

Examples of Simulations with OpenFOAM

Complex Physics and Industrial CFD

Hrvoje Jasak

h.jasak@wikki.co.uk, hrvoje.jasak@fsb.hr

Wikki Ltd, United Kingdom

Faculty of Mechanical Engineering and Naval Architecture

University of Zagreb, Croatia

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Background



Complex Physics Topics and New Capabilities

- Viscoelastic flow modelling
- Free surface flows with compressibility effects: under-water explosions
- Flash boiling simulations
- Block matrix in use: strong coupling in multi-phase VOF
- Some new fluid-structure interaction results
- New mesh handling features: Overset Grid Method, Immersed Boundary Method, remeshing with Tetrahedral Edge Swapping

Industrial CFD Topics

- External aerodynamics with LES
- Simulations in metallurgical industry
- Radial Basis Function (RBF) and geometric shape optimisation
- OpenFOAM Turbo Tools
- Automotive Simulations
- Complex mesh motion cases



Examples of Simulation



Example of Capabilities of OpenFOAM in Complex Physics and Industrial CFD

- This is only a part of the OpenFOAM capabilities!
- Chosen for relevance and illustration of the range of capabilities rather than exhaustive illustration of range of capabilities
- In some cases, simplified geometry is used due to confidentiality
- Regularly, the work resulted in a new solver; in many cases, it is developed as an extension or combination of existing capabilities

Description of Simulation and Setup

- Physics and numerical method setup
- Standard or customised solver; details of mesh resolution and customisation



Viscoelastic Flow Model



MSc Thesis: Jovani Favero, Universidade Federal de Rio Grande del Sul, Brazil

• Viscoelastic flow model:

 $\nabla \mathbf{u} = 0$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \bullet (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \bullet \boldsymbol{\tau}_{\mathbf{s}} + \nabla \bullet \boldsymbol{\tau}_{\mathbf{p}}$$

where $\tau_s = 2\eta_s \mathbf{D}$ is the solvent stress contribution and τ_p is the **polymeric part** of the stress, non-Newtonian in nature

- Depending on the model, $au_{\mathbf{p}}$ is solved for: saddle-point problem
- Models introduce "upper", "lower" or Gordon-Schowalter derivatives, but we shall consider a general form: standard transport equation in relaxation form

$$\frac{\partial \boldsymbol{\tau}_{\mathbf{p}}}{\partial t} + \nabla_{\bullet}(\mathbf{u}\boldsymbol{\tau}_{\mathbf{p}}) = \frac{\boldsymbol{\tau}^{*} - \boldsymbol{\tau}_{\mathbf{p}}}{\delta}$$

where δ is the relaxation time-scale

• Problem: $au_{\mathbf{p}}$ dominates the behaviour and is explicit in the momentum equation



Viscoelastic Flow Model

Model Implementation Recipe

• Recognise τ^* as the equilibrium stress value: make it implicit!

$$\nabla \bullet \boldsymbol{\tau}^* = \nabla \bullet \left[\boldsymbol{\kappa} \bullet \frac{1}{2} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right]$$

• Calculate implicit viscoelastic viscosity:

$$\boldsymbol{\kappa} = \boldsymbol{\tau}^* \bullet \left[\frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right]^{-1}$$

• Split complete stress into implicit and explicit component

$$egin{aligned}
ablaullet au_{\mathbf{p}} &=
ablaullet au^* +
ablaullet au_{\mathbf{corr}} \ &=
ablaullet (oldsymbol{\kappa}ullet
abla \mathbf{u}) +
ablaullet oldsymbol{\tau}_{\mathbf{corr}} \end{aligned}$$



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Implemented Viscoelastic Models

