFD



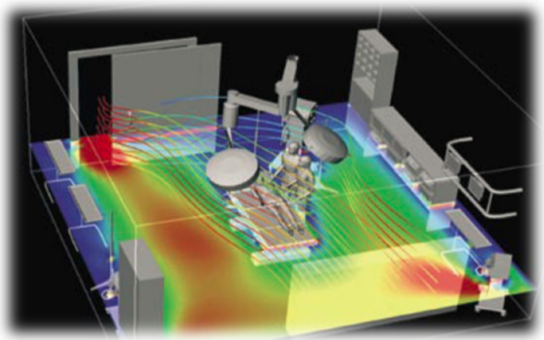
- Practical Preprocessing Steps
  1. Geometry (physical bounds) of the problem space is defined
  2. Volume occupied by the fluid is divided into discrete cells (aka ‘mesh‘)
  3. Physical modeling is defined (e.g. equations of motion)
  4. Boundary conditions (e.g. specify fluid behaviour & boundary properties)
- Computational simulation
  - Equations are solved iteratively via time-steps over space →

- Postprocessing Steps
  - Further simulation output data analysis and/or visualization

Selected Libraries & Methods – OpenFOAM & iFluids

- OpenFOAM Selected Facts
  - Free and open source software & maintained by OpenFOAM foundation
  - Use of object oriented programming (e.g. C++ classes, etc.)
- OpenFOAM Parallelization
  - Several methods for Domain decomposition (cf. Lecture 3)
  - Distributed memory with MPI(cf. Lecture 2)
- OpenFOAM Examples
  - Dispersion of stack exhaust above a pitched roof (e.g. environmental consulting)
- Library Example iFluids
  - Example for computational steering

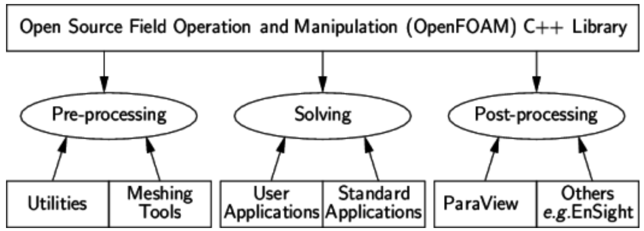
> - **iFluids is a parallel software for CFD simulations in general & for indoor air flow simulations in particular being also augmented with computational steering capabilities & online visualizations**



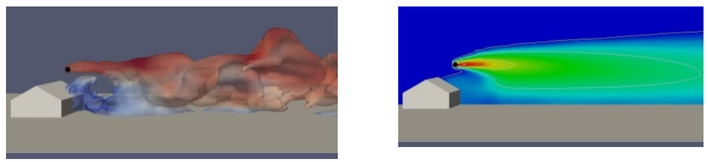
[33] P. Wenisch et al.

> - **Open source field operation & manipulation (OpenFOAM) is a C++ toolbox of numerical solvers & pre-/post processing utilities for the solution of CFD problems used in HPC simulations**

modified from [32] OpenFOAM Web page



(Parallelization is inherent in the OpenFOAM design)



