Numerics Improvements in OpenFOAM with Examples of Industrial CFD

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Outline

Objective

- Give an update on ongoing technical developments with OpenFOAM
- Present improvements in numerics and methodology needed to meet industrial CFD requirements

Topics

- Landscape of industrial and academic CFD: 2016-2020 and beyond
- The Naval Hydro Pack: OpenFOAM in naval hydrodynamic
- Features and performance update for the coupled p-U solver
- Coupled solver methodology
- Harmonic balance for turbo-machinery simulations
- Complex physics models
- Summary

CFD: 2016-2020 and Beyond

Status of the CFD Market

- **The end of an era for general purpose CFD codes**
  - Tools that do all things for all people no longer exist: consider using ANSYS CFX for wave modelling or internal combustion engines
  - A CFD engineer who “knows all the models” belongs to a previous age
- Customised problem-oriented tools (not physics-oriented!)
- Integration, automatisation and transfer of knowledge: collaborative model development, validation and verification

Customised Problem-Specific CFD Simulation Tool

- Extension from “general CFD” to problem-specific tools, eg. turbo-machinery rotor-stator interfaces or free surface wave modelling
- **20-click CFD** (or no-click CFD): general purpose GUIs front-end no longer answers users’ needs: application language, minimal controls, scripted interface

Integration of Simulation Tools in Industrial Design

- Automated simulation (+meshing) with **rapid turn-around**: 8 hrs max!
- At least 99% simulation reliability; known scope of model applicability and achievable accuracy of simulated results (error bars!)

Why Does Open Source Matter

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Open Source Simulation Tools

- Historically, CFD tools are treated as “black magic boxes” capable of solving all problems for all people (provided not many questions are asked)
- . . . but to achieve a solution to known accuracy this is not sufficient
- **Application-specific extensions** are critical
    - Cannot do added resistance for a ship in waves simulation unless the solver can generate waves in a reliable and efficient manner
    - Implementation of application-specific auxiliary models is sometimes more complex than the basic fluid flow solver
    - Black box user coding is not sufficiently flexible (data access? HPC? parallel scaling?)
- **This is no longer a general-purpose CFD solver** (!)
- Ability to inspect, correct and modify the source code gives confidence in results
- Shared validation effort with third parties requires control over the code base
- Ideally, **code validation is a shared industry effort**: better simulation tools benefit everyone!

Open Source simulation toolbox is the best way to design and deploy problem-specific tools while re-using base building blocks

Validation and Verification

Validation and Verification: Beyond the Basics

- Requirement on validation and verification of CFD tools is well beyond the traditional “does this model produce the data that matches (one) experiment?”:
  - What is the range of applicability of the model? At what uncertainty?
  - What is the mesh resolution requirement? Time-step requirement? Grid uncertainty? Non-linear iteration coupling accuracy? Periodic uncertainty?
- Validation and verification studies of this type are extremely challenging and limited in scope to the problem at hand

Example: CFD Validation of Added Resistance in Naval Hydrodynamics

- Guidance on mesh resolution relative to wave height/length, size or relaxation zones, time-step size, number of non-linear correctors, number of simulated wave encounters (periodic uncertainty)
- Multi-code, multi-experiment (public) validation exercise: Tokyo 2015 Workshop
- Validation effort: 16 person/months!

Naval Hydro Pack

Numerical Simulations in Naval Hydrodynamics

- Traditionally, potential flow methods are widely used in naval hydrodynamics
  - Potential flow solver captures waves accurately
  - Interaction with a static and moving hull can be captured
  - Ability to operate in spectral space
  - (Some) viscous effects can be captured using ITTC procedures
- ...but limits of applicability are upon us: forward speed, viscous drag, turbulence modelling, breaking waves, non-linearity
- The cost of CFD has only recently become acceptable
- **Objective: Extract significant added value from CFD** to justify substantial increase in computational cost

Limitations on CFD Methodology

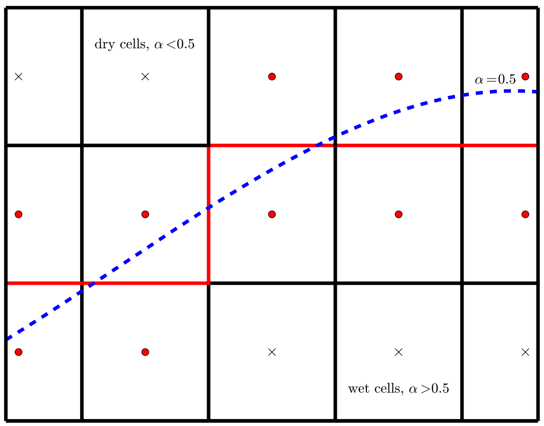
- Range of scales and extreme Re number: 1e9 or 1e10
- Sea-keeping simulations need to account for 30-50 wave encounters in regular sea states. In freak waves or irregular sea states the statistics requirement is even more severe
- Free surface flow solver needs to operate at extreme CFL number: 500 to 10 000

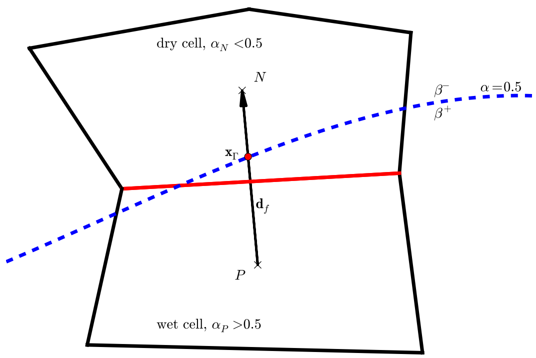
A complete re-think and re-implementation of the naval hydro solver is required!

Interface Jump Conditions

Naval Hydro Pack: Interface Jump Conditions for Free Surface Flows

- In free surface flows, a discrete surface discontinuity exists with a sharp change in properties: ρ, ν: proper handling is needed for accurate free surface simulations
- Huang et.al. (2007) describe a ghost fluid single-phase formulation of interface jump conditions in CFD-Ship Iowa
- Extended, modified and numerically improved treatment by Vukčević and Jasak (2015) with 2-phase handling is implemented in the Naval Hydro pack
  - Perfectly clean interface: no surface jets
  - Pressure force evaluated exactly even for a smeared VOF interface
  - Dramatically increased efficiency and accuracy of wave modelling





Interface Jump Conditions

Interface Jump Conditions: Derivation

- **Conditionally averaged** momentum equation:

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla_{\bullet}(\rho\mathbf{u}\mathbf{u}) = \nabla_{\bullet}\sigma_{eff} - \nabla p_d - (\mathbf{g}_{\bullet}\mathbf{x}\nabla\rho)$$

- Looking at the RHS of the equation, the gradient of dynamic pressure (∇p_d) is balanced by the density gradient ($\nabla\rho$).
- The balance between **pressure and density gradients happens in the momentum equation...**
- ...which in turn causes spurious air velocities because the pressure–density coupling should not be resolved in the momentum equation using a segregated solution algorithm

Interface Jump Conditions

Interface Jump Conditions: Derivation

- "Mixture formulation" of the momentum equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla_\bullet(\mathbf{u}\mathbf{u}) - \nabla_\bullet\left(\nu_e \nabla \mathbf{u}\right) = -\frac{1}{\rho}\nabla p_d$$

- Dynamic pressure jump conditions at the interface:

$$[p_d] = -[\rho]\mathbf{g}_\bullet\mathbf{x}$$

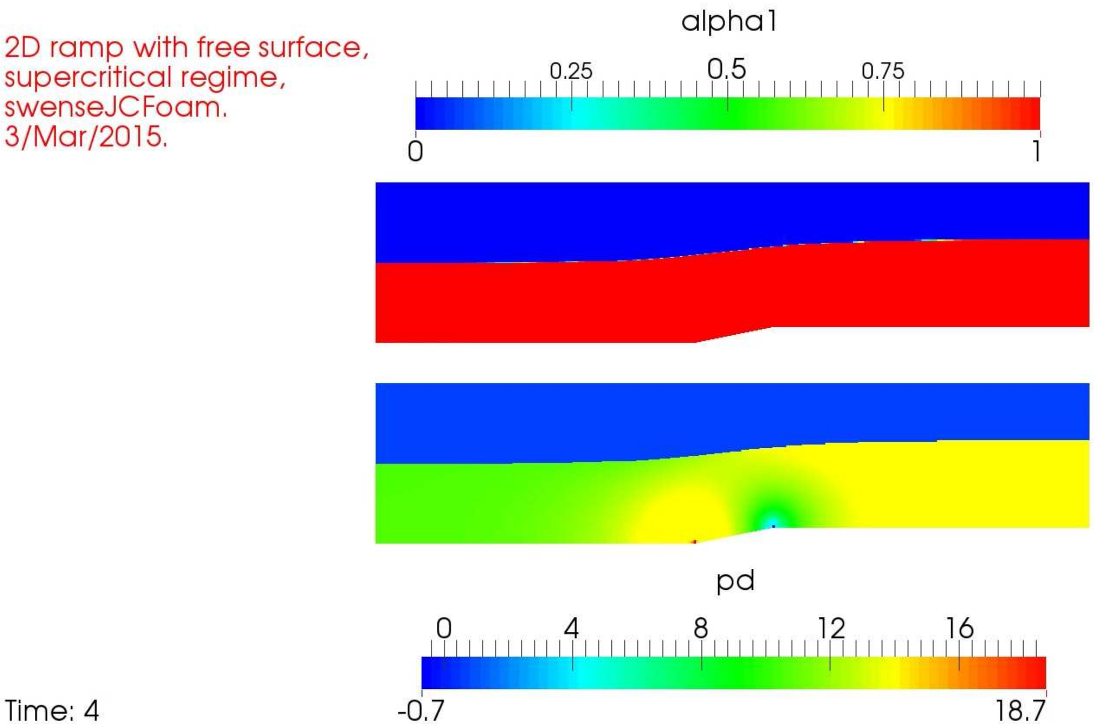
$$\left[\frac{1}{\rho}\nabla p_d\right] = 0$$

- Interface jumps implemented directly in discretisation operators
- Interface jump condition can be used both with level set and VOF
- ...and smearing of the surface in VOF no longer affects the pressure forces!
- Extension to viscous force jump can be performed but currently not used

Interface Jump Conditions

Interface Jump Conditions: Results

- Example: 2D ramp with free surface
- Relative error for water height at the outlet is -0.34% compared to analytical solution
- Note sharp p_d jump and α distribution
- The simulation with `interFoam` is not stable due to spurious air velocities



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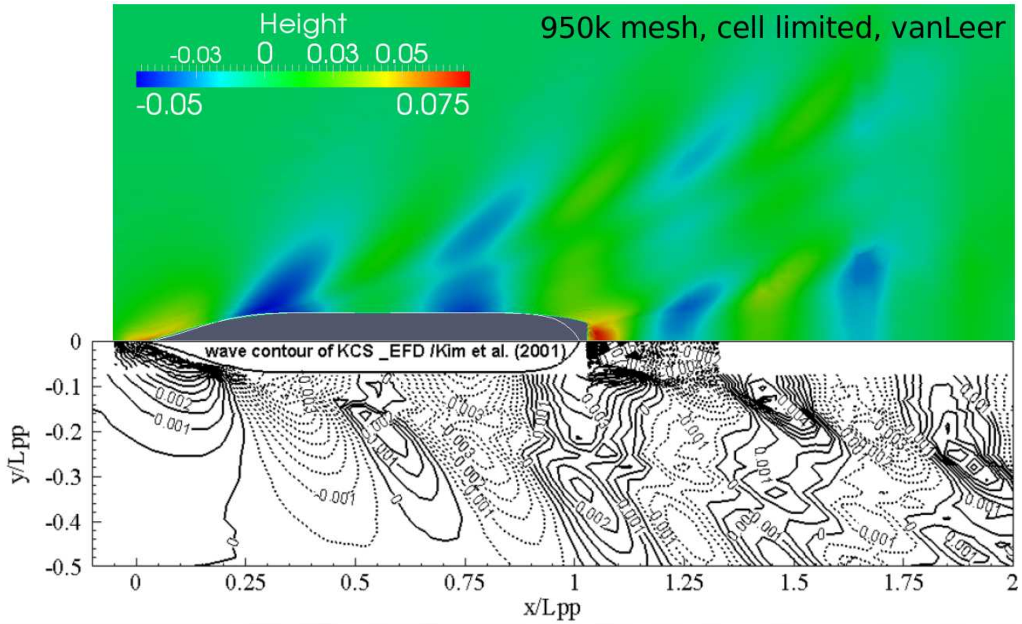
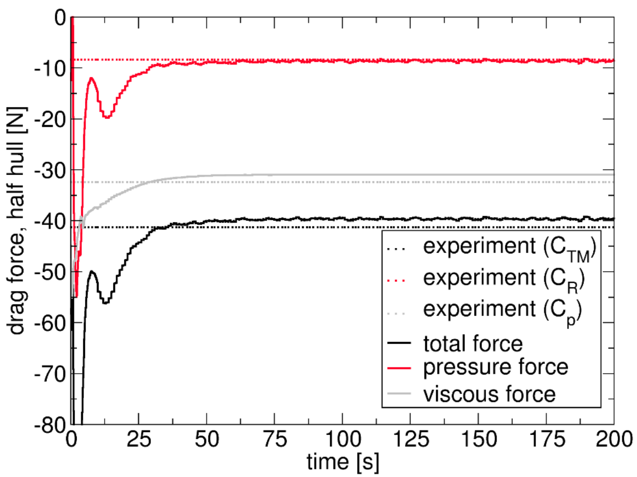
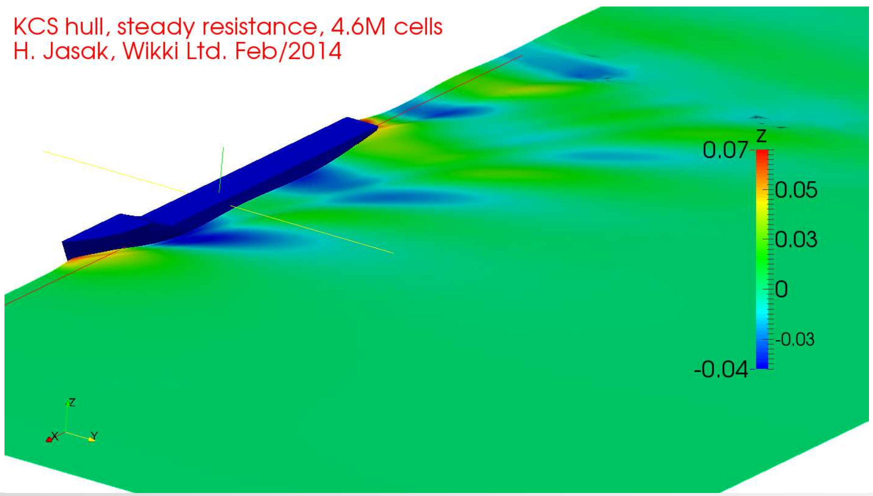
Steady Resistance in Calm Water for a Displacement Hull