- **Kinetic Theory Models**: Maxwell linear; UCM and Oldroyd-B; White-Metzner; Larson; Cross; Carreau-Yasuda; Giesekus; FENE-P; FENE-CR
- Network Theory of Concentrated Solutions and Melts Models: Phan-Thien-Tanner linear (LPTT); Phan-Thien-Tanner exponential (EPTT); Feta-PTT
- Reptation Theory / Tube Models: Pom-Pom model; Double-equation eXtended Pom-Pom (DXPP); Single-equation eXtended Pom-Pom (SXPP); Double Convected Pom-Pom (DCPP)
- Multi-Mode Form: The value of $au_{\mathbf{p}}$ is obtained by the sum of the K modes

$$oldsymbol{ au}_{\mathbf{p}} = \sum_{K=1}^n oldsymbol{ au}_{\mathbf{p}_K}$$

Flow Solvers Implemented by Jovani Favero: Example Simulation

- Single-phase non-Newtonian solver based on transient SIMPLE
- Multi-phase free surface VOF solver: viscoelastic in each phase
- Support for topological changes: syringe ejection



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Multi-Phase Compressibility

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Simulation of Under-Water Explosions

- This is ongoing collaboration with Johns Hopkins APL, Penn State University and Wikki: working hard for almost a year
- Dominating effects of compressibility in air and water: massive change in density, with propagating pressure waves
- Pressure ranges from 500 bar to 20 Pa
- Stiff numerics: collapse of over-expanded bubble due to combined compressibility of both phases are the basis of the phenomenon
- Test cases: Rayleigh-Plesset oscillation, undex under a plate, explosion
- Eric Paterson, Scott Miller, David Boger, Penn State; Ashish Nedungadi, JHU-APL





Multi-Phase Compressibility



First Simulations of Under-Water Explosions: Eric Paterson, Penn State

- Bubble of high initial pressure expands after explosion
- Initial pressure pulse is very fast with little effect
- Bubble collapse creates re-entrant jer which pierces the free surface
- Stability problems resolved in segregated solver
- Next phase: block-coupled $p \alpha$ solution algorithm







Flash-Boiling Flows: Shiva Gopalakrishnan, David P. Schmidt, UMass Amherst

- The fundamental difference between flash boiling and cavitation is that the process has a higher saturation pressure and temperature: higher density
- Enthalpy required for phase change is provided by inter-phase heat transfer
- Jakob number: ratio of sensible heat available to amount of energy required for phase change

$$Ja = \frac{\rho_l c_p \Delta T}{\rho_v h_{fg}}$$

 Equilibrium models are successful for cavitation since Ja is large and timescale of heat transfer is small. Flash boiling represents a finite rate heat transfer process: Homogeneous Relaxation Model (HRM)

$$\frac{Dx}{Dt} = \frac{\bar{x} - x}{\Theta}; \qquad \Theta = \Theta_0 \epsilon^{-0.54} \phi^{1.76}$$

x is the quality (mass fraction), relaxing to the equilibrium \bar{x} over a time scale Θ

• The timescale Θ is obtained from empirical relationship: Downar–Zapolski [1996]. ϵ is the void fraction and ϕ is the non–dimensional pressure.



Flash-Boiling Simulations

Flash-Boiling Flows: Numerical Method

• Conservation of Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\phi_v \rho \right) = 0$$

Conservation of Momentum

$$\frac{(\partial \rho U^0)}{\partial t} + \nabla \cdot \left(\phi U^0\right) = -\nabla p^n + \nabla \cdot \left(\mu \nabla U^0\right)$$

• Pressure Equation

$$\frac{1}{\rho} \frac{\partial \rho}{\partial p} \Big|_{x,h} \left(\frac{\partial (\rho p^{k+1})}{\partial t} + \nabla \cdot (\rho U p^{k+1}) \right) + \rho \nabla \cdot \phi^* - \rho \nabla \frac{1}{a_p} \nabla p^{k+1} + M \left(p^k \right) + \frac{\partial M}{\partial p} \left(p^{k+1} - p^k \right) = 0$$

The HRM model term is denoted as $M(=\frac{Dx}{Dt})$. The superscripts k and k + 1 are the corrector steps for the pressure equation.