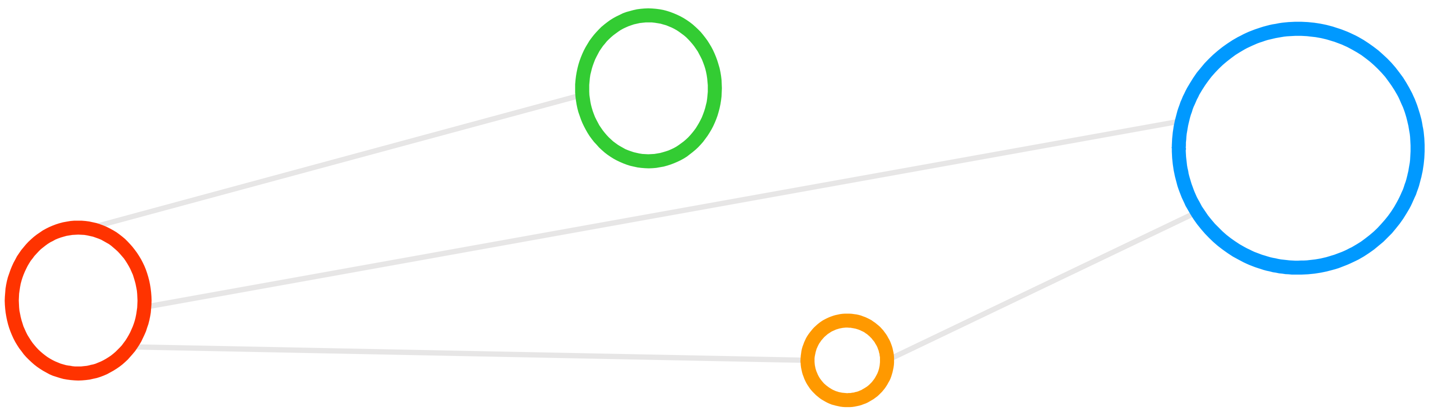
(using the LES mode within OpenFOAM)

[31] Lohmeier Consulting Engineers

[Video] CFD Summary

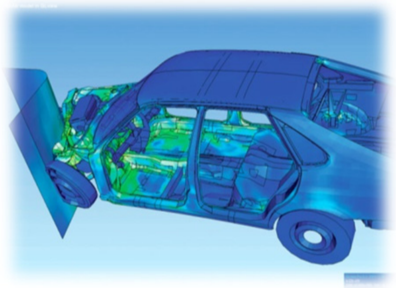
[16] YouTube Video, CFD

Finite Elements Method (FEM)



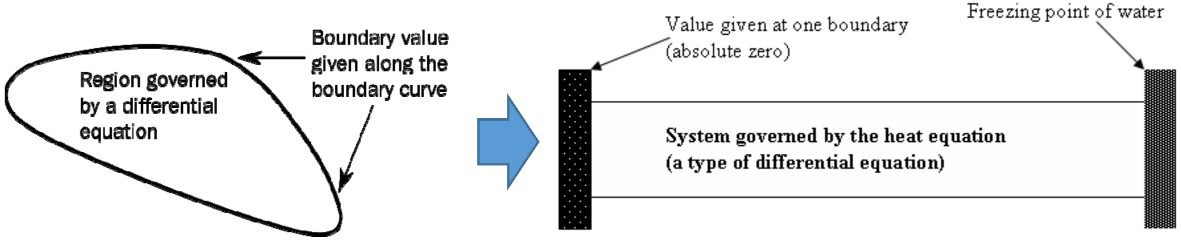
Finite Elements Methods (FEM) – Terminology & Motivation

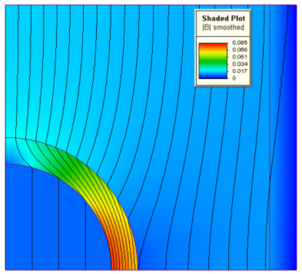
- Approach
  - Approximate 'complex equations over a large domain' (i.e. resulting mesh)
  - Connecting many simple element equations over many small subdomains (i.e. finite elements)
  - Fixed vs. dynamic domain decompositions
- Boundary value problems
  - Boundary outlines a region governed by partial differential equations (PDEs)



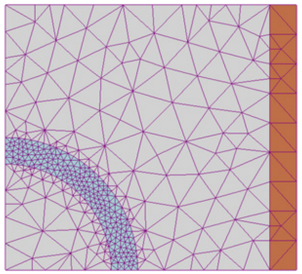
- **Finite Elements Methods (FEM) is a numerical method to find approximate solutions to boundary value problems (governed by partial differential equations) by connecting many simple elements**