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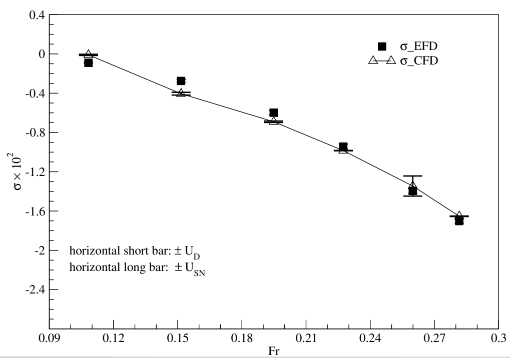
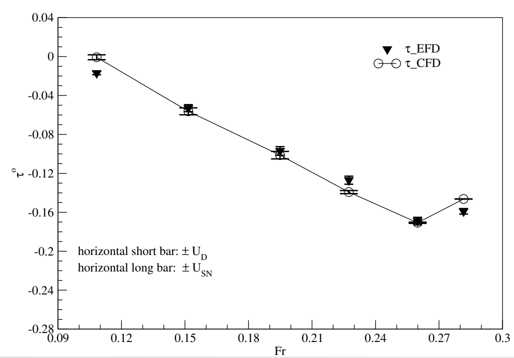
Steady Resistance in Calm Water: **KRISO Container Ship (KCS)**

- Computer: Single processor Intel I7 4820K, 3.7 GHz, 4 cores , 16 GB RAM
- **A converged and accurate resistance force in 30 min on 1 CPU!**

Mesh size	Drag [N]	Simulation Time for 200 s	Converged Force Simulation Time [s]
600k	41.93	1153 = 19 min	50
700k	41.09	1285 = 21 min	50
950k	40.35	1752 = 29 min	50
1.6M	39.93	2996 = 50 min	50
2.6M	38.91	14249 = 4.0 hrs	125/75
4.6M	38.58	27888 = 7.7 hrs	125/75

- Computational and experimental uncertainty in sinkage and trim simulations





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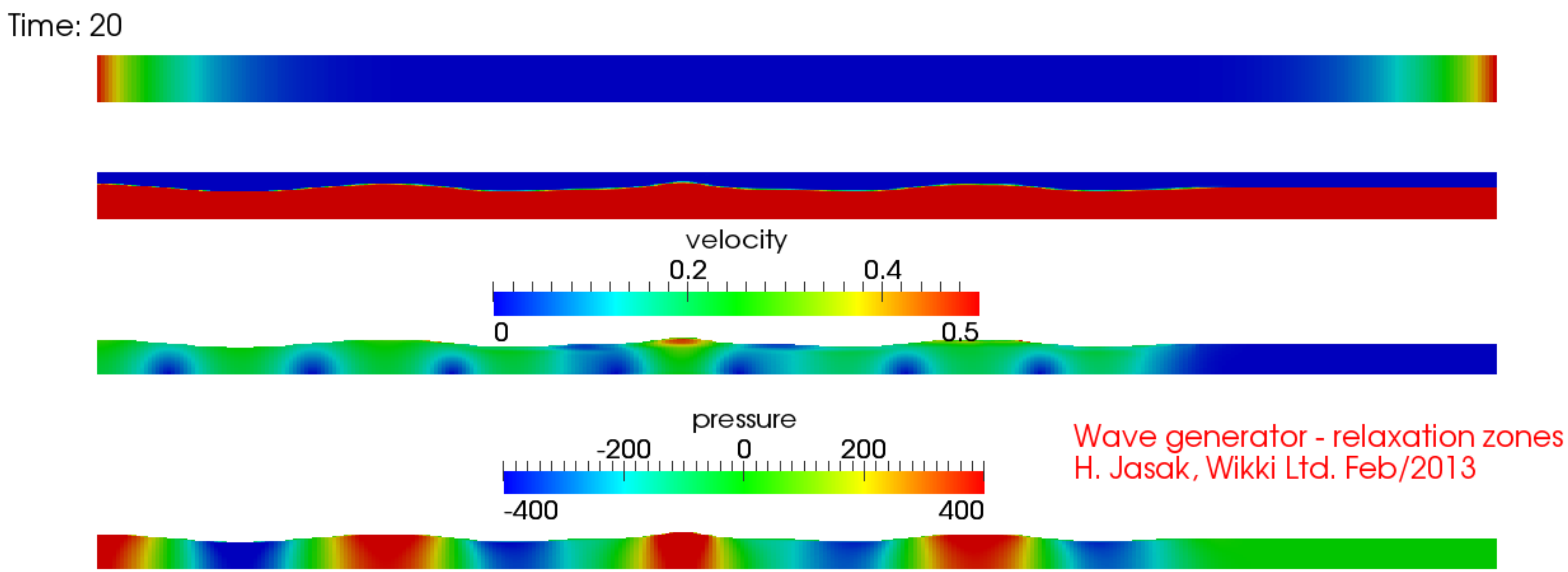
Example: Wave Generator and Potential Current

- Inlet wave relaxation zone: regular Stokes waves with soft ramp time
- Outlet relaxation zone: potential current, fixed water table



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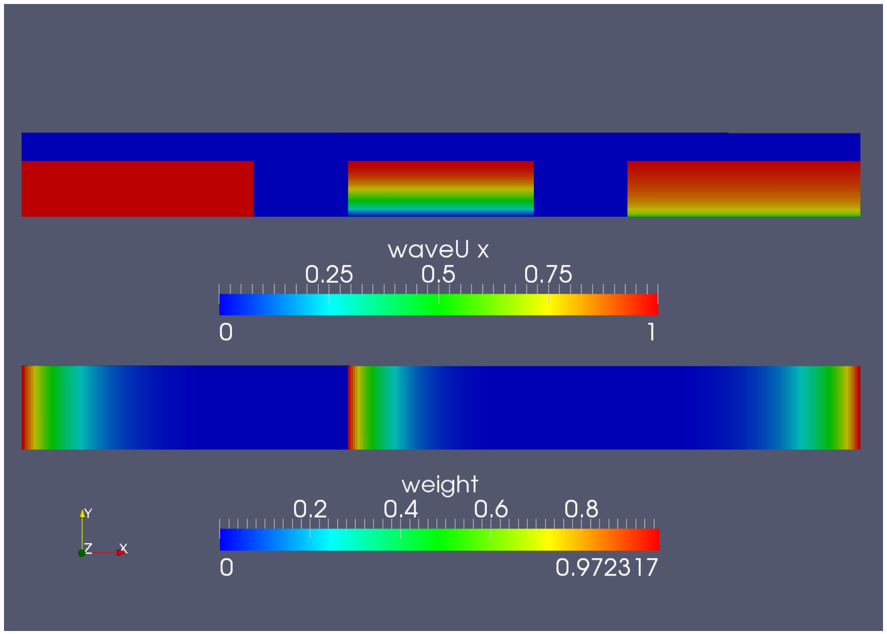
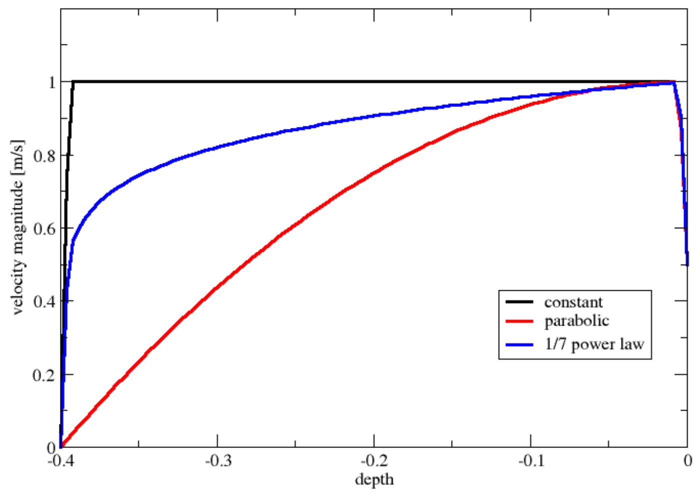
Prescription of Mean Current Profile in Wave Trains

- In shallow seas, boundary layer at the seabed may be important
- Example: wave force loading on static structures rising from seabed; sediment transport driven by wave action
- Wave profile follows action of the wave train, with specified depth-wise profile, imposed via the relaxation zones



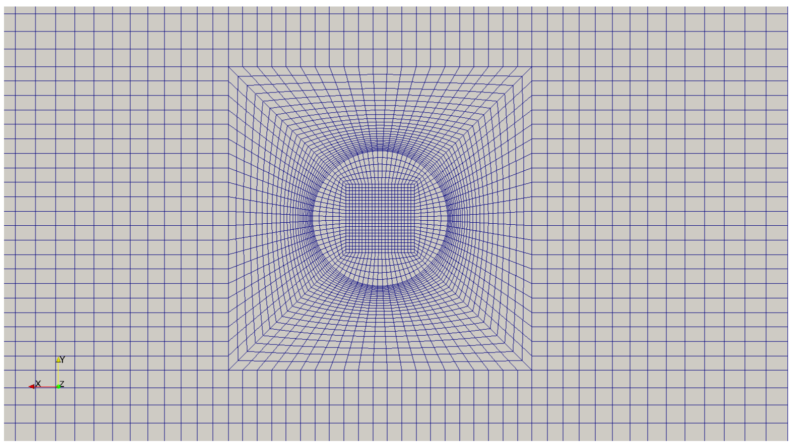


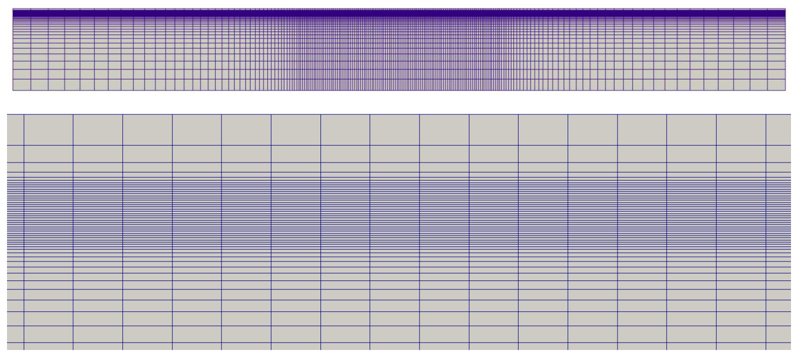
Regular Wave Impact on a Semi-Submersed Trunk

- Incident wave parameters

	Frequency	Wave height	Wave length	Period
N	f, h	h, m	λ, m	T, s
1	0.70	0.060	3.19	1.43
2	0.70	0.120	3.19	1.43
3	0.90	0.123	1.93	1.11
4	1.10	0.050	1.30	0.90
5	1.43	0.049	0.76	0.70

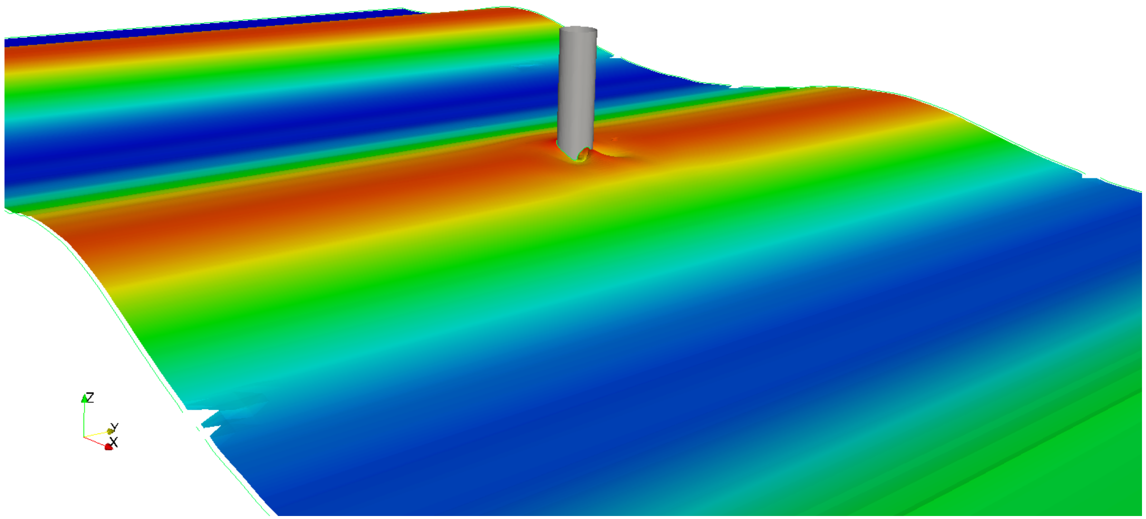
- Mesh structure around the cylinder and free surface: high cell aspect ratio

