Initial and Boundary Conditions for Viscous-Flow Problems

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Why are ICs and BCs needed?

- Solutions to ODEs are usually not unique (integration constants exist), which is also a problem for PDE’s.
- PDE’s are usually specified through a set of ICs and BCs.
- A BC expresses the behavior of a function on the boundary of the domain. An IC specifies the value of the function in time direction, at time $t = 0.0$.
- The GDEs to be discussed next constitute an IBVP for a system of 2nd order nonlinear PDE, which require IC and BC for their solutions, depending on physical problem and appropriate approximations.
Initial Conditions

- Initial conditions (ICS, steady/unsteady flows)
  - ICs should not affect final results and only affect convergence path, i.e. number of iterations (steady) or time steps (unsteady) need to reach converged solutions.
  - More reasonable guess can speed up the convergence
  - For complicated unsteady flow problems, CFD codes are usually run in the steady mode for a few iterations for getting a better initial conditions
Boundary Conditions

Types of BCs: can be defined/categorized mathematically, physically, and numerically.

- **Mathematical definitions**

<table>
<thead>
<tr>
<th>Name</th>
<th>Form</th>
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<tbody>
<tr>
<td>Dirichlet</td>
<td>$\phi = f$</td>
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<tr>
<td>Neumann</td>
<td>$\frac{\partial \phi}{\partial n} = f$</td>
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<td>Robin</td>
<td>$C_0 \phi + C_1 \frac{\partial \phi}{\partial n} = f$</td>
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<tr>
<td>Mixed</td>
<td>$\phi = f$, $C_0 \phi + C_1 \frac{\partial \phi}{\partial n} = f$</td>
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<tr>
<td>Cauchy</td>
<td>$\phi = f$ and $C_0 \frac{\partial \phi}{\partial n} = g$</td>
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- **For flow variables**
  - Kinematic BCs: motion without regard for the cause
  - Dynamic BCs: the causes of motion
Boundary Conditions

• Physical domain boundaries:
  - Solid Surface
    - Fixed, moving wall, Deforming wall, FSI
    - Permeable Interface, Porous Surface
  - Free Surface, Wave Boundary
  - Two-Phase Interface Internal Jump conditions
  - Inlet/exit/outer
  - Fairfield/Open

![Diagram of boundary conditions with labels for x/H, z/H, Slip Wall, Jump Conditions, Non-slip Wall, Inlet, and Outlet.]
Boundary Conditions

• For grid and numerical treatment:
  - Symmetric BC
  - Periodic BC
  - Numerical beach, absorbing BC
  - Multiblock/Overset overlapping grid BC
  - Convection BC
  - Pole BC (singularity)
  - Global mass conservation enforcing BC

Overset and patched multiblock grids for airfoil.
Examples of Boundary conditions

1. Solid Surface
   - Fixed, moving wall
   - Permeable interface, porous surface
   - Deforming wall, FSI

2. Single phase flows: Free surface BCs

3. Multiphase flows: Two-phase interface jump conditions

4. Inlet/exit/outer

Pipe flow with no-slip (A) and slip (B) boundary conditions. (Berg et al., 2021).

Free surface flow: droplet

Two-phase interfacial flow: bubble
Examples of Boundary conditions

1. Solid Surface

**No-slip BCs:** No-slip BC widely used for most macroscopic flows without loss of accuracy

- \( \ell = \text{mean free path of a moving molecular particle} \ll \text{fluid motion}; \) therefore, macroscopic view is “no slip” condition, i.e. no relative motion or temperature difference between liquid and solid.

\[
\begin{align*}
\underline{V_{\text{liquid}}} &= \underline{V_{\text{solid}}} \\
T_{\text{liquid}} &= T_{\text{solid}}
\end{align*}
\]

- Exception for gas and contact line problem

---

Smooth wall:
Specular reflection
Conservation of tangential momentum
\( u_w = 0 = \text{fluid velocity at wall} \)

Rough wall:
Diffuse reflection. Lack of reflected tangential momentum balanced by \( u_w \)
Examples of Boundary conditions

**Slip-wall BCs:**

\[
\tau_w = \mu \left( \frac{du}{dy} \right)_w \\
1 = \frac{\mu}{\frac{2}{3} \rho a} \\
u_w = \frac{3 \mu \tau_w}{2 \rho a \mu} \\
Ma = \frac{U}{a} \\
Cf = \frac{\tau_w}{\frac{1}{2} \rho U^2}
\]

\[
u_w / U = 0.75 Ma \ C_f
\]

High Re:

\[C_f \sim 0.005 \quad \text{Say} \ Ma \sim 20 \quad \Rightarrow \quad \frac{u_w}{U} < 0.01\]