[19] Wikipedia on FEM





[18] Wikipedia on Boundary value problems



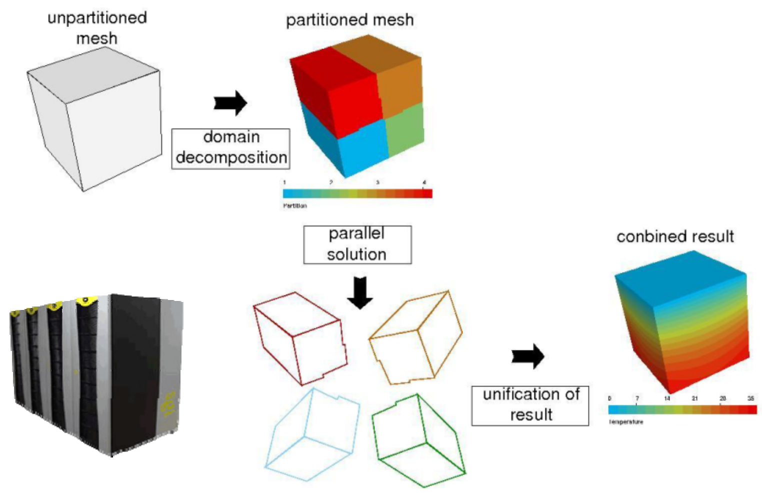
(FEM mesh to solve a magnetic problem)

FEM – Mesh Generation Technique

- Practice 'mesh creation'
  - Tools offer the creation of meshes in a straightforward way
  - For large complex geometry objects parallelization should be used
  - Result is an 'unpartitioned mesh'
- Parallelization
  - Domain decomposition (cf. Lecture 3)
  - Solving 'partitioned mesh' in parallel
- Wide variety of different mesh types
  - Uniform meshes or non-uniform meshes
  - (also cf. Short Lecture 11 on visualization)

- **Mesh generation (aka grid generation) refers to generating a polygonal or polyhedral mesh that approximates a geometric domain and that is used in a wide variety of CFD and FEM simulations**

[20] Wikipedia on Mesh



[21] T. Zwinger et al.

FEM – Adaptive Mesh Refinement (AMR)

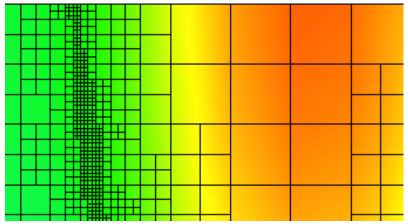
- Overcome 'static mesh' limits
  - 'Discrete mesh' spacing resolution simple approach in numerical analysis
  - No solutions of the numerical analysis on scales smaller then mesh spacing
  - AMR dynamically changes the spacing & shape of the mesh (i.e. dynamic grid)
  - Useful for very large range of scales
- Selected benefits
  - Increased computational savings over static grids
  - Flexible control of grid resolution as needed compared to the static grids or static mesh refinement
  - Increased storage savings over static grid

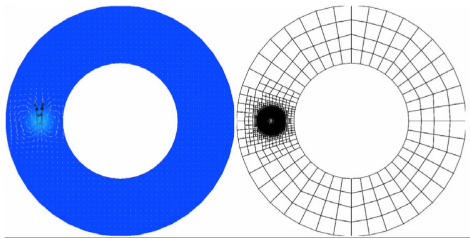
(static mesh refinement can be used for some regions that do not change shape over time)

- **Adaptive mesh refinement (AMR) is a method in numerical analysis & HPC to dynamically change the accuracy of a solution in certain regions during the time the solution is calculated as simulation**

modified from [22] Wikipedia on AMR

(use of adaptive mesh refinement as a method for reduction of big data outcomes of simulations)



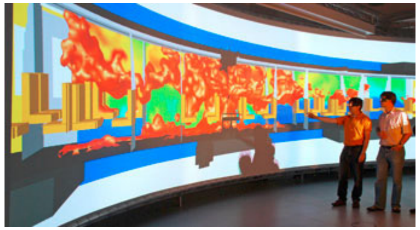


(e.g. fire and heat transfer requires AMR as interesting regions vary over time)