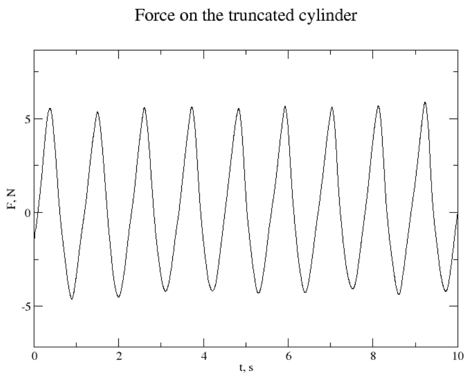


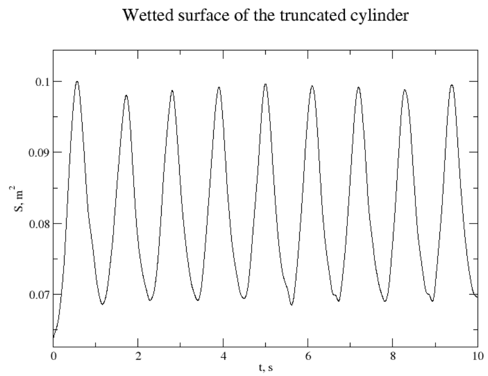


Regular Wave Impact on a Semi-Submersed Trunk

Wave loads on vertical cylinder







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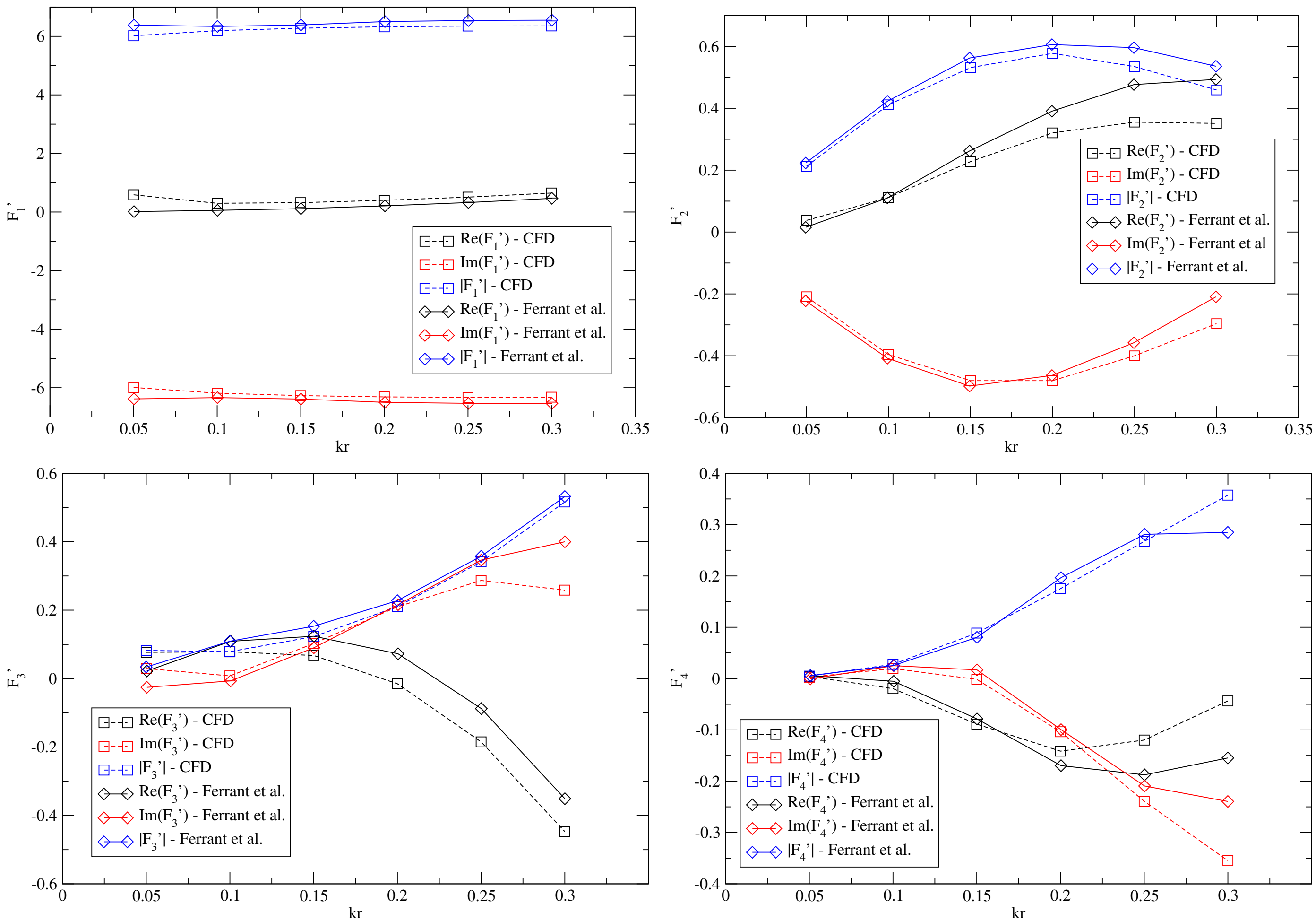
Example: Regular Wave Impact on a Semi-Submersed Trunk

- Wave number study of diffraction: normalised harmonic force coefficients
- First to fourth order harmonics Re and Im part, comparison with Ferrant (1999)



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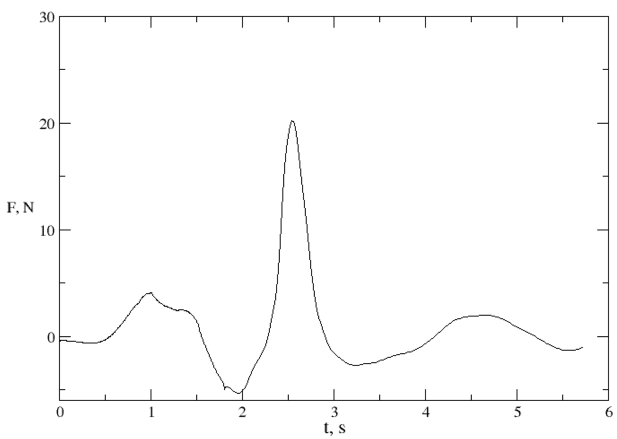
Example: Freak Wave Impact on a Semi-Submersed Trunk

- Wave components correspond to the Pierson-Moskowitz sea energy spectrum
- **Wave focusing method** was used to create a freak wave at a given point in time-space
  - 30 harmonic wave components
  - Phase shifts for individual wave components set up using optimisation
  - Sea spectrum significant height $h_s = 0.12\,\mathrm{m}$
  - Optimisation achieves freak wave height $H = 0.28\,\mathrm{m}$
- Domain layout and mesh identical to wave train simulation



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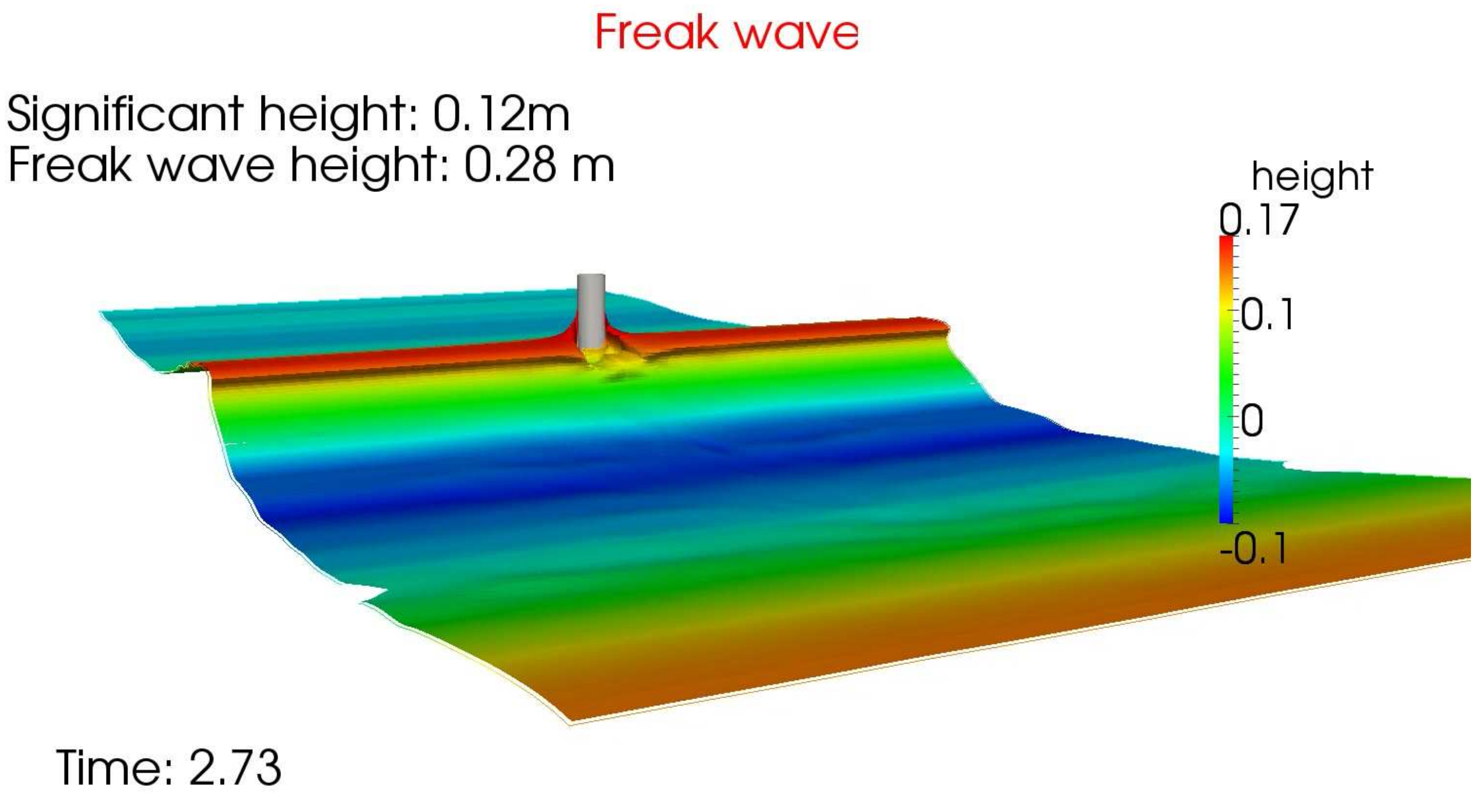
Example: Freak Wave Impact on a Semi-Submersed Trunk

- Characteristics of a desired freak wave prescribed at the point of impact
- Freak wave model describes decomposition into amplitudes, frequencies and phase lags required to produce the freak wave at point of impact



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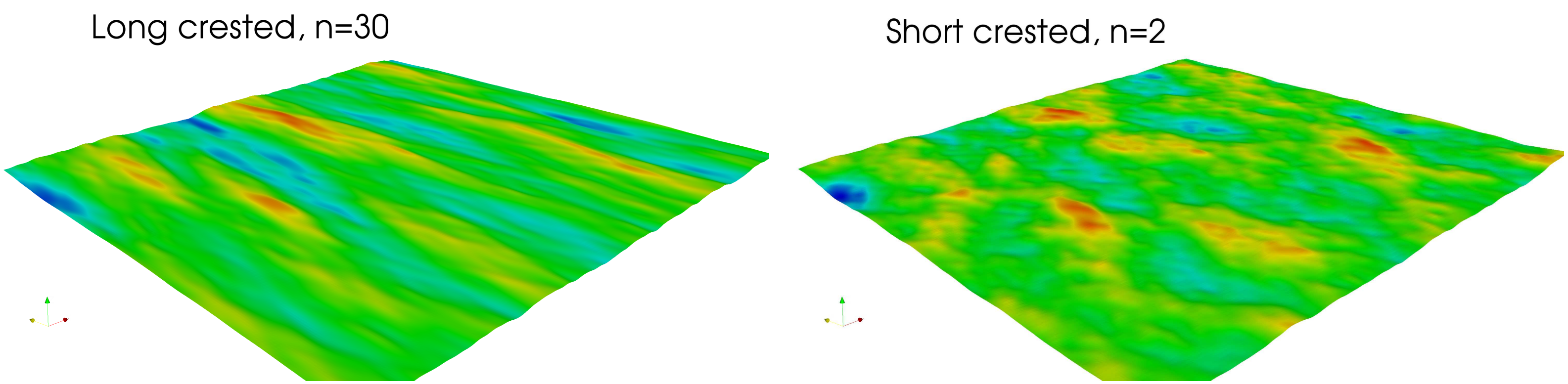
Irregular Sea States and Directional Sea Spectra

- Realistic sea states cannot be described using one-dimensional sea spectra: there exists a substantial scatter in directionality which needs to be accounted for
- Two-dimensional sea spectrum is applied in spectral components and in spreading direction
- Typical number of spectra/directional components is approx 600
- HOS is necessary to capture the interaction between frequencies: more consistent results than in linear superposition of spectral components
- “Short-crested” and “long-crested” waves can be created via variation of the spectral directionality parameter m



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Sea-Keeping Validation in Regular Head Waves: Tokyo 2015 Workshop C 2.10 Case

- Towed ship in head waves at design Froude number: $F_n = 0.26$
- Model scale: $L_{PP} = 6.0702$ m
- 5 wave conditions (and a steady resistance test)
  1. C1; $\lambda/L_{PP} = 0.65$, $H = 0.062$ m
  2. C2; $\lambda/L_{PP} = 0.85$, $H = 0.078$ m
  3. C3 (resonant case); $\lambda/L_{PP} = 1.15$, $H = 0.123$ m
  4. C4; $\lambda/L_{PP} = 1.37$, $H = 0.149$ m
  5. C5; $\lambda/L_{PP} = 1.96$, $H = 0.196$ m
- Experimentally measured heave, pitch and total resistance
- No experimental uncertainty reports
- Complete CFD validation and verification study
  - Spatial and temporal resolution requirement
  - Periodic uncertainty study
  - Hydro-mechanical coupling study

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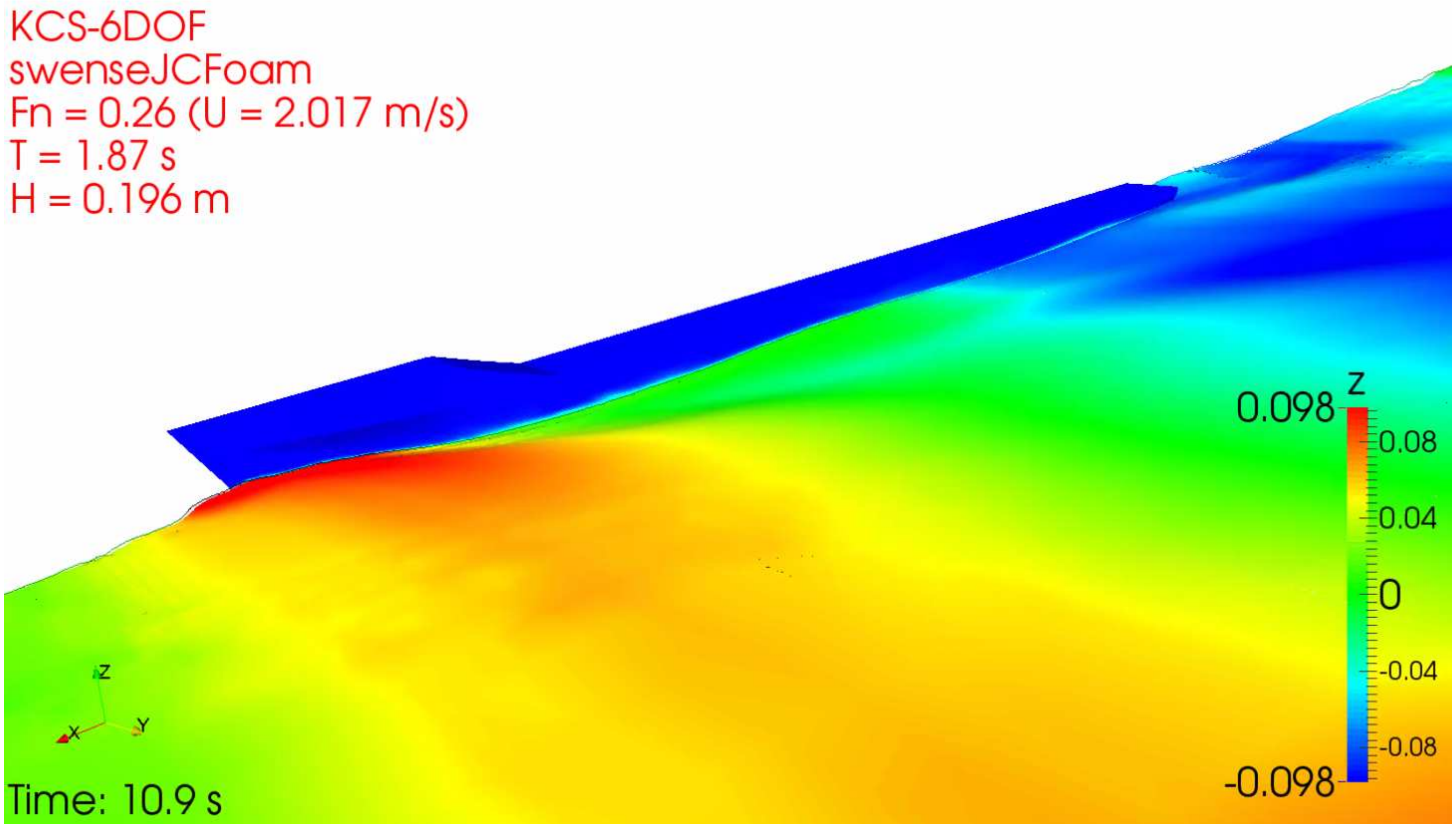
Sea-Keeping Validation in Regular Head Waves: Tokyo 2015 Workshop C 2.10 Case