Low Re:

\[C_f \sim 0.6 Re_x^{1/2} \quad Re_x = Ux/\nu\]

\[
u_w / U = \frac{0.4 Ma}{Re_x^{1/2}}
\]

Significant slip possible at low Re, high Ma: “Hypersonic LE Problem”

**Similar for T:**

High Re:

\[T_{gas} = T_w\]

Low Re:

\[
\frac{T_{gas} - T_w}{(T_r - T_w)} = 0.87 Ma \ C_f
\]

Ref. T

Air
Examples of Boundary conditions

Contact line problem:

• No-slip BCs used for most macroscopic flows without loss of accuracy but pose a problem in viscous flows at contact lines.

• For small scale flows, slip BC with a finite slip length is usually used: $u_0 = b \left| \frac{\partial u}{\partial y} \right|$. The contact line movement is also dependent to the contact angle, but the mechanism is not fully understood.

• For large scale flows with high Reynolds numbers, very small grid spacing is usually used near the wall in order to resolve the boundary layer.

• In CFDSHIP-Iowa, a blanking distance ($b$) is used for the interface functions, which is chosen based on the $y^+$. The recommended value is $y^+ > 30$ (outside of the turbulence buffer region), and $y^+ = 100$ is usually used for most simulations of ship flows according to the numerical experiments.
Examples of Boundary conditions

Permeable interface, porous surface:

**Suction or Injection**

\[ u = 0, \text{no slip} \]

\[ v = v_s \text{ or } v = v_i, \text{flow through the wall} \]

\[ T_{\text{fluid}} = T_{\text{wall}}, \text{no temperature jump} \]

\[ q_w = hT_y|_w = \rho_i v_i c_p (T_w - T_i), \text{energy at the wall} \]
Examples of Boundary conditions

Fluid Structure Interaction (FSI) BCs:

Kinematic continuity between the fluid and the structure is ensured by the non-slip wall condition:

\[ \mathbf{u}_w = \frac{\partial \mathbf{x}}{\partial t}, \mathbf{v}_w = \frac{\partial \mathbf{y}}{\partial t}, \mathbf{w}_w = \frac{\partial \mathbf{z}}{\partial t} \]

where \( \mathbf{u}_w = \{u_w, v_w, w_w\} \) is the velocity of the fluid particle and \( \mathbf{x} = \{x, y, z\} \) are the coordinates of the solid wall. The continuity of the momentum is ensured by the continuity of the stress across the fluid-structure interface:

\[ \tau_{ij} \cdot n_i|_w = \tau_{ij} \cdot n_i|_s \]

The energy conservation, considering the first law of thermodynamics

\[ \delta Q - \delta W = \frac{dE}{dt} \]

The energy equation for adiabatic CV,

\[ -\frac{\delta W}{dt} = \frac{dE}{dt} = \frac{\partial}{\partial t} \iiint_{V(t)} \rho e \, dV + \int_{S(t)} \rho (\mathbf{u} \cdot \mathbf{n}) dS \]

\[ E = k_e + p_{ee} + p_{eg}, k_e, p_{ee}, p_{eg} \text{ are the kinetic and elastic} \]

and gravitational potential energies.

The work rate flows are exchanged between the water CV and the structure CV.

\[ \dot{W} = \dot{W}_{shaft} + \dot{W}_p + \dot{W}_v \]

\( \dot{W}_p \) and \( \dot{W}_v \) are the pressure and viscous work rates done by the CV.

Within the fluid CV, \( \dot{W}_{shaft} = 0 \). Within the structure CV, \( \dot{W}_{shaft} \) is the work rate done by the plate’s mount on the system and is hereafter named \( \dot{W}_M \).

The pressure and viscous work done on solid = pressure and viscous work done on fluid and vice versa, which are equivalent to separate \( \frac{dE}{dt} \) for solid which includes \( E = k_e + p_{ee} + p_{eg} \) and fluid which only includes \( E = k_e + p_{eg} \). In most cases net outflux of energy from the CV is zero.