[23] Civil Security & Traffic Group

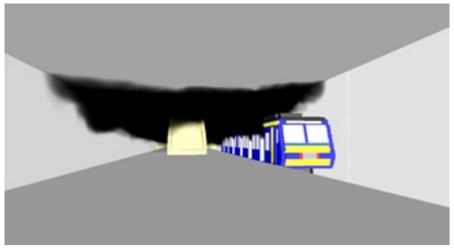
FEM – AMR Fire Dynamics Simulator (FDS) – Application Example

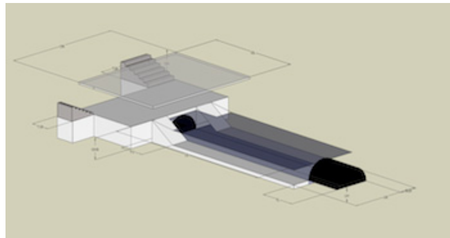
- Selected Facts
  - Open source package
  - Includes visualization tool SmokeView
- Parallelization
  - MPI (cf. Lecture 2) & OpenMP (cf. Lecture 6)
  - Hybrid programming (cf. Lecture 10)
  - Uses Adaptive Mesh Refinement (AMR)
- Examples
  - Smoke and heat transport from fires in underground stations (e.g. fire safety / civil engineering)
  - Fire simulations in trains, constructions, and generally objects

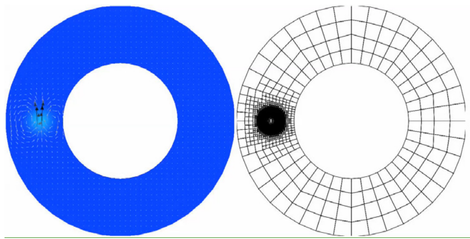


- **Fire Dynamics Simulator (FDS) is a CFD simulation package solving simplified forms of the Navier-Stokes equations and enables large-eddy simulations (LES) for low-speed flows (i.e. smoke/fire)**

modified from [29] FDS Web page



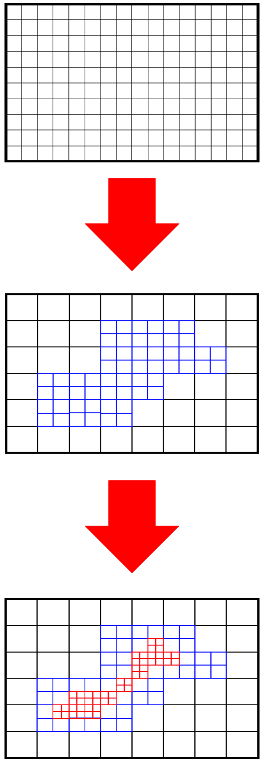




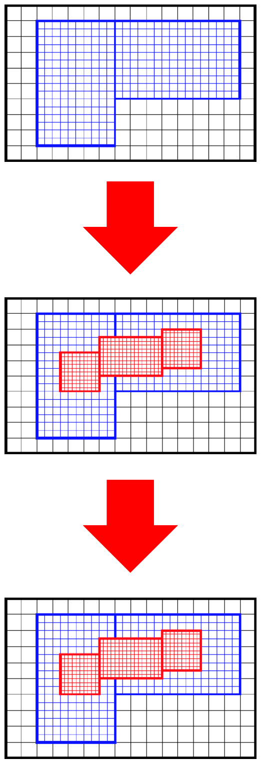
[23] Civil Security & Traffic Group

FEM – Adaptive Mesh Refinement – Tree-Code Example (cf. Lecture 5)

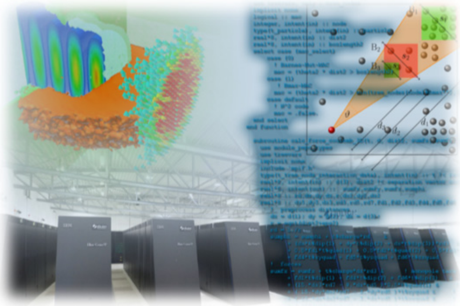
- Different approaches

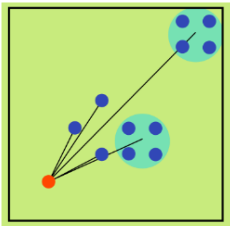


(point-based)