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Performance test results

- Results correspond to temporal resolution study with 25 time steps per encounter period
- This case represents trade–off between performance and accuracy (mean values and phases are affected by such a low temporal resolution)
- Simulated time

$$\begin{array}{rl} & 1.87276 \text{ s (encounter period)} \\ \times & 30 \text{ (number of periods simulated)} \\ = & 56.1828 \text{ s of simulated time} \end{array}$$

- **Total execution time = 1677.87 s $\approx$ 30 minutes**
- ... yielding approximately **30 s of CPU time for 1 s of real time**
- If better accuracy is desired, good results can be obtained with 200 time steps per encounter period = **4 min of CPU time for 1 s of real time $\approx$ 2 min of CPU time per encounter period**

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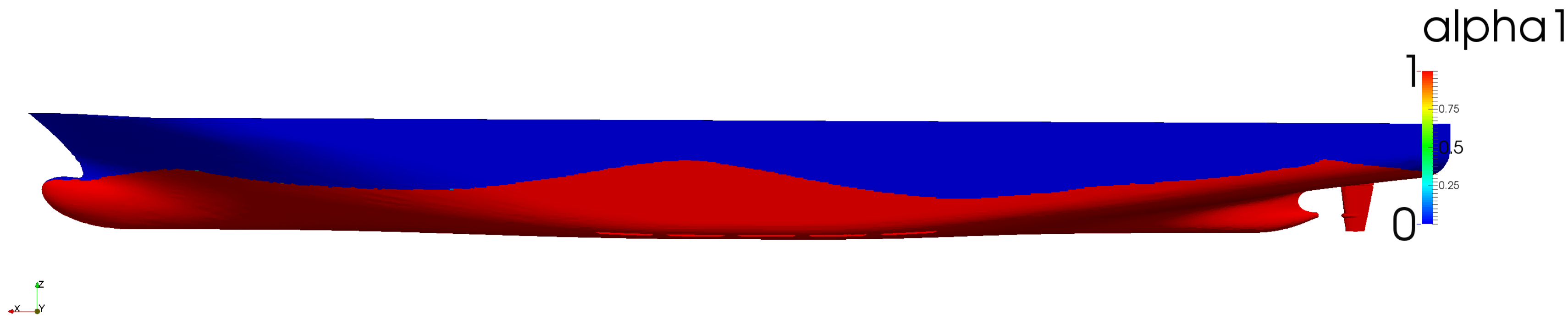

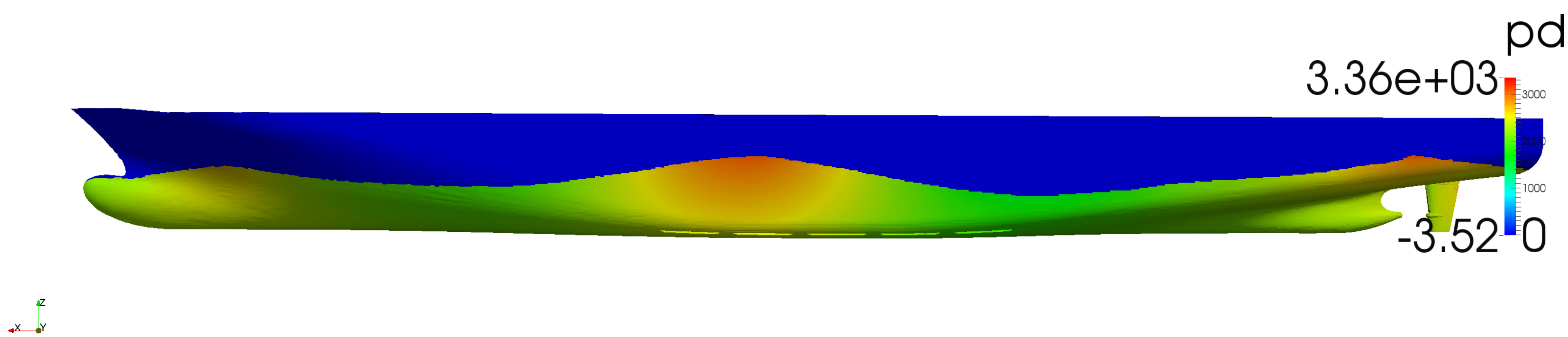

Sharp, non–ventilating free surface

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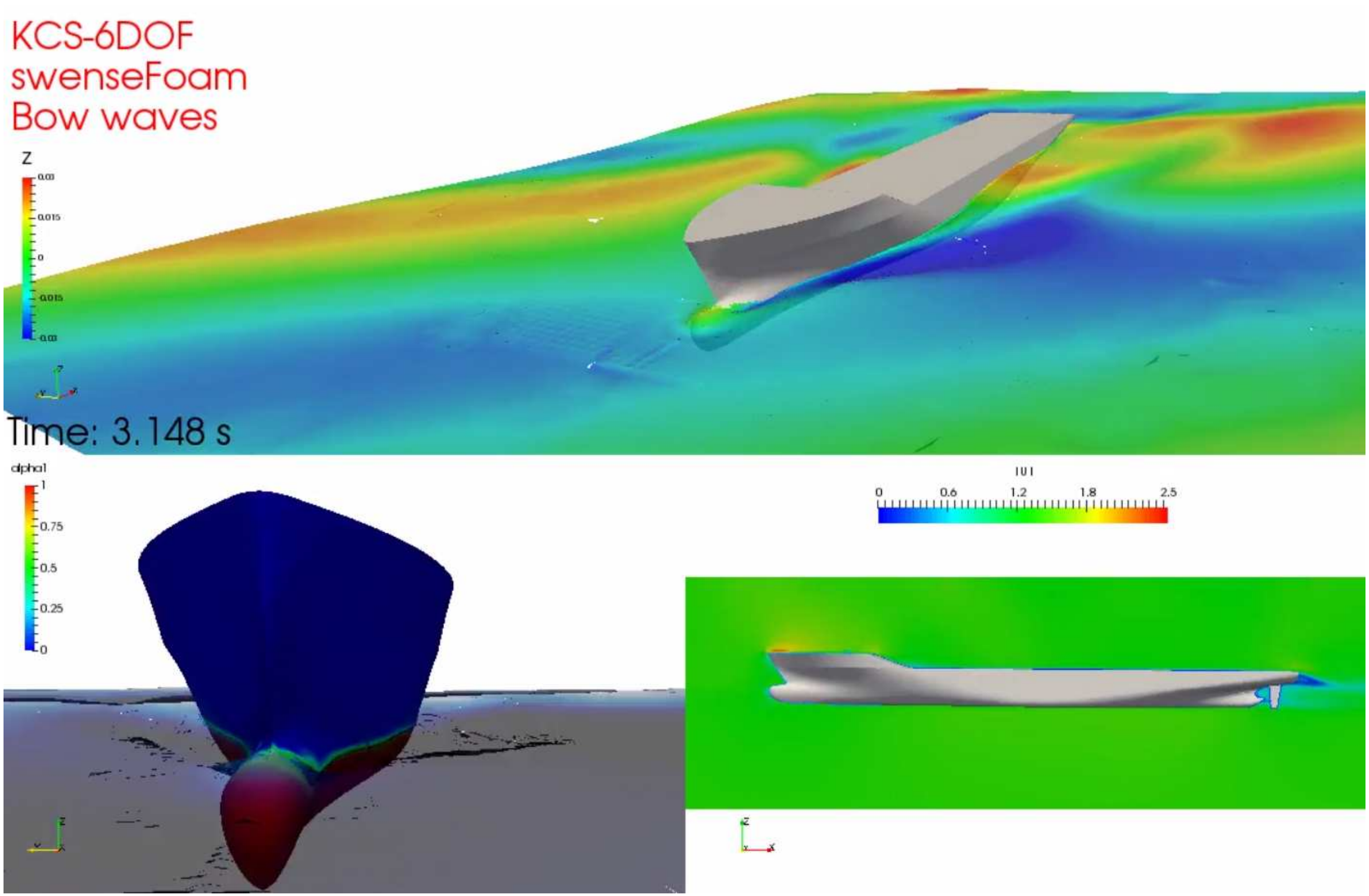

KCS 2.11–C2 seakeeping case, 45°

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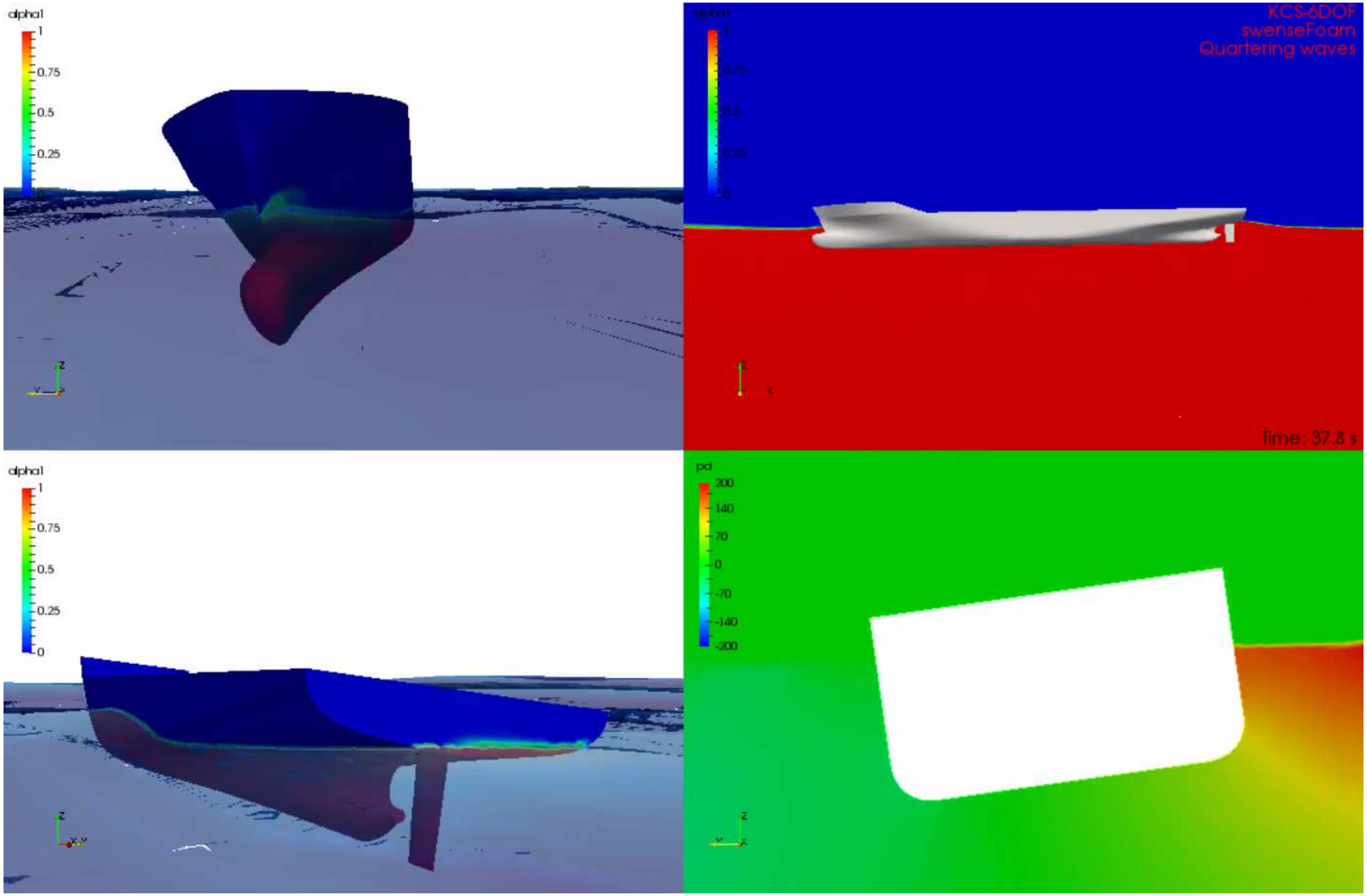

KCS 2.11–C4 seakeeping case, 135°

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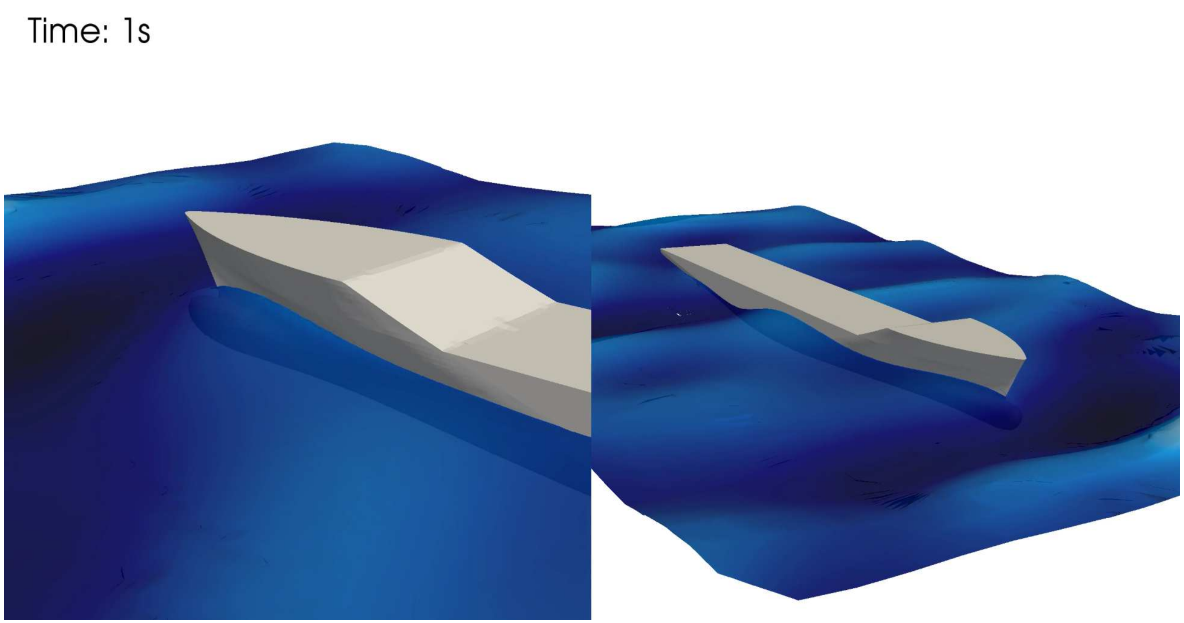
Sea-Keeping, Irregular Sea States and 2-D HOS Spectrum Freak Wave

- Combining the wave modelling and sea-keeping features in a simulation of a focused freak wave impact on a floating object: barge and full-scale KCS hull
- Freak wave has developed naturally from a 2-D spectrum without focusing
  - Long time-series simulation of potential theory HOS model
  - Screening wave elevation for a freak wave event
  - Coordinate transformation for wave impact on a floating object
  - Using HOS data to initialise CFD simulation



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Total resistance grid uncertainties for 5 cases:

1. Mean value average uncertainty 10%
2. First order harmonic uncertainties less than 3%, except for the beam waves C3 case with $U_G = 59\%$ (note: **very small response**)

Heave grid uncertainties for 5 cases:

1. Mean value uncertainties range from 2% for head waves case to 27% for the quartering waves case
2. First order harmonic uncertainties are less than 2%, except for the following waves case with $U_G = 18\%$

Roll grid uncertainties for 5 cases:

1. Mean value: 3% and 7% for bow and quartering waves, respectively
2. Mean value for beam waves is high: 63%–needs further investigation
3. First order harmonic average grid uncertainty approximately 4%.