Thus for the fluid

\[ \frac{dE}{dt} = \frac{\partial}{\partial t} \iiint_{V_w} \rho_w \left( g z + \frac{||\mathbf{u}_w||^2}{2} \right) dV_w \]

And for the solid

\[ \frac{dE}{dt} = \frac{\partial}{\partial t} \iiint_{V(t)} \rho dV \]
Examples of Boundary conditions

Single flow free surface BCs:

- Free surface problems since interface is unknown and part of the solution, but effect gas on liquid idealized.
- Assume the upper fluid (air) is an “atmosphere” that merely exerts pressure on the lower fluid (water), with shear and heat conduction negligible.
- Kinematic FSBC: free surface is stream surface
- Dynamic FSBC: stress continuous across free surface (similar for mass and heat flux)

Approximations:

\[ p \approx p_a = 0, \text{ neglect air viscosity and surface tension} \]

\[ \xi_x \sim \xi_x \sim 0, \text{ small slope} \]

\[ w_x \sim w_y \sim w_z = 0, \quad \frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = 0 \]

small normal velocity gradient
Examples of Boundary conditions

Two-phase interface jump conditions:

The velocity fields in fluids 1 and 2 are continuous across the interface if there is no phase change and mass transfer across the interface,

\[ \mathbf{u}_1 = \mathbf{u}_2 \]  \hspace{1cm} (1)

where \( \mathbf{u} \) is the velocity vector. The interface velocity \( V_I \) is the normal velocity and is the same on both sides of the interface:

\[ V_I = \mathbf{u}_1 \cdot \mathbf{n} = \mathbf{u}_2 \cdot \mathbf{n} \] \hspace{1cm} (kinematic condition) \hspace{1cm} (2)

where \( \mathbf{n} \) is the unit normal vector.

The continuity of the tangential velocities is analogous to the no-slip boundary condition on a wall,

\[ \mathbf{u}_1 - (\mathbf{u}_1 \cdot \mathbf{n})\mathbf{n} = \mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{n})\mathbf{n} \] \hspace{1cm} (continuity of the tangential velocity) \hspace{1cm} (3)
Examples of Boundary conditions

Stress conditions:
The stress tensor is defined in terms of the local fluid pressure and velocity field as

\[ T = -pI + \tau = -pI + \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \]  (4)

where \( I \) is the unit tensor, \( \tau \) is viscous stress tensor, \( p \) is pressure, and \( \mu \) is the dynamic viscosity. The stress vector, the force (per unit area) exerted by the fluid on the interface, is defined as,

\[ t(n) = n \cdot T \]  (5)

Note that the stress vector in the above equation generally includes both the normal and tangential stress components.

The exact interface stress condition is given in the stress balance equation below:

\[ n \cdot T_1 - n \cdot T_2 = \sigma n (\nabla \cdot n) - \nabla \sigma \]  (6)

where \( \nabla \sigma \) is tangential stress associated with gradients of the surface tension. The divergence of the unit normal is related to the mean curvature:

\[ \nabla \cdot n = \kappa \]  (7)

The stress jump condition can be rewritten as

\[ n \cdot (T_1 - T_2) = \sigma \kappa n - \nabla \sigma \]  (8)
Examples of Boundary conditions

Note that both normal and tangential stresses must be balanced at the interface. The condition can be written separately as the “normal stress balance” and “tangential stress balance”.

Normal stress balance

Projection of Eq. (8) along the unit normal \( \mathbf{n} \) obtains,

\[
\mathbf{n} \cdot (\mathbf{T}_1 - \mathbf{T}_2) \cdot \mathbf{n} = \sigma \mathbf{n} \cdot \mathbf{n} = \sigma \kappa
\]  

(9)

Tangential stress balance

Taking dot product of Eq. (8) with any unit tangential vector \( \mathbf{t} \) yields the tangential stress balance,

\[
\mathbf{n} \cdot (\mathbf{T}_1 - \mathbf{T}_2) \cdot \mathbf{t} = \nabla \sigma \cdot \mathbf{t}
\]  

(10a)

The surface tension \( \sigma \) depends on temperature and composition of the interface, which can be treated as a constant. The gradient of surface tension will vanish and the tangential stress is continuous across the interface.

\[
\mathbf{n} \cdot (\mathbf{T}_1 - \mathbf{T}_2) \cdot \mathbf{t} = 0
\]  

(10b)
Examples of Boundary conditions

Numerical approximation of the jump conditions

The viscous stress tensor $\tau$ can be written as,

$$\tau = \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] = \mu \begin{pmatrix} \nabla u \\ \nabla v \\ \nabla w \end{pmatrix} + \mu \begin{pmatrix} \nabla u \\ \nabla v \\ \nabla w \end{pmatrix}^T$$  \hspace{1cm} (11)