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Flash-Boiling Simulations

Conservation of Mass

```
solve
(
    fvm::ddt(rho) + fvm::div(phiv, rho)
);
```

Conservation of Momentum

```
fvVectorMatrix UEqn
(
    fvm::ddt(rho, U) + fvm::div(phi, U) - fvm::laplacian(mu, U)
);
solve(UEqn == -fvc::grad(p));
Pressure Equation
fvScalarMatrix pEqn(fvm::laplacian(rUA, p));
solve
(
    psi/sqr(rho)*(fvm::ddt(rho, p) + fvm::div(phi, p))
    + fvc::div(phivStar) - pEqn
    + MSave + fvm::SuSp(dMdp, p) - dMdp*pSave
);
```



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Flash-Boiling Simulations



Asymmetric Fuel Injector Nozzle-Design from Bosch GmbH.









Multi-Phase Volume-of-Fluid Solver

- System of equations contains multiple VOF equations and global continuity handled by a pressure equation in standard form
- The phase for which VOF is solved first dominates the other phases: this is not acceptable; flipping the order of solution moves the problem around
- Aim: Coupled pressure based approach to achieve physical behaviour
- Solution strategy: solve α_i transport equations, volumetric continuity and closure equation in a strongly coupled manner, making the coupling terms implicit!
- To make this run, we shall use the block matrix and block solver (Jasak and Clifford, 2009)
- Credit goes to Kathrin Kissling and Julia Springer, NUMAP-FOAM 2009



Block Matrix in Use: Multi-Phase VOF

Multi-Phase Volume-of-Fluid Solver: Equation Set and Coupling

• Volume fraction transport equation, with separated pressure-driven flux terms

$$\begin{bmatrix} \frac{\partial \left[\alpha_{i}\right]}{\partial t} \end{bmatrix} + \left[\nabla \bullet \left(\left(\left(\frac{A_{H}}{A_{D}} \right)_{f} \bullet \mathbf{s}_{f} + \frac{1}{A_{D}} (\sigma \kappa)_{f} \nabla_{f}^{\perp} \alpha + \frac{1}{A_{D}} (\mathbf{g} \bullet \mathbf{x})_{f} |\mathbf{s}_{f}| \nabla_{f}^{\perp} \rho \right) [\alpha_{i}] \right) \right] \\ - \left[\nabla \bullet \left(\left(\frac{1}{A_{D}} \right) \nabla p^{*} [\alpha_{i}] \right) \right] + \left[\nabla \bullet \left([\alpha_{i}] \sum_{k=1, k \neq i}^{N} \alpha_{k} \phi_{r, ij} \right) \right] = 0$$

• Pressure equation, with separated phase fluxes (coupling terms)

$$\left[\nabla \bullet \left[\left(\frac{1}{A_D} \right)_f \nabla [p^*] \right] \right] = \nabla \bullet \left(\sum_{i=1}^N \alpha_i \phi^* \right)$$

• Closure equation and definition of fluxes

$$\sum_{i} \alpha_{i} = 1 \quad \phi^{*} = \sum_{i} \alpha_{i}^{N} \phi^{*}$$



Block Matrix in Use: Multi-Phase VOF

Multi-Phase Volume-of-Fluid Solver: Solution Strategy

- Above equations are dumped into a block matrix format, with coefficient size N + 1: (p^*, α_i) and solved in a block-coupled manner
- Result: strong coupling between α s and p: no dominant phase







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Fluid-Structure Coupling Capabilities in OpenFOAM

- As a Continuum Mechanics solver, OpenFOAM can deal with both fluid and structure components: easier setup of coupling
- (Parallelised) surface coupling tools implemented in library form: facilitate coupling to external solvers without "coupling libraries" using proxy surface mesh
- Structural mechanics in OpenFOAM targeted to non-linear phenomena: consider best combination of tools
 - Large deformation formulation in absolute Lagrangian formulation
 - Independent parallelisation in the fluid and solid domain
 - Parallelised data transfer in FSI coupling
- Dynamic mesh tools and boundary handling used to manipulate the fluid mesh







foamedOver: Overset Grid Technology in OpenFOAM

- Work by David Boger, Penn State University using SUGGAR and DirtLib libraries developed by Ralph Noack, Penn State (must mention Eric Paterson!)
- Overset Grid Technology
 - Multiple components meshed individually, with overlap
 - Hole cutting algorithm to remove excess overlap cells
 - Mesh-to-mesh interpolation with implicit updates built into patch field updates and linear solver out-of-core operations
- Body-fitted component meshes: preserving quality and near-wall resolution
- Simple mesh motion and geometrical studies (replacing individual components)
- Overset grid is physics-neutral! Currently testing for free surface flows