Pitch grid uncertainties for 5 cases:

1. First order harmonic uncertainties below 2%, except for the beam waves case (very small pitch response)

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Feasibility Estimate of a Head Wave Seakeeping Study

- Performed 33 simulations in total:
  - 6 simulations for the temporal resolution study
  - 4 simulations for the hydro–mechanical coupling study
  - 7 short simulations for parallel scaling test
  - 1 performance test
  - 15 simulations for grid refinement study
- In approximately 2 weeks using 56 cores, one can get a good estimate of transfer functions at design Froude number, including numerical uncertainty assessment!
- Without uncertainty assessment, the transfer function can easily be obtained within a few days
- Note: **it is feasible** to run a 3–hour storm simulations with CFD

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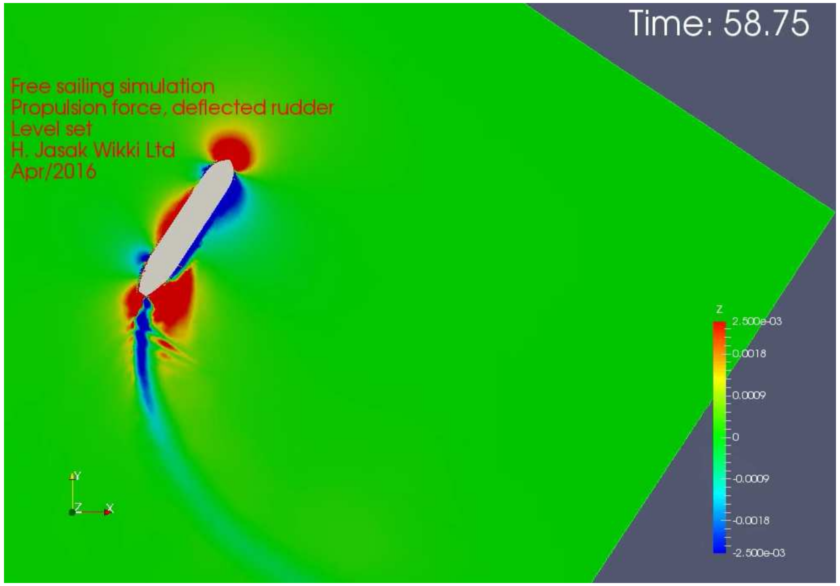
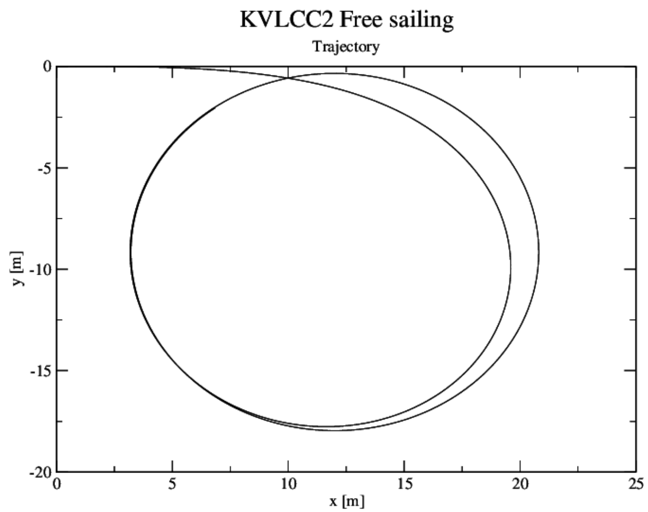
Manoeuvring Simulations: Propeller (Sail?) Modelling

- Prescribed trajectory simulations performed routinely: turning circle, zig-zag manoeuvre
- Manoeuvring validation under way: free sailing or thruster performance for global positioning for off-shore objects





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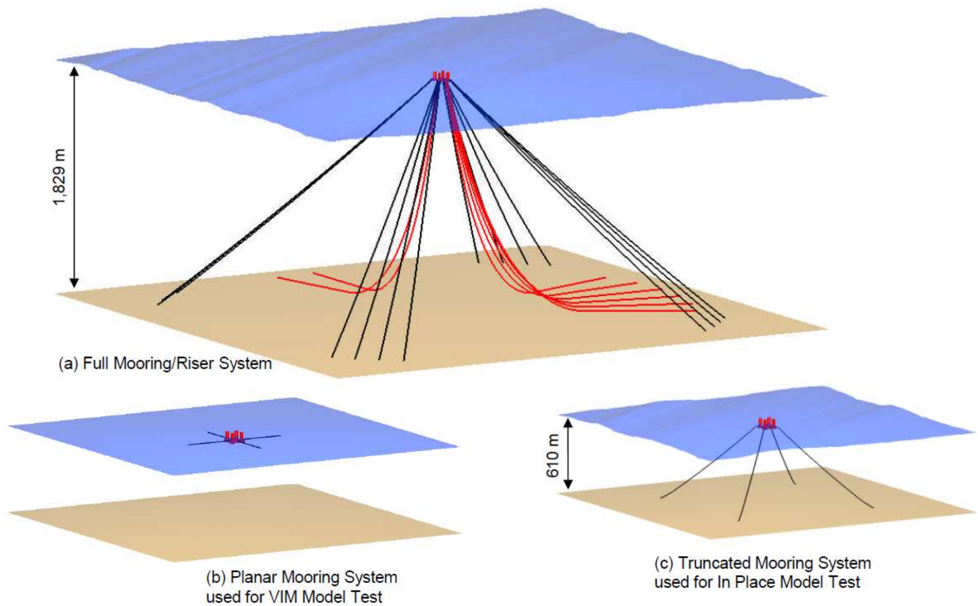
Simulation of Mooring Systems for Global Performance of Off-Shore Objects

- Mooring forces are modelled via addition of explicit force, added mass or added damping to the 6-DOF motion equation
- Currently, only simple mooring models are implemented in the Naval Hydro pack: single- and multiple-point spring damper systems. Kinematic constraints currently not handled
- **Interface to external mooring system libraries**: in collaboration with Technip and SHI: OTC 2016 paper



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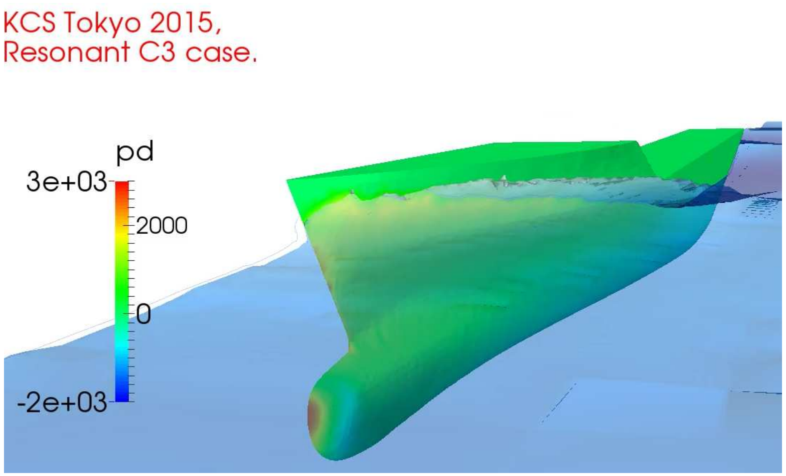
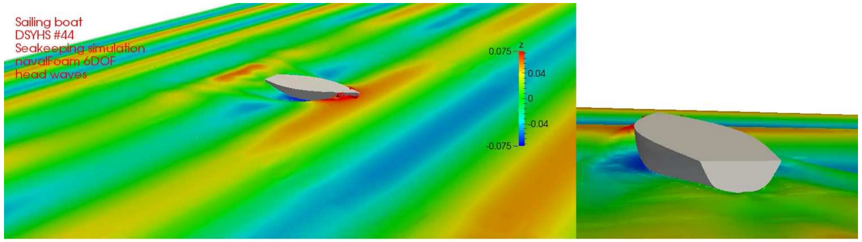
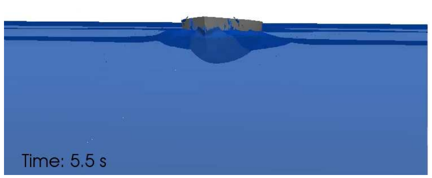
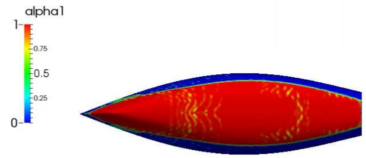
Violent Free Surface Flow Simulations

- Options on sloshing/slamming motion
  1. Static mesh with time-varying direction of gravity + acceleration
  2. Dynamic mesh: prescribed rigid body motion, either harmonic or graph-based
  3. 6-DOF motion of the hull, as a part of sea-keeping simulations: slamming occurs in hull-wave interaction, eg. resonant case
     - Solid body domain motion with CFD boundary conditions which allow "far-field" condition on the complete outside boundary
     - New feature: zonal algebraic mesh deformation around moving body









Block Matrix in OpenFOAM

Background

- OpenFOAM uses equation mimicking to perform field algebra and discretisation: **perfect for simple PDE-s or segregated solution algorithms**
- . . . but sometimes we use equation segregation inappropriately
- There exists a family of problems that cannot be solved efficiently without inter-equation coupling; some simulations "that work" can be performed 10-s or 100-s of times faster than with equivalent segregated algorithms

Objective

- Implement flexible and efficient block-coupled solution infrastructure
- Re-use all operator-based discretisation schemes, parallelisation and boundary condition tools already available in OpenFOAM
- Optimise top-level code for efficient execution and ease of assembly

Examples

- Incompressible steady pressure-velocity system (with turbulence)
- Compressible multi-phase free surface simulations: under-water explosions

Block Matrix in OpenFOAM

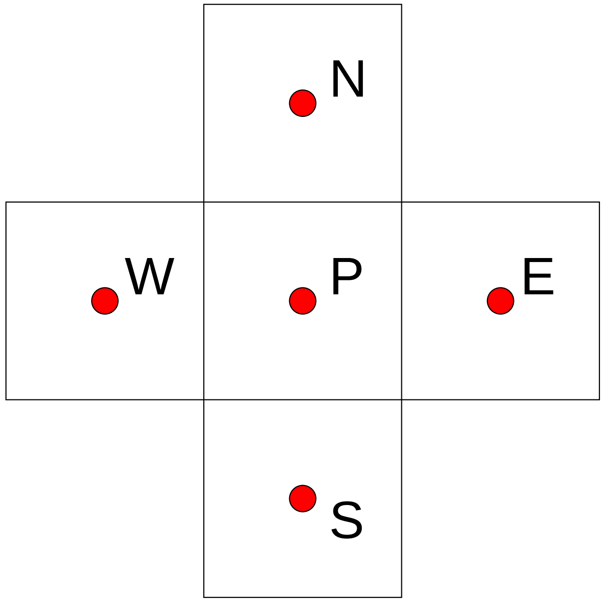
Block-Coupled Solution Algorithms

- For cases of strong coupling between the components of a vector, the components can be solved as a **block variable**: (u_x, u_y, u_z) will appear as variables in the same linear system
- In spite of the fact that the system is much larger, the coupling pattern still exists: components of $\mathbf{u}$ in cell P may be coupled to other components in the same point or to vector components in the neighbouring cell
- With this in mind, we can still keep the sparse addressing defined by the mesh: if a variable is a vector, a tensorial diagonal coefficients couples the vector components in the same cell. A tensorial off-diagonal coefficient couples the components of $\mathbf{u}_P$ to all components of $\mathbf{u}_N$, which covers all possibilities
- For **multi-variable block solution** like the compressible Navier-Stokes system above, the same trick is used: the cell variable consists of $(\rho, \rho\mathbf{u}, \rho E)$ and the coupling can be coupled by a 5×5 matrix coefficient
- Important disadvantages of a block coupled system are
    - Large linear system: several variables are handled together
    - Different kinds of physics can be present, *e.g.* the transport-dominated momentum equation and elliptic pressure equation. At matrix level, it is impossible to separate them, which makes the system more difficult to solve

Block Matrix in OpenFOAM

Matrix Connectivity and Mesh Structure

- Irrespective of the level of coupling, the FVM dictates that a cell value will depend only on values in surrounding cells



- We still have freedom to organise the matrix by ordering entries for various components of the solution variable x
- Global sparseness pattern related to mesh connectivity: easier coefficient assembly

Block Matrix in OpenFOAM

Coupling Coefficient

- Matrix implemented with **block coefficients**
- Consider general linear dependence between two vectors $\mathbf{m}$ and $\mathbf{n}$

$$\mathbf{m} = \mathbf{A}\,\mathbf{b}$$

- Component-wise coupling describes the case where m_x depends only on n_x, m_y on n_y and m_z on n_z
  1. Scalar component-wise coupling
  2. Vector component-wise coupling
  3. Full (block) coupling
- Explicit methods do not feature here because it is not necessary to express them in terms of matrix coefficients
- For reference, the linear equation for each cell featuring in the matrix reads

$$\mathbf{A}_P \mathbf{m}_P + \sum_N \mathbf{A}_N \mathbf{m}_N = \mathbf{R}$$

Coupled p-U Solver

Turbulent Steady Incompressible Flows: SIMPLE or Coupled System

- Equation set contains linear p-U and non-linear U-U coupling

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla\bullet(\mathbf{u}\mathbf{u}) - \nabla\bullet\left(\nu\nabla\mathbf{u}\right) = -\nabla p$$

$$\nabla\bullet\mathbf{u} = 0$$

- Traditionally, this equation set is solved using the **segregated SIMPLE algorithm**
  - Low memory peak: solution + single scalar matrix in peak storage
  - p-U coupling is handled explicitly: loss of convergence (under-relaxation)
  - Number of iterations is substantial; not only due to non-linearity
  - Convergence dependent on mesh size: SIMPLE slows down on large meshes
- **Block-implicit p-U coupled solution**
  - Coupled solution significantly increases matrix size: 4 blocks instead of 1
  - . . . but the linear p-U coupling is fully implicit!
  - Iteration sequence only needed to handle the non-linearity in the U-equation
  - Net result: **significant convergence improvement** (steady or transient) at a cost of increase in memory usage: **reasonable performance compromise!**