(patch-based)

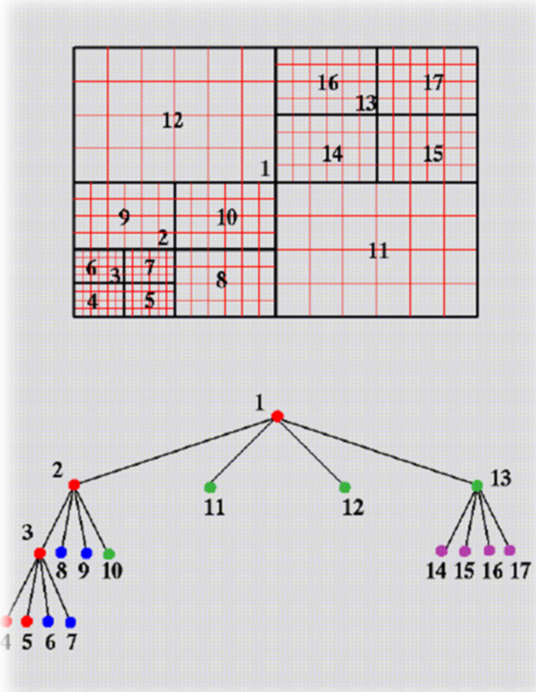




[25] PEPC Web page

[26] F. Salvatore et al.

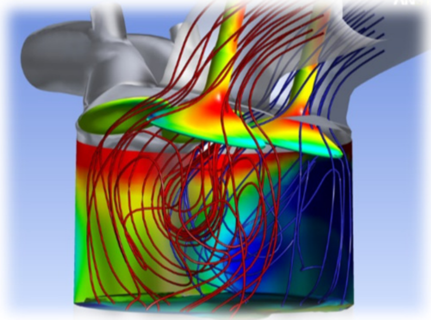
- Often tree-based implementation



(block-based tree)

Selected Libraries & Methods – Ansys

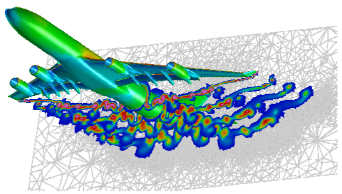
- Selected Facts
  - Strong commercial software tools w.r.t. functionality (although commercial available at many HPC centers)
  - Enables predictions how manufactured products will operate in real world
  - Offers FEM, structural analysis, CFD, etc.



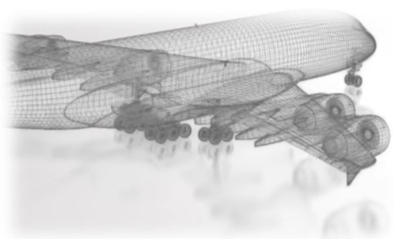
- Ansys is a commercial software package that consists of a wide variety of tools that enable HPC simulation-driven product development with several dedicated HPC packs & GPU support

modified from [34] Ansys Web page

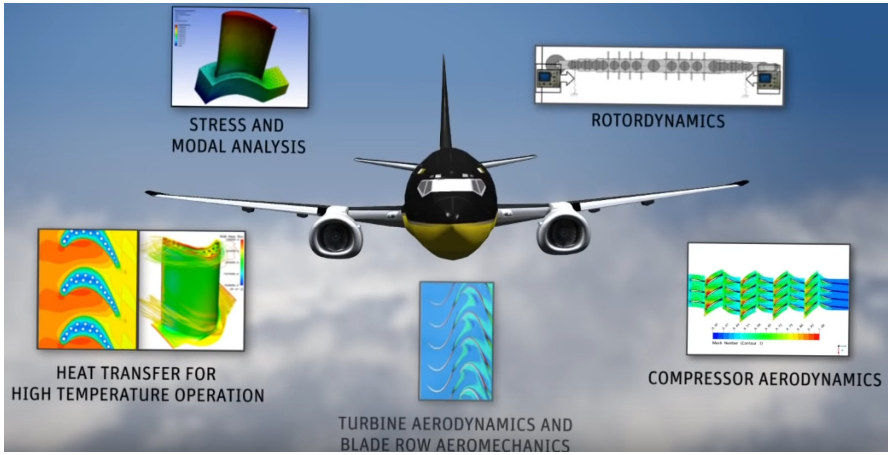
- Parallelization
  - Different 'HPC packs' across multiple physics problems packages
  - GPU enabled (cf. Lecture 7) package
  - Stores grids in HDF files (cf. Lecture 5)