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Immersed Boundary Method

- Handling of moving obstacles in the flow domain whose size is larger than mesh resolution: covering multiple cells
- Mesh topology and connectivity does not change: immersed STL surface
- Presence of boundary implicitly accounted for in discretisation, with appropriate handling of boundary conditions





Immersed Boundary Method



Immersed Boundary Method: Examples

• Laminar flow around a 2-D moving circular cylinder in a channel



• Laminar flow around two counter-rotating elements in a cavity





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Re-Meshing with Tetrahedral Edge Swapping

• In cases where mesh motion involves topological change at the boundary or unpredictable mesh deformation, topological change machinery is impractical: cannot decide a-priori where to place topology modifiers

• Dynamic remeshing using tetrahedral edge swapping

- Motion is prescribed on external boundaries
- Tetrahedral cell quality examined continuously: bad cells trigger automatic remeshing without user interaction: answers to dynamicMesh interface
- Implemented by **Sandeep Menon**, **UMass Amherst** as a ready-to-use library
- Example: viscoelastic droplet collision using free surface tracking
- Can be used for all dynamic mesh cases: ultimate ease of mesh setup!







- Pushing state-of-the-art by applying Detached Eddy Simulation (DES) to full car body external aerodynamics simulations: native solver and mesher, no change
- Increase in simulation cost over transient RANS is over 1 order of magnitude!
- Controlling the Cost of Full Car DES:
 - Automated meshing and simulation environment, from STL surface of the car body to averaged DES results and forces
 - Hex-core mesher with near-wall layers and local refinement: mesh is designed to make it good for second-order LES numerics with minimal cost
 - No parallel license cost of CFD solver: simulations run on approx. 200 CPUs
- Improvement in C_D, C_L and force-per-component predictions due to better capturing of turbulence and transient flow features





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CFD in Metallurgical Applications



Three-Phase Free Surface Flow in a Tundish

- 3 phases with extreme density ratio: liquid steel, liquid slag, air (7000:2500:1)
- Note the presence of multiple phase-to-phase interfaces: using consistent discretisation for multiple phase α equations
- Temperature-dependent properties of slag and steel
- Simultaneous filling and pouring with large outlet velocity
- Examples
 - Simulation of a Turbo-Stop device for initial fill
 - Simulated break-down of a slag layer: detail of flow at exit nozzle





CFD in Metallurgical Applications



Assembling a Matrix for Conjugate Heat Transfer Problems

- OpenFOAM supports multi-region simulations, with possibility of separate addressing and physics for each mesh: multiple meshes, with local fields
- Some equations present only locally, while others span multiple meshes

```
coupledFvScalarMatrix TEqns(2);
TEqns.hook
(
    fvm::ddt(T) + fvm::div(phi, T)
    - fvm::laplacian(DT, T)
);
TEqns.hook
(
    fvm::ddt(Tsolid) - fvm::laplacian(DTsolid, Tsolid)
);
```

```
TEqns.solve();
```

• Coupled solver handles multiple matrices together in internal solver sweeps: arbitrary matrix-to-matrix and domain-to-domain coupling



CFD in Metallurgical Applications



Conjugate Heat Transfer and Thermal Shock

- Coupling may be established geometrically: adjacent surface pairs
- Each variable is stored only on a mesh where it is active: (U, p, T)
- Choice of conjugate variables is completely arbitrary: e.g. catalytic reactions
- Coupling is established only per-variable: handling a general coupled complex physics problem rather than conjugate heat transfer problem specifically
- Allows additional models to be solved on each region without overhead: structural stress analysis, turbulence or LES





Radial Basis Function

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Radial Basis Function Interpolation