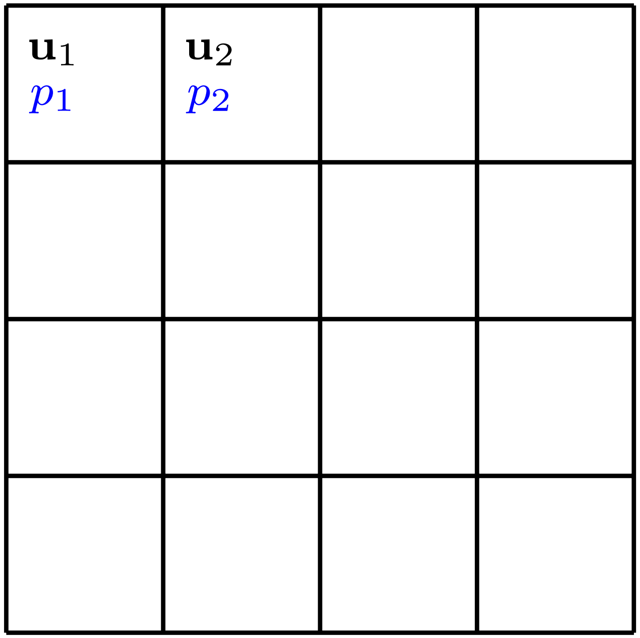
Coupled p-U Solver

SIMPLE-Based Segregated p-U Solver

```
// Momentum equation assembly and solution
fvVectorMatrix UEqn
(
    fvm::div(phi, U)
  + turbulence->divDevReff(U)
);
UEqn.relax();
solve(UEqn == -fvc::grad(p));

// Pressure equation assembly and solution
U = UEqn().H()/UEqn.A();
phi = fvc::interpolate(U) & mesh.Sf();
fvScalarMatrix pEqn
(
    fvm::laplacian(1/UEqn.A(), p) == fvc::div(phi)
);
pEqn.solve();
phi -= pEqn.flux();
p.relax();
```

Block Matrix in OpenFOAM

Block-Coupled $\mathbf{u} - p$ System Matrix Structure



$$
\begin{bmatrix}
\begin{pmatrix} a_{P\,(\mathbf{u}\,\mathbf{u})} & a_{P\,(\mathbf{u}\,p)} \\ a_{P\,(p\,\mathbf{u})} & a_{P\,(p\,p)} \end{pmatrix} & \begin{pmatrix} a_{N\,(\mathbf{u}\,\mathbf{u})} & a_{N\,(\mathbf{u}\,p)} \\ a_{N\,(p\,\mathbf{u})} & a_{N\,(p\,p)} \end{pmatrix} & \dots \\
. & \begin{pmatrix} a_{P\,(\mathbf{u}\,\mathbf{u})} & a_{P\,(\mathbf{u}\,p)} \\ a_{P\,(p\,\mathbf{u})} & a_{P\,(p\,p)} \end{pmatrix} & \dots \\
\vdots & \vdots & \ddots
\end{bmatrix}
\begin{bmatrix} \mathbf{u}_1 \\ p_1 \\ \mathbf{u}_2 \\ p_2 \\ \vdots \end{bmatrix}
=
\begin{bmatrix} b_{\mathbf{u}\,1} \\ b_{p\,1} \\ b_{\mathbf{u}\,2} \\ b_{p\,2} \\ \vdots \end{bmatrix}
$$

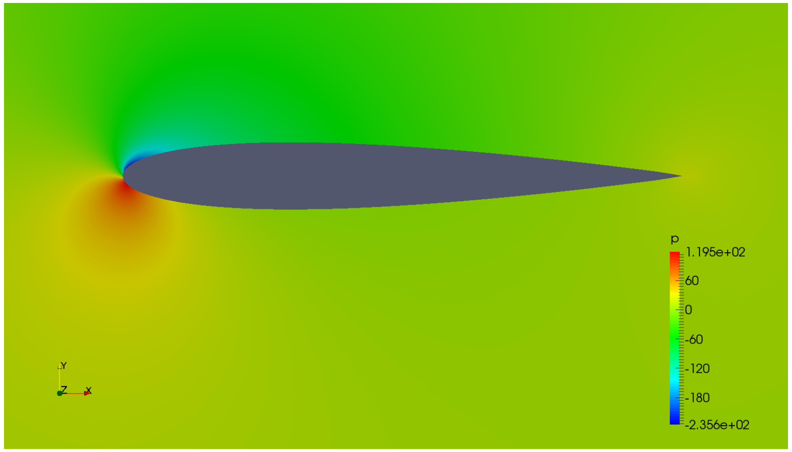
Coupled p-U Solver

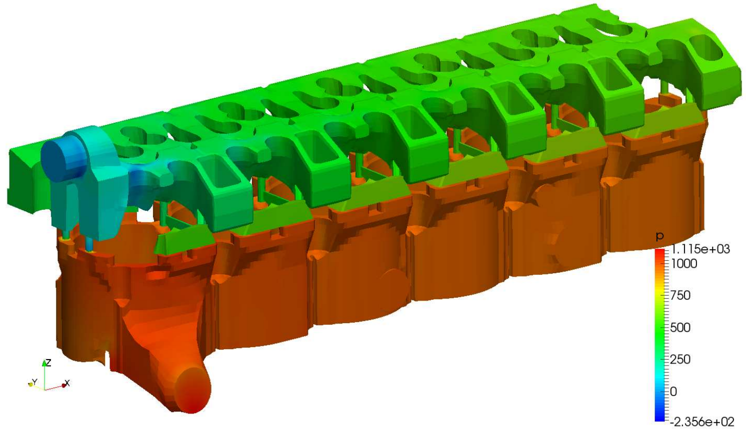
Coupled Implicit p-U Solver: Source Code

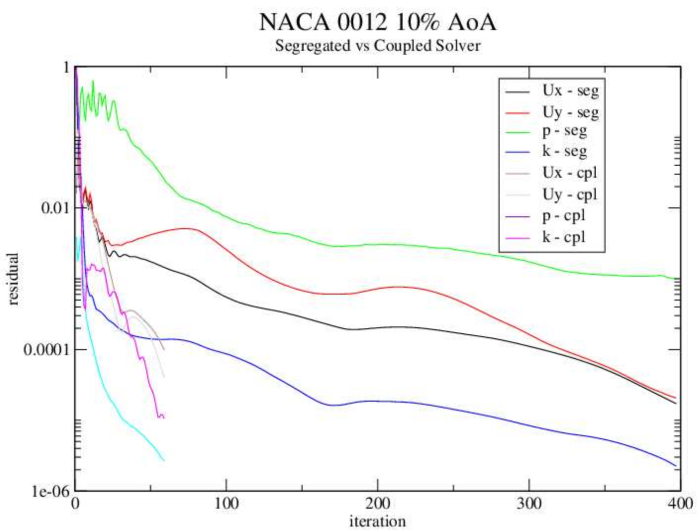
```
fvVectorMatrix UEqn
(
    fvm::div(phi, U)
  + turbulence->divDevReff(U)
);
fvScalarMatrix pEqn
(
   - fvm::laplacian(rUAf, p) == -fvc::div(fvc::grad(p))
);
blockVectorSystem pInU(fvm::grad(p));
blockVectorSystem UInp(fvm::div(U));

BlockLduMatrix<vector4> A(mesh);
blockMatrixTools::insertEquation(0, UEqn, A, x, b);
blockMatrixTools::insertEquation(3, pEqn, A, x, b);
blockMatrixTools::insertBlockCoupling(3, 0, UInp, U, A, b, false);
blockMatrixTools::insertBlockCoupling(0, 3, pInU, p, A, b, true);

BlockLduSolver<vector4>::New("Up", A, dict)->solve(Up, b);
blockMatrixTools::retrieveSolution(0, U.internalField(), Up);
blockMatrixTools::retrieveSolution(3, p.internalField(), Up);
```

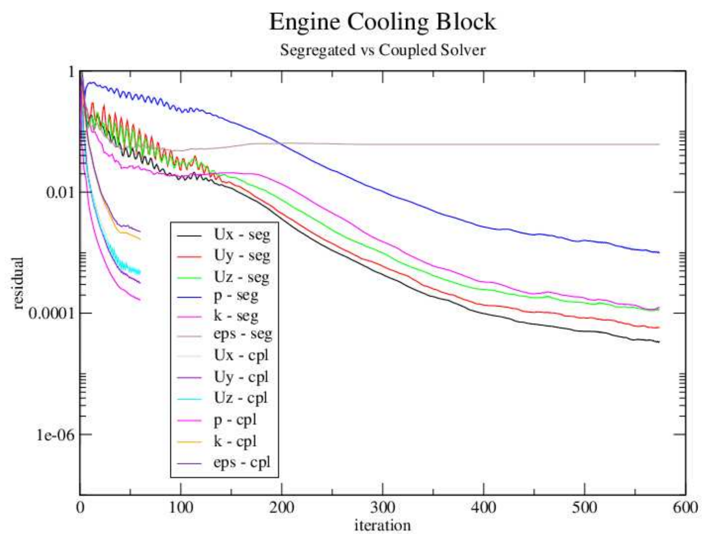
Coupled p-U Solver

Performance Improvements of the Coupled p-U Solver: Speed and Robustness



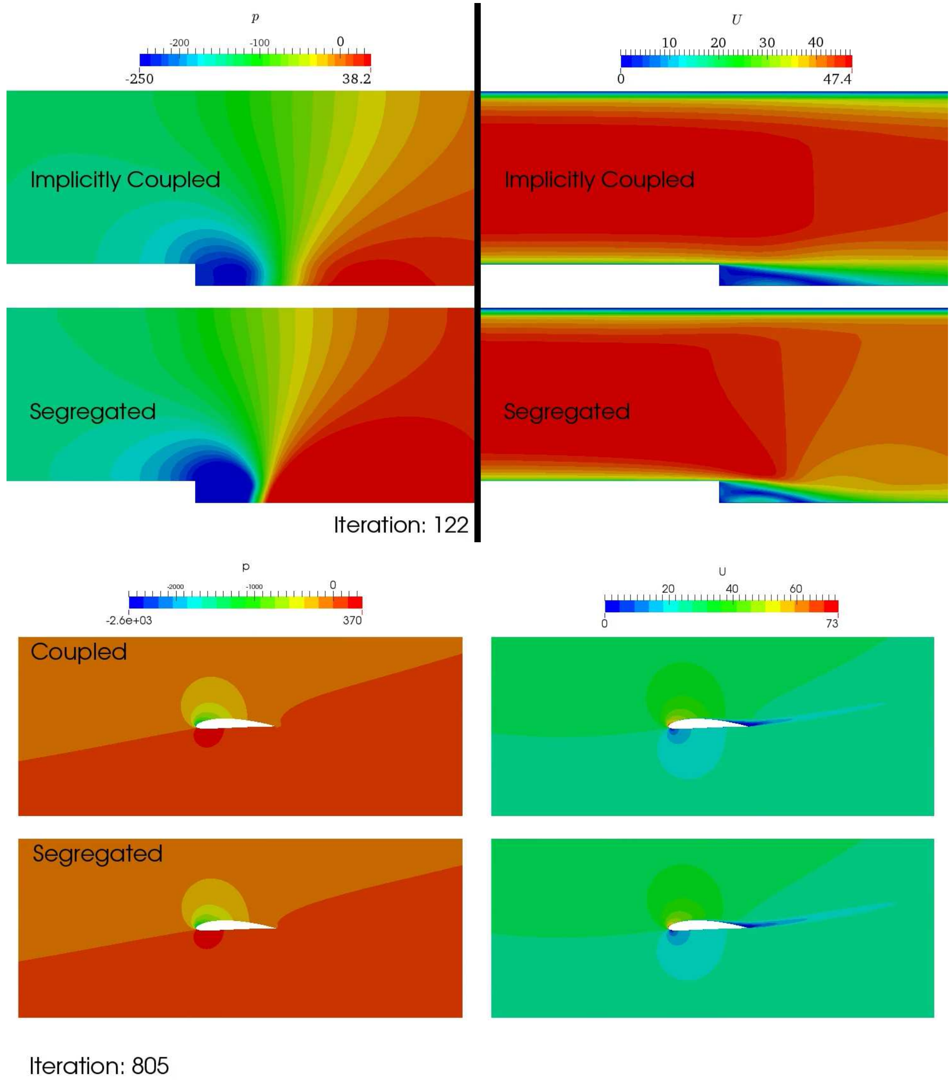






Coupled p-U Solver

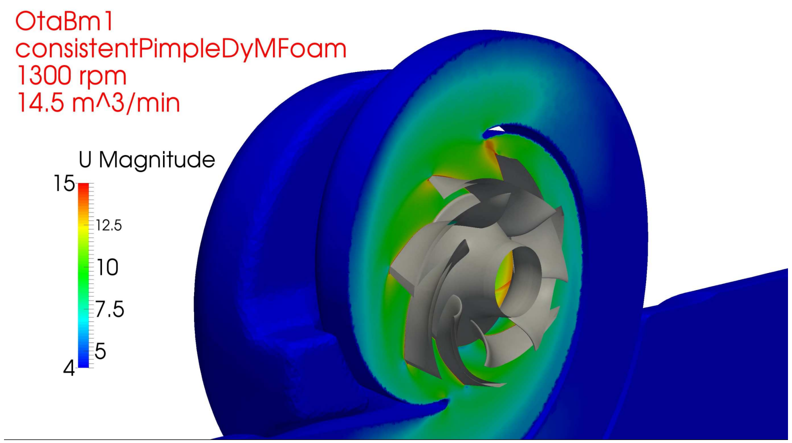
Performance Improvements of the Coupled p-U Solver: Speed and Robustness