- Example
  - Internal combustion engine modeled using ANSYS Fluent
  - Aerospace engineering

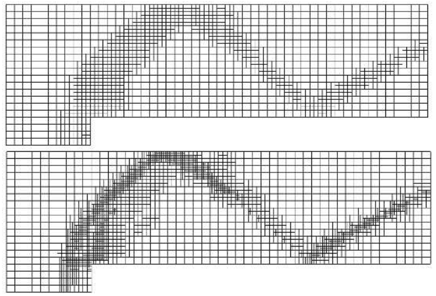


modified from [35] Ansys YouTube Video



Selected Libraries & Methods – OpenFOAM Revisited & Code_Aster

- OpenFOAM Selected Facts
  - Open source and many other features
- OpenFOAM Parallelization
  - Implementation of AMR (and coarsening)
- OpenFOAM Example
  - Automatic resolution control for the finite volume method
  - Error guides the refinement process & updates mesh
- Code_Aster Selected Facts
  - Free and open source software tool for FEM and related methods
  - Integrated with Salome-Meca platform (GUI functions, visualization, etc.)

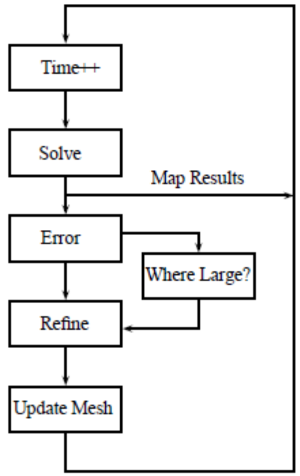


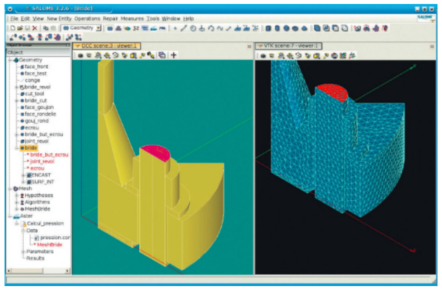
- **Open source field operation & manipulation (OpenFOAM) is a C++ toolbox of numerical solvers & pre-/post processing utilities for the solution of CFD problems used in HPC simulations**

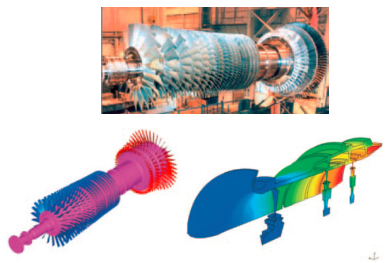
modified from [32] OpenFOAM Web page

[36] OpenFOAM Tutorial

(automatically improve the accuracy of CFD and FEM simulations in interesting regions)







- **Code_Aster offers a full range of multiphysical analysis and modelling approaches useful for computer aided engineering (CAE) and takes also partly advantage of parallelization methods**

modified from [37] Code_Aster Manual

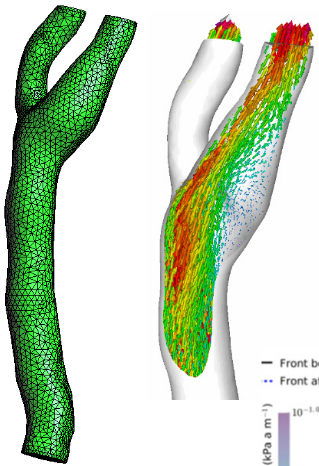
Selected Libraries & Methods – Elmer Package & Application Example