Using the jump notation $[x] = x_1 - x_2$, and $\mathbf{t}_I$ and $\mathbf{t}_{II}$ the orthogonal unit tangential vectors, the stress jump conditions Eqs. (9) and (10b) can be rewritten as three separate jump conditions,

$$[p - 2\mu(\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{n}] = \sigma \kappa$$  \hspace{1cm} (12)

$$[\mu(\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{t}_I + \mu(\nabla u \cdot \mathbf{t}_I, \nabla v \cdot \mathbf{t}_I, \nabla w \cdot \mathbf{t}_I) \cdot \mathbf{n}] = 0$$  \hspace{1cm} (13)

$$[\mu(\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{t}_{II} + \mu(\nabla u \cdot \mathbf{t}_{II}, \nabla v \cdot \mathbf{t}_{II}, \nabla w \cdot \mathbf{t}_{II}) \cdot \mathbf{n}] = 0$$  \hspace{1cm} (14)

The velocity is continuous and the tangential velocity derivatives are also continuous,

$$[\nabla \mathbf{u} \cdot \mathbf{t}_I^T] = 0 \hspace{1cm} \text{or} \hspace{1cm} [\nabla u \cdot \mathbf{t}_I] = [\nabla v \cdot \mathbf{t}_I] = [\nabla w \cdot \mathbf{t}_I] = 0$$ \hspace{1cm} (15)

$$[\nabla \mathbf{u} \cdot \mathbf{t}_{II}^T] = 0 \hspace{1cm} \text{or} \hspace{1cm} [\nabla u \cdot \mathbf{t}_{II}] = [\nabla v \cdot \mathbf{t}_{II}] = [\nabla w \cdot \mathbf{t}_{II}] = 0$$ \hspace{1cm} (16)
Examples of Boundary conditions

Numerical approximation of the jump conditions

The normal stress condition can be written as,

\[ [p] - 2[\mu](\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n = \sigma_k \]  (17)

The tangential jump conditions

\[ [\mu \nabla u] = [\mu](\nabla u) \begin{pmatrix} 0 \\ t_I \\ t_{II} \end{pmatrix}^T \begin{pmatrix} 0 \\ t_I \\ t_{II} \end{pmatrix} + [\mu] n^T n (\nabla u)^T n - [\mu] \begin{pmatrix} 0 \\ t_I \\ t_{II} \end{pmatrix}^T \begin{pmatrix} 0 \\ t_I \\ t_{II} \end{pmatrix} (\nabla u)^T n^T n \]  (18)

Note that the right-hand side of the above equation only involves velocity derivatives that are continuous across the interface. If \( [\mu] = 0 \), then \([\nabla u] = 0\).

If the viscosity is smoothed to be continuous across the interface, the normal jump condition

\[ [p] = \sigma_k \]  (19)

The tangential viscous stress jump condition,

\[ [(\nabla u \cdot n^T) \cdot t_I] + [(\nabla u \cdot t_I^T) \cdot n] = 0 \]  (20)

According to Eq. (18), with a constant viscosity, all the velocity derivatives will be continuous across the interface which implies that both jump terms on the left hand side of the above equation are zero.
Examples of Boundary conditions

Vorticity condition across the interface

The vorticity in the normal direction is written as,

\[ \mathbf{n} \cdot \omega = \mathbf{n} \cdot (\nabla \times \mathbf{u}) = (\mathbf{t}_I \times \mathbf{t}_{II}) \cdot (\nabla \times \mathbf{u}) \quad (21) \]

Using the identity \((\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c})\), Eq. (21) can be rewritten as,

\[ \mathbf{n} \cdot \omega = (\mathbf{t}_I \cdot \nabla)(\mathbf{t}_{II} \cdot \mathbf{u}) - (\mathbf{t}_I \cdot \mathbf{u})(\mathbf{t}_{II} \cdot \nabla) \quad (22) \]

which is continuous across the interface since the right hand side of the above equation only involves tangential derivatives of the velocity.

The vorticity in the tangential directions,

\[ \mathbf{t}_I \cdot \omega = \mathbf{t}_I \cdot (\nabla \times \mathbf{u}) = (\mathbf{t}_{II} \times \mathbf{n}) \cdot (\nabla \times \mathbf{u}) = (\mathbf{t}_{II} \cdot \nabla)(\mathbf{n} \cdot \mathbf{u}) - (\mathbf{t}_{II} \cdot \mathbf{u})(\mathbf{n} \cdot \nabla) \quad (23) \]

\[ \mathbf{t}_{II} \cdot \omega = \mathbf{t}_{II} \cdot (\nabla \times \mathbf{u}) = (\mathbf{n} \times \mathbf{t}_I) \cdot (\nabla \times \mathbf{u}) = (\mathbf{n} \cdot \nabla)(\mathbf{t}_I \cdot \mathbf{u}) - (\mathbf{n} \cdot \mathbf{u})(\mathbf{t}_I \cdot \nabla) \quad (24) \]

The tangential vorticities are generally not continuous across the interface since the normal derivatives, \((\mathbf{t}_{II} \cdot \mathbf{u})(\mathbf{n} \cdot \nabla)\) and \((\mathbf{n} \cdot \nabla)(\mathbf{t}_I \cdot \mathbf{u})\), are involved in the above equations, respectively.