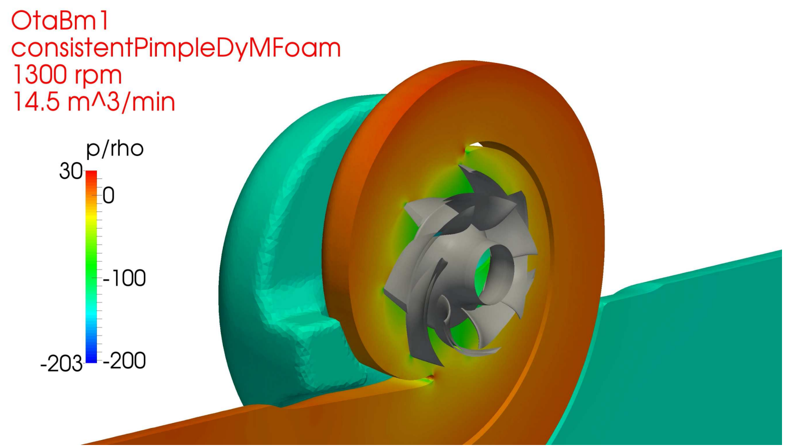


Coupled p-U Solver

Performance Improvements and Extensions in the Coupled p-U Solver

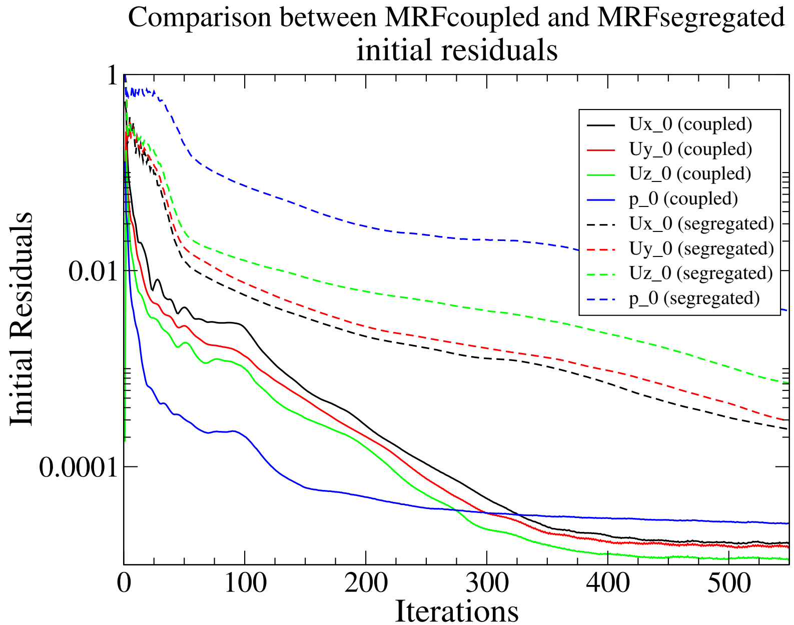
- Improvements in performance for the coupled solver: consistency, numerics
- Extension to compressible flows, MRF and porous media (implicit!)
- Major performance jump: block-coupled AMG with additive correction (Hutchinson 1988)
- **Block-coupled $k-\epsilon$ and $k-\omega$ SST turbulence models**
  - Turbulence equations solved in a single block-coupled system
  - Analysis of source terms to establish favourable cross-equation coupling
  - Implemented in Diploma Thesis assignment: Robert Keser, Uni Zagreb
- Example: steady (MRF) and transient centrifugal pump

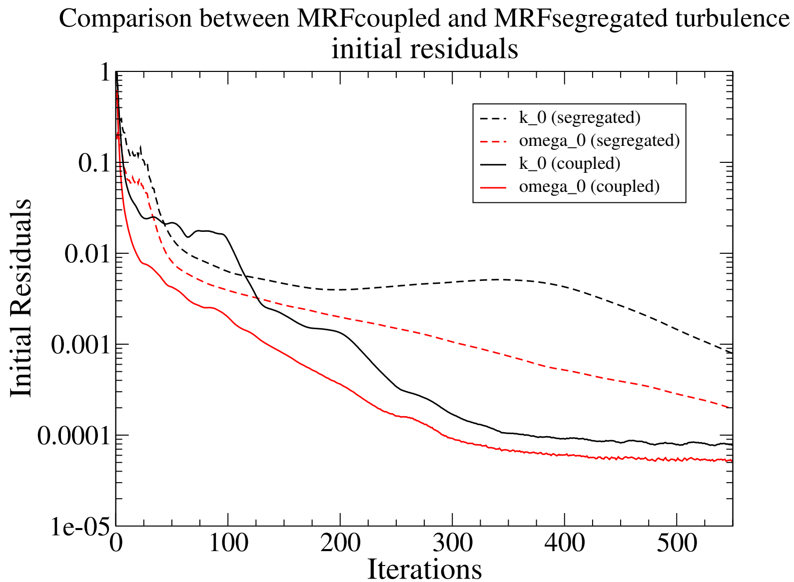


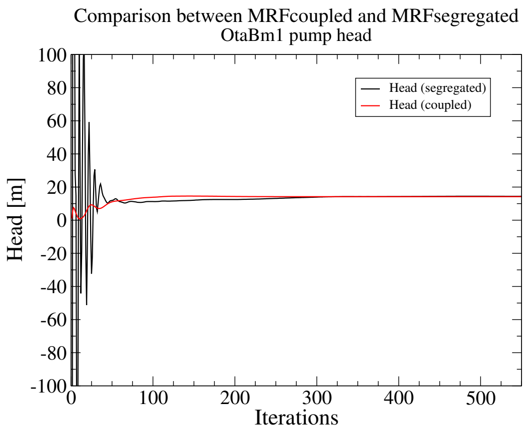


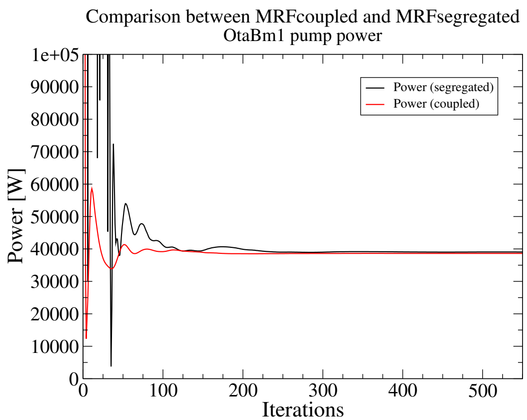
Coupled p-U Solver

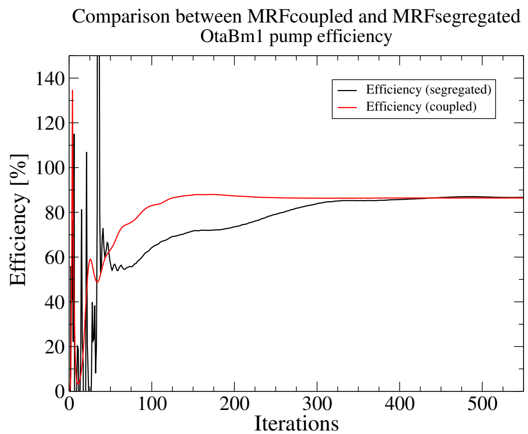
Performance Improvements and Extensions in the Coupled p-U Solver











Coupled Solution

Coupled Solution Algorithms: Consequences

- Coupled algorithms are still used rarely because of code complexity and guidance on “appropriate coupling formulation”: **problem solved**
- NUMAP-FOAM Summer School 2016: Dominated by projects on coupled implicit solution for complex non-linear problems
  - Coupled eddy viscosity turbulence models
  - Coupled visco-elasto-plastic rheology solver (double Rhie-Chow)
  - Coupled poly-dispersed multi-phase DQ-MOM solver: moment equation
  - Coupled lift/drag terms in multi-phase momentum equations
  - Coupled solid mechanics: better non-linear convergence
  - Coupled Finite-Volume to Finite Area solver: cracking porous media
- There are many more problems where linearised implicit inter-equation coupling may prove a game-changer: accelerated convergence, increased robustness, improved

New Solution Algorithms

Expanding the Horizons: Spectral Modelling of Time-Periodic Flows

- Many CFD problems involve temporally periodic flows
  - Flows induced by periodic boundary condition
  - Flows with periodically moving objects
  - Wave-like phenomena
- To remove irregular start-up unsteadiness, a number of periods is simulated: expensive, complicated – periodic uncertainty issues

Harmonic Balance Method: **n coupled quasi-steady coupled equations**

- Variables are developed into Fourier series in time with n-harmonics and substituted into transport equation independently for each computational point
- Example: Harmonic Balance scalar equation set

$$\nabla \bullet (\mathbf{u} \mathsf{Q}_{t_\mathrm{j}}) - \nabla \bullet (\gamma \nabla \mathsf{Q}_{t_\mathrm{j}}) = -\frac{2\omega}{2n+1} \left(\sum_{i=1}^{2n} \mathsf{P}_{(\mathrm{i}-\mathrm{j})} \mathsf{Q}_{t_i} \right)$$

$$\mathsf{P}_i = \sum_{k=1}^{n} k \sin(k \omega i \Delta t), \qquad \text{for} \quad i = \{1{,}2n\}.$$

New Solution Algorithms

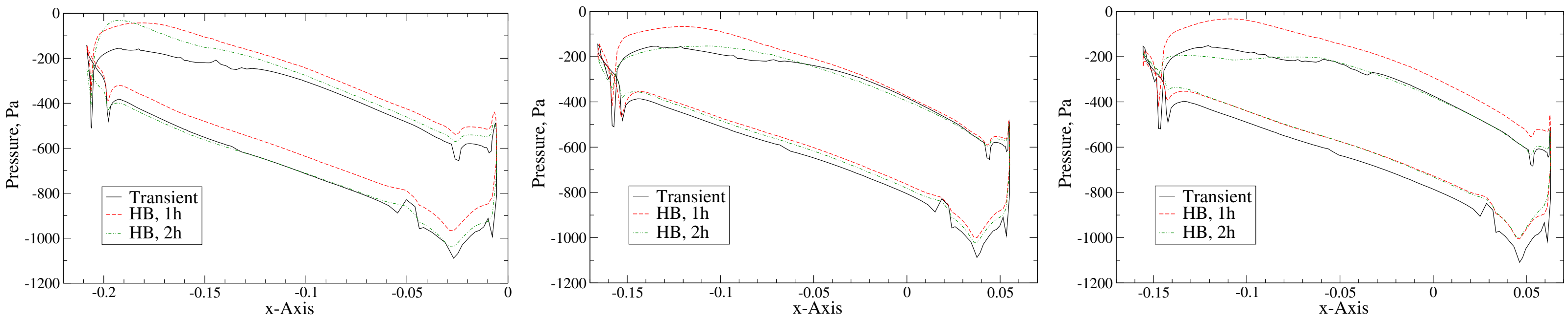
Harmonic Balance Solver: ERCOFTAC Centrifugal Pump

- Validation of harmonic balance in turbulent incompressible periodic flow
- HB simulations performed using 1 and 2 harmonics: rotor and stator blade count
- Results compared against full transient simulation: excellent agreement
  - **Integral properties: typical error of 2%**
  - **Local solution features: pressure on surface in time**
  - **Mode and nature of flow instability**
- Results are **significantly better than expected!**
- Substantial reduction in simulation time:
  - Intel Core i5-3570K, 3.4 GHz computer with 16 GB memory
  - Transient run needs approx. 50 blade passages to become quasi-periodic

	Transient	HB, 1 h	HB, 2 h
Simulation time	5 hrs/rotation	52 mins	78 mins
Iterations	600, dt = 5e-5 s 1 rotation = 0.03 s	3000	2400

New Solution Algorithms

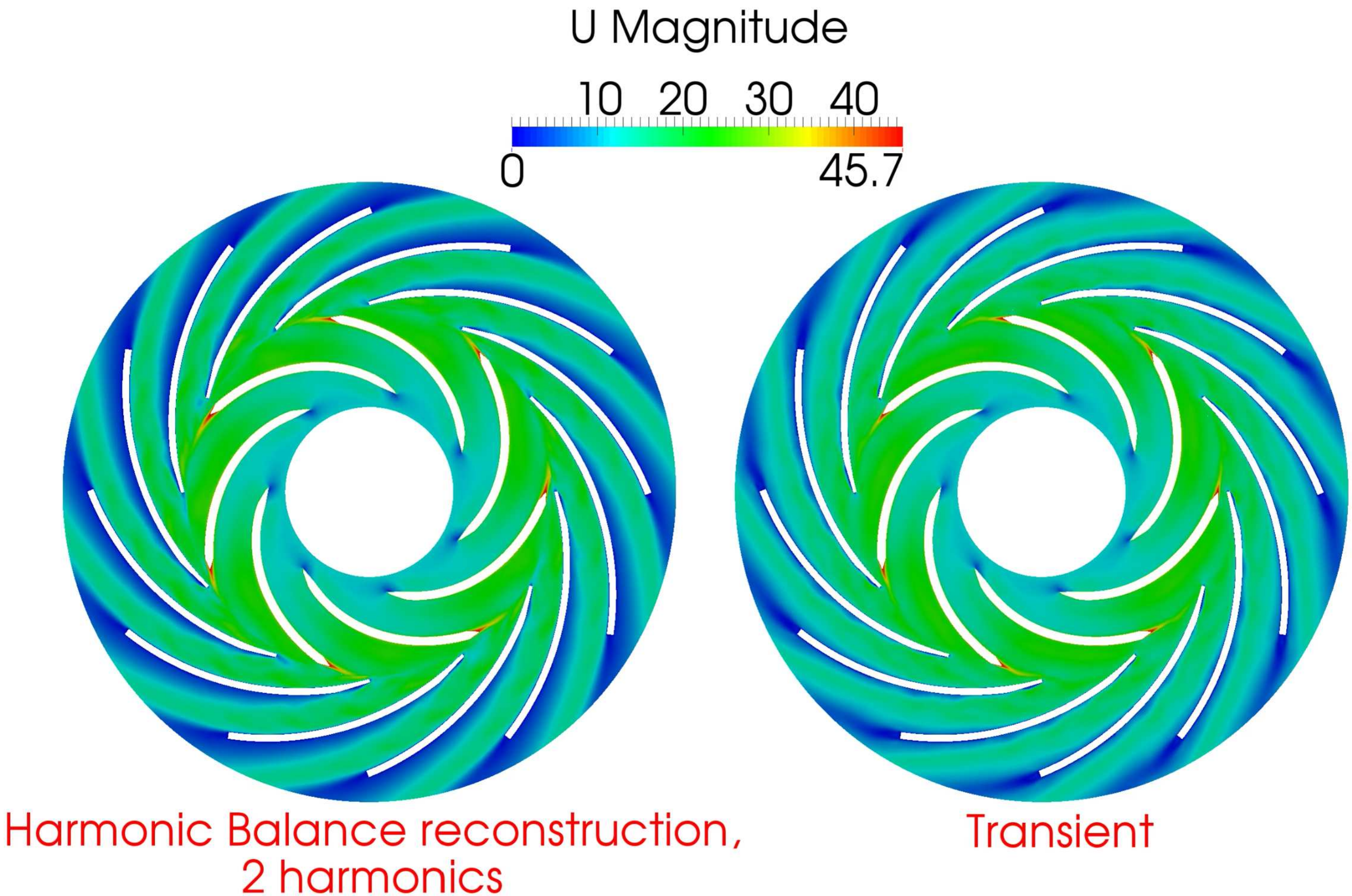
Harmonic Balance Solver: ERCOFTAC Centrifugal Pump



		Transient	HB, 1h	err, %	HB, 2h	err, %	MRF	err, %
$t = \frac{T}{3}$	Efficiency	89.72	88.80	1.0	89.76	0.0	89.65	0.07
	Head	81.48	81.80	0.4	80.45	1.3	84.12	3.14
	Torque	0.0297	0.0302	1.7	0.0294	0.9	0.0308	3.57
$t = \frac{2T}{3}$	Efficiency	89.92	88.78	1.3	89.81	0.1		
	Head	81.48	81.85	0.4	80.6	1.1		
	Torque	0.0296	0.0302	2.0	0.0295	0.4		
$t = T$	Efficiency	89.83	88.85	1.1	89.71	0.1		
	Head	81.49	81.79	0.4	80.39	1.3		
	Torque	0.0297	0.0302	1.6	0.0294	1.0		