- Selected Facts
  - Open source multi-physical simulation software
  - Includes physical models of structural mechanics, electromagnetics, heat transfer, accoustics, etc.
  - Differen tools ElmerGUI, ElmerSolver, ElmerPost
- Parallelization
  - Distributed memory with MPI (cf. Lecture 3)
- Example
  - Blood flow in carotid artery (poses a fluid-structure interaction challenge)
  - Ice dynamic models (e.g. for ice calving)

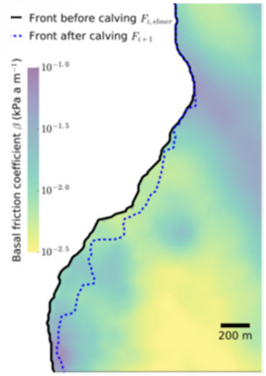
▪ Elmer is an open source multi-physical simulation software package that solves physical models described by partial differential equations via FEM and is used in a wide variety of HPC simulations

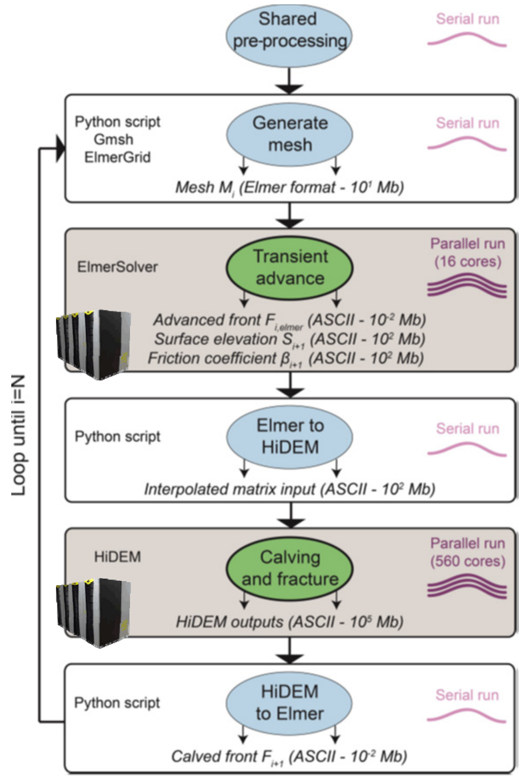
modified from [28] Elmer Web page

(e.g. research on calcification that reduces elasticity of arteries)