However, as shown in Eq. (20), all the velocity derivatives will be continuous if the viscosity jump \([\mu] = 0\), then tangential vorticities will also be continuous.
Examples of Boundary conditions

For two immiscible fluids with different density and viscosity:
Velocity, velocity gradient, viscosity, and shear stress distribution

Velocity, Uz, viscosity, and Taw profile for a layered two fluid flow.
Examples of Boundary conditions

Inlet/outlet/exit/outer/far-field BCs:

- **Inlet**: $V$, $p$, $T$, specified, e.g., constant values are used, $V = V_{in}$, $p = 0$, $T = T_{in,0}$
- **Outer or far-field**: $V$, $p$, $T$, specified similarly as inlet
- **Exit**: depends on the problems, but
  - often use $U_{xx} = 0$ and $\frac{\partial p}{\partial n} = 0$.
  - For external flow, zero stream wise diffusion
  - For fully developed internal flow and wave problem, periodic BCs can be used
  - For unsteady internal flow, global mass conservation enforcement may be needed: $U_{out} = U_{out} \frac{Q_{in}}{Q_{out}}$, where $Q_{in}$ and $Q_{out}$ is the total inlet and outlet and flux, respectively.
<table>
<thead>
<tr>
<th>IBTYP</th>
<th>Description</th>
<th>$U$</th>
<th>$V$</th>
<th>$W$</th>
<th>$P$</th>
<th>$k$</th>
<th>$\omega$</th>
<th>$\nu_1$</th>
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<tr>
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<td>Inlet</td>
<td>UINF</td>
<td>VINF</td>
<td>WINF</td>
<td>$\partial P/\partial \xi_i = 0$</td>
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<td>Exit</td>
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<td>Impermeable slip (calculate forces)</td>
<td>Eq. (78)</td>
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<td>Eq. (78)</td>
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<td>Impermeable slip (no forces)</td>
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<td>Eq. (78)</td>
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<td>41</td>
<td>Translational periodicity, w/ ghost cells</td>
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<td>43</td>
<td>Pole (i-around)</td>
<td>Eq. (80)</td>
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<td>Pole (j-around)</td>
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<td>No-slip/centerplane</td>
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<td>z-axis symmetry</td>
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<tr>
<td>91</td>
<td>Multi-block w/ ghost cells</td>
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<td>92</td>
<td>Multi-block w/o ghost cells</td>
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<tr>
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<td>Blanked out points</td>
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</table>

* See text for detailed description
Simulation Examples using CFDShip-Iowa

Plunging wave breaking:

- **Inlet:**
  \[ u = \text{constant}, \, v = w = 0 \]

- **Exit:**
  \[ \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = \frac{\partial w}{\partial n} = 0 \]

- For pressure, \( \frac{\partial p}{\partial n} = 0 \) for all the boundaries.

- Mass balance needed at the outlet.

Wave breaking in bump flow simulation: 2.2 billion grid points

Movie
Simulation Examples using CFDShip-Iowa

Wedge flow:

- The $j_{max}$ boundary is split into two parts: inlet and exit.
- **Inlet**: $u = \text{constant}, v = w = 0$
- **Exit**: $\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = \frac{\partial w}{\partial n} = 0$
- Slip BCs at both top and bottom.
- For pressure, $\frac{\partial p}{\partial n} = 0$ for all the boundaries.
- Mass balance needed at the outlet.
Simulation Examples using CFDShip-Iowa

Stokes wave breaking
Slip wall BCs at top and bottom
Periodic BCs at inlet, exit, and two sides.

Stokes wave breaking: 3.2-12 Billion Grid Points

Movie
Simulation Examples using CFDShip-Iowa

NSWC15E Planing Hull

- Water is moving, ship-fixed system
- **Inlet (10):**
  \[ u = u_{\text{inflow}}, \; v = w = 0 \]
- **Exit(11):**
  \[ \frac{\partial^2 u}{\partial n^2} = 0, \; \frac{\partial p}{\partial n} = 0 \]

Movies: bottom view side view
Simulation Examples using CFDShip-Iowa

KCS free running

- Symmetric BC can not be used, use full ship
- Inlet (10): \( u = v = w = 0 \), since the ship is moving, earth fixed system (inertial)
- Exit (11)

Movies: free running