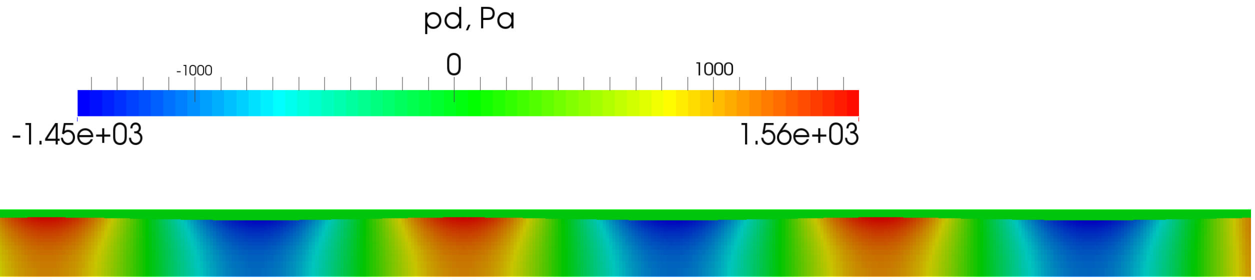
New Solution Algorithms

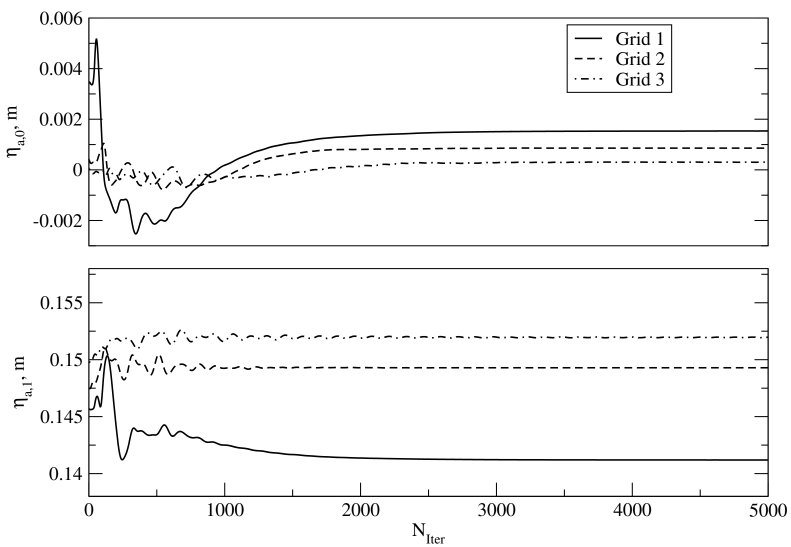
Harmonic Balance Solver: ERCOFTAC Centrifugal Pump



New Solution Algorithms

Harmonic Balance Solver: Periodic Two-phase Surface Flow





New Solution Algorithms

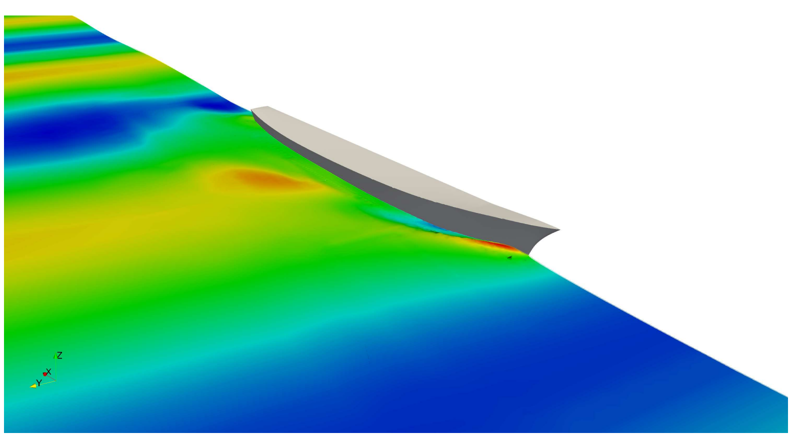
Harmonic Balance Solver: Periodic Two-phase Surface Flow

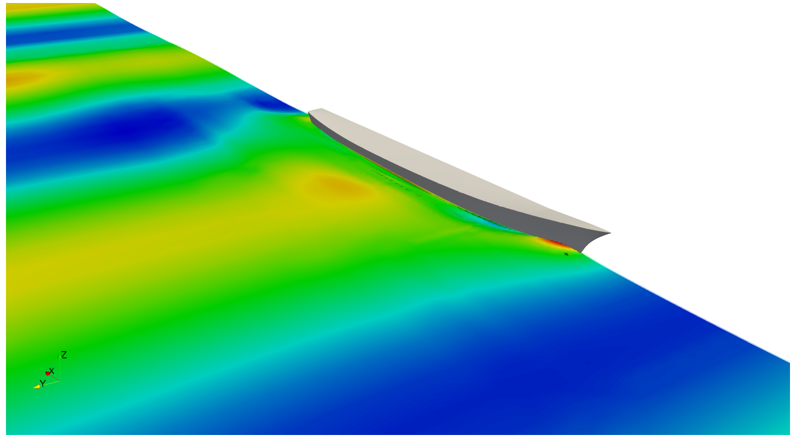
- Zeroth and 1th order harmonic amplitudes of the free surface with iterative uncertainty obtained with different spectral resolution

No. Harmonics	$\eta_{a,0}$, m	$\eta_{a,1}$, m	$U_{I,0}$, %	$U_{I,1}$, %	ϵ_0, m	ϵ_1, %
1	0.001898	0.1531	0.5962	0.03494	-0.0006	-0.328
2	0.000302	0.1520	0.9360	0.01349	0.0010	0.393
3	0.000411	0.1519	0.3916	0.01975	0.0009	0.459
4	0.000394	0.1518	0.1845	0.00099	0.0009	0.524
5	0.000352	0.1517	0.1215	0.00033	0.0009	0.590
6	0.000438	0.1517	0.1651	0.00033	0.0009	0.590
7	0.000337	0.1516	0.1386	0.00033	0.0010	0.655
8	0.000332	0.1516	0.1008	0.00033	0.0010	0.655

New Solution Algorithms

Harmonic Balance Solver: DTMB Ship on Waves



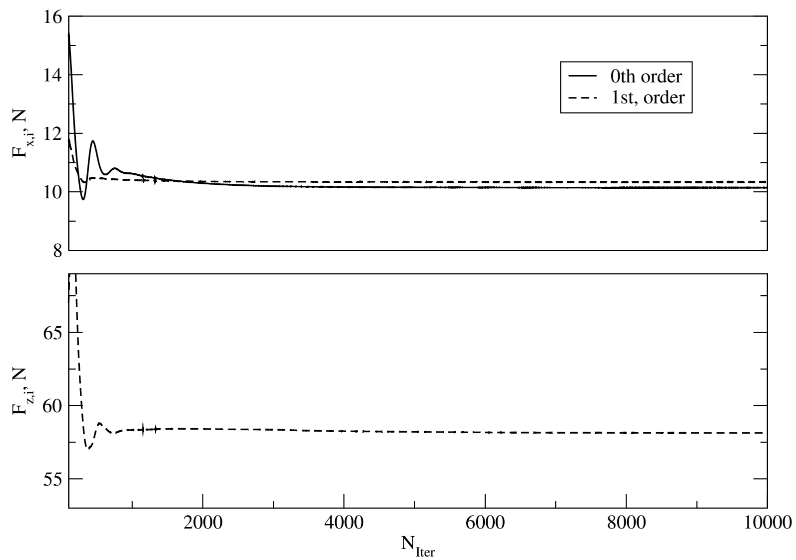


- Ship model parameters: $L = 3.05$ m
- Froude number: $F_r = 0.28$, $U = 1.52$ m/s
- Wave parameters: $H = 0.036$ m, $T = 1.09$ s, $\lambda = 4.57$ m
- 2 harmonics are used in the HB simulation
- 200 time steps per encounter wave period are used in the transient simulation

New Solution Algorithms

Harmonic Balance Solver: DTMB Ship on Waves

- Convergence of longitudinal and vertical force harmonics

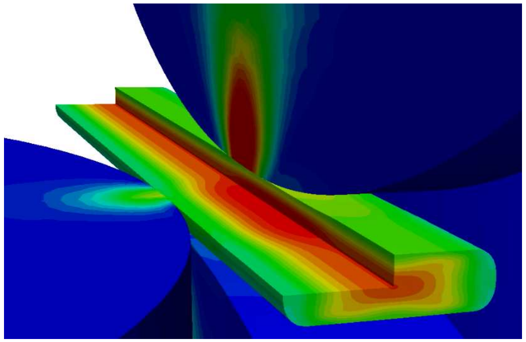


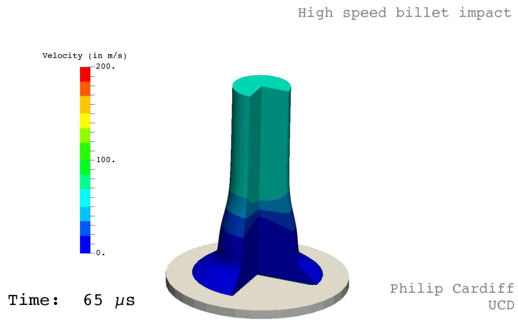
Item	Transient	Harmonic Balance	ε, %
$F_{x,0}$, N	9.20	10.14	-10.2
$F_{x,1}$, N	10.70	10.34	3.36
$F_{z,0}$, N	784.88	785.72	-0.11
$F_{z,1}$, N	62.63	58.14	7.17

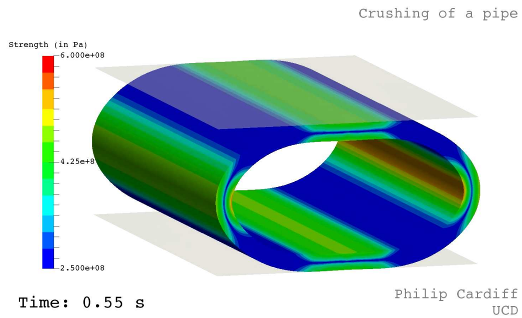
Complex Physics Models

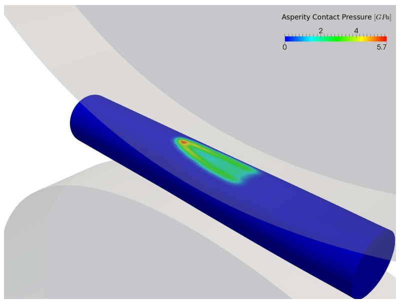
Non-Linear Solid Mechanics Simulations

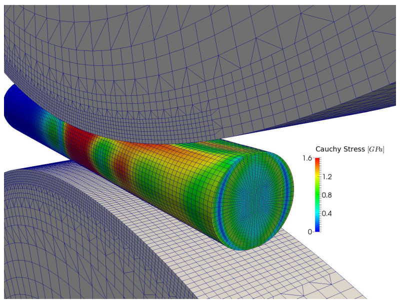
- Geometric and material non-linearity, large deformation, modelling of contact (linear and non-linear) with complex friction models
- Textbook example of practical collaborative development: academia + industry
- New generation of mixed mode lubricated contact modelling

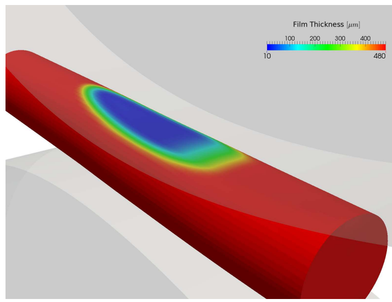


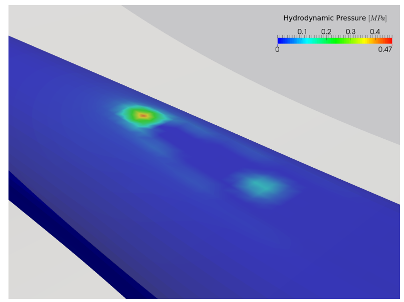








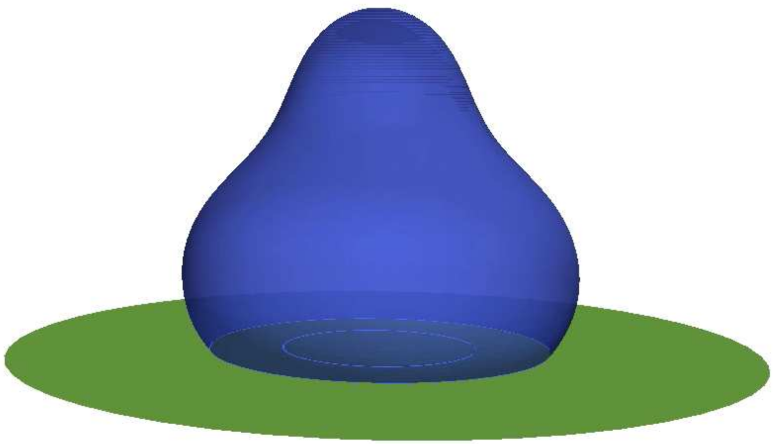


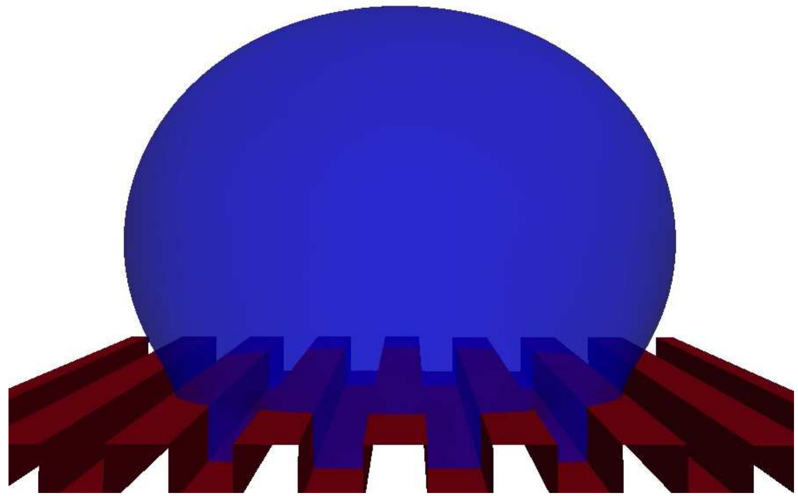


Complex Physics Models

Complex Physics of Wetting Processes: TU Darmstadt

- Modelling of interaction of individual droplets and complex surfaces
- Free surface is modelled using interface capturing and interface tracking models
- Stabilisation library for visco-elastic rheology at extreme Weissenberg numbers
- Excellent example of building research on top of existing capabilities





Summary

Summary

- CFD 2020 is moving beyond general-purpose CFD products and “universal solution providers”
- Outlook: Vertically integrated problem-specific applications
  - Application-specific extensions to complete the modelling
  - User interface speaking language of the application
- Strict requirements on solution accuracy and uncertainty; guidance on mesh resolution, discretisation settings, choice of physical models
- Practical use requires automated or script-driven tools with turn-around time below 8 hours
- **Validation and verification** effort is the major challenge!
- Open Source libraries are a natural baseline for such environment: low-level CFD discretisation is re-used across the board
- Handling complex physics brings CFD closer to the user requirements: new algorithms, execution environments and multi-scale modelling data exchange