- General interpolation for clouds of points
- Mathematical tool which allows data interpolation from a small set of control points to space **with smoothness criteria** built into the derivation
- Used for mesh motion in cases of large deformation: no inverted faces or cells
- Implemented by Frank Bos, TU Delft and Dubravko Matijašević, FSB Zagreb





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RBF Mesh Morphing Object

- RBF morphing object defines the parametrisation of geometry (space):
 - 1. Control points in space, where the parametrised control motion is defined
 - 2. Static points in space, whose motion is blocked
 - 3. Range of motion at each control point: $(\mathbf{d}_0, \mathbf{d}_1)$
 - 4. Set of scalar parameters δ for control points, defining current motion as

 $\mathbf{d}(\delta) = \mathbf{d}_0 + \delta(\mathbf{d}_1 - \mathbf{d}_0), \quad \text{where} \quad 0 \le \delta \le 1$

- For each set of δ parameters, mesh deformation is achieved by interpolating motion of control points d over all vertices of the mesh: new deformed state of the geometry
- Mesh in motion remains valid since RBF satisfies smoothness criteria

Using RBF in Optimisation

- Control points may be moved individually or share δ values: further reduction in dimension of parametrisation of space
- Mesh morphing state is defined in terms of δ parameters: to be controlled by the optimisation algorithm



RBF Morphing

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RBF Morphing Example: Morphing of a Cylinder

• Control points in motion:

Point	Motion range	
(-0.02 -0.02 0)	((0 0 0) (-0.01 0.01 0))	
(0.02 -0.02 0)	((0 0 0) (0.2 0.0 0))	
(-0.02 0.02 0)	((0 0 0) (-0.01 -0.01 0))	
(0.02 0.02 0)	((0 0 0) (0.02 0 0))	

• Note: parametrisation uses a single parameter δ for this motion





RBF Morphing

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RBF Morphing Example: Morphing of a Sphere

• Control points in motion:

Point	Motion range	
(-0.3 ±0.3±0.3)	((0 0 0) (±0.1 ±0.1 ±0.1))	
($0.3 \pm 0.3 \pm 0.3$)	((0 0 0) (±0.1 ±0.1 ±0.1))	
(0.7 0 0)	((0 0 0) (0.3 0 0))	

- Note: parametrisation uses a single parameter δ for this motion
- Optimisation shall be performed with 3 parameters: front, back, tail







Geometric Shape Optimisation with Parametrised Geometry

• Specify a desired object of optimisation and use the parametrisation of geometry to explore the allowed solution space in order to find the **minimum of the optimisation objective**

 $objective = f(\mathbf{shape})$

- 1. Parametrisation of Geometry
 - Computational geometry is complex and usually available as the computational mesh: a large amount of data
 - Parametrisation tool: **RBF mesh morphing**, defining deformation at a small number of mesh-independent points in space
- 2. **CFD Flow Solver** is used to provide the flow solution on the current geometry, in preparation for objective evaluation
- 3. Evaluation of Objective: usually a derived property of the flow solution
- 4. **Optimiser Algorithm**: explores the solution space by providing sets of shape coordinates and receiving the value of *objective*. The search algorithm iteratively limits the space of solutions in search of a minimum value of *objective*



3-D Sphere: Minimising Drag Force

- Using 9 control points in motion, with symmetry constraints: 4 points in front square, radial motion; 4 points in back square, radial and axial motion; 1 tail point, axial motion only
- Optimisation is performed with 3 parameters:

iter = 1 pos = $(0.2 \ 0.7 \ 0.2)$ v = 147.96 size = 0.2997iter = 5 pos = $(0.06111 \ 0.7092 \ 0.7092)$ v = 106.26 size = 0.2153iter = 12 pos = $(0.03727 \ 0.9354 \ 0.3830)$ v = 77.934 size = 0.0793iter = 22 pos = $(0.04095 \ 0.9458 \ 0.3413)$ v = 75.821 size = 0.006610





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HVAC 90 deg Bend: Flow Uniformity at Outlet