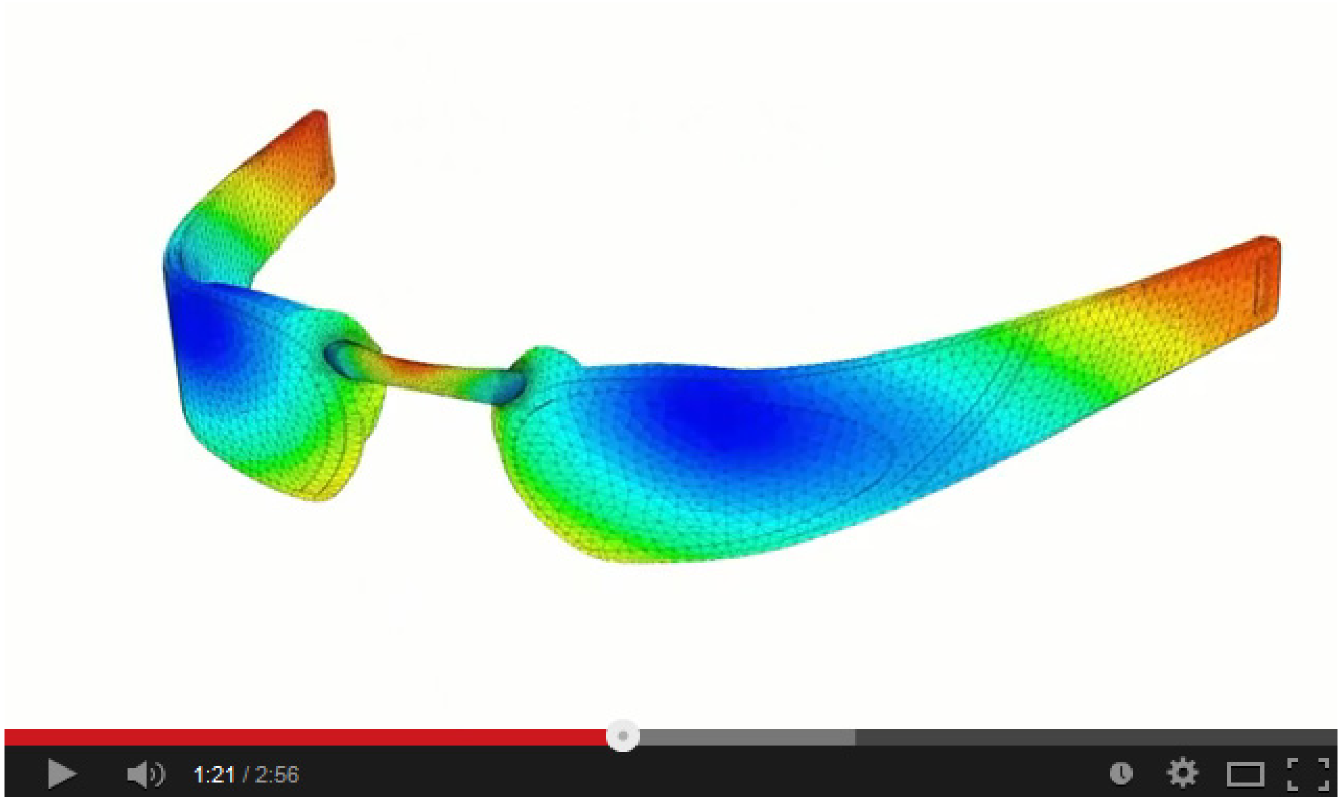
[24] Elmer Para2012 Tutorial





[30] M.S. Memon and M. Riedel et al., 'Scientific workflows applied to the coupling of a continuum (Elmer v8.3) and a discrete element (HiDEM v1.0) ice dynamic model', Geoscientific Model Development (GMD), Vol 12 (7), 2019

[Video] Speedo Application Use Case



[17] YouTube Video, 'Ansys Speedo Use Case'

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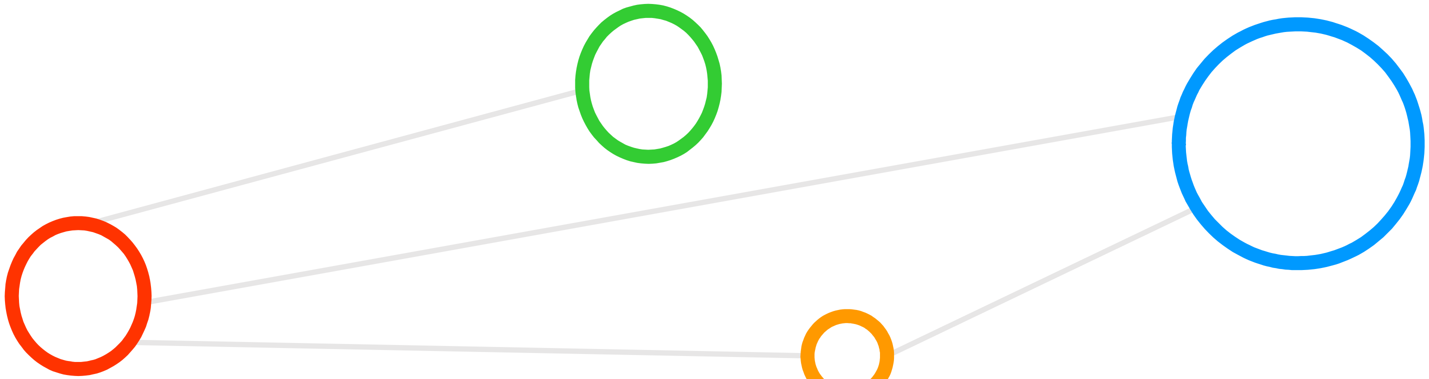

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