- Flow solver: incompressible steady-turbulent flow, RANS $k \epsilon$ model; coarse mesh: 40 000 cells; 87 evaluations of objective with CFD restart
- RBF morphing: 3 control points in motion, symmetry constraints; 34 in total
- Objective: flow uniformity at outlet plane

iter = 0 pos = $(0.9 \ 0.1 \ 0.1)$ v = 22.914 size = 0.69282 iter = 5 pos = $(0.1 \ 0.1 \ 0.1)$ v = 23.0088 size = 0.584096 iter = 61 pos = $((0.990164 \ 0.992598 \ 0.996147)$ v = 13.5433 size = 0.00095





OpenFOAM Turbo Tools

General Grid Interface

- Turbomachinery CFD requires additional features: implemented in library form
- General Grid Interface (GGI) and its derived forms
 - Cyclic GGI
 - Partial overlap GGI
 - Mixing plane interface (under testing)
- Implementation and parallelisation is complete: currently running validation cases in collaboration with commercial clients and Turbomachinery Working Group
- Other turbo-related components in pipeline: harmonic balance solver solver
- Library-level implementation allows re-use of GGI beyond turbomachinery





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Modelling Diesel Particular Filters: Federico Piscaglia, Politecnico di Milano

- Steady-state compressible flow through thin porous layers
- Detailed 3-D meshing of channels expensive: mesh resolution requirements
- ... but due to flow non-uniformity, channel-scale simulations cannot provide the answer: not all channels are equally loaded and energy equation is solved globally
- Solution: multi-scale filter model
 - Each channel is one cell thick: (1-D) simulation
 - Porosity is a face property; flow friction is a volumetric sink
 - Porous faces are assigned time-dependent filtration efficiency due to soot deposition, affecting the flow and species distribution
- Automatic meshing tool for the monolith, unstructured mesh for inlet and outlet







Spray, Wall Film and Combustion Simulations in Internal Combustion Engines

- Complete simulation of spray injection, evaporation, wall film and combustion in a GDI engine. Mesh motion and topological changes as shown before
- Basic flow solver, **automatic mesh motion**, topological changes used in standard form. Simulation includes intake stroke (moving piston + valves): **reverse tumble**
- Full suite of Diesel spray modelling using Lagrangian modelling framework
- Implementation of wall film and spray-film interaction: Željko Tuković, FSB
- Mesh sensitivity of **spray penetration**: solved with adaptive refinement!
- Authors of engine simulations: Tommaso Lucchini, Gianluca D'Errico, Daniele Ettore, Politecnico di Milano and Dr. Federico Brusiani, University of Bologna





Complex Mesh Motion



6-DOF Floating Body in Free Surface Flow

- Flow solver: turbulent VOF free surface, with moving mesh support
- Mesh motion depends on the forces on the hull: 6-DOF solver
- 6-DOF solver: ODE + ODESolver energy-conserving numerics implemented using quaternions, with optional elastic/damped support
- Variable diffusivity Laplacian motion solver with 6-DOF boundary motion as the boundary condition for the mesh motion equation
- Topological changes to preserve mesh quality on capsize
- Coupled transient solution of flow equations and 6-DOF motion, force calculation and automatic mesh motion: custom solver is built from library components





Summary

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Project Status Summary

- OpenFOAM is a free software, available to all at no charge: GNU Public License
- Object-oriented approach facilitates model implementation
- Equation mimicking opens new grounds in Computational Continuum Mechanics
- Extensive capabilities already implemented; open design for easy customisation
- Solvers are validated in detail and match the efficiency of commercial codes
- Open Source model dramatically drops the cost of industrial CFD

OpenFOAM in Research and Industry

• Technical development driven by **Special Interest Groups** & **Birds-of-a-Feather**

Turbomachinery	Ship Hydrodynamics	Simulation of Engines
Turbulence	Fluid-Structure Interaction	Multiphase Flows
Aeroacoustics	Combustion and explosions	Solid Mechanics
Documentation	High Performance Computing	OpenFOAM in Teaching

• Sixth OpenFOAM Workshop: Penn State University 13-16 June 2011 http://www.openfoamworkshop.org

