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Target Simulation

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Talk Outline



- New development of models for cavitation/phase transitions
 - Heterogeneous method (Direct Numerical Simulation)
 - Riemann problem for the phase boundary
 - Adaptive mesh refinement (AMR)
 - Applications to targets
- Mercury jet entering a 15 T magnetic solenoid
- Current study: role of the mercury reservoir in the formation of the jet
- Conclusions and future plans





We have developed two models for cavitating and bubbly fluids

 Heterogeneous method (Direct Numerical Simulation): Each individual bubble is explicitly resolved using FronTier interface tracking technique.



Homogeneous EOS model. Suitable average properties are determined and the mixture is treated as a pseudofluid that obeys an equation of single-component flow.



Homogeneous isentropic two phase EOS model (summary)

- Correct dependence of the sound speed on the density (void fraction). The EOS is applicable if properties of the bubbly fluid can be averaged on the length scale of several bubbles. Small spatial scales are not resolved.
- Enough input parameters (thermodynamic/acoustic parameters of both saturated points) to fit the sound speed in all phases to experimental data.
- Absence of drag, surface tension, and viscous forces. Incomplete thermodynamics.



Experimental image (left) and numerical simulation (right) of the mercury jet.





Potential features of the heterogeneous method

- Accurate description of multiphase systems limited only by numerical errors.
- Resolves small spatial scales of the multiphase system
- Accurate treatment of drag, surface tension, viscous, and thermal effects.
- Mass transfer due to phase transition (Riemann problem for the phase boundary)
- Models some non-equilibrium phenomena (critical tension in fluids)



5



Validation of the direct method: linear waves and shock waves in bubbly fluids

Good agreement with experiments (Beylich & Gülhan, sound waves in bubbly water) and theoretical predictions of the dispersion and attenuations of sound waves in bubbly fluids

- Simulations were performed for small void fractions (difficult from numerical point of view)
- Very good agreement with experiments of the shock speed
- Correct dependence on the polytropic index





Application to SNS target problem





Left: pressure distribution in the SNS target prototype. Right: Cavitation induced pitting of the target flange (Los Alamos experiments)

- Injection of nondissolvable gas bubbles has been proposed as a pressure mitigation technique.
- Numerical simulations aim to estimate the efficiency of this approach, explore different flow regimes, and optimize parameters of the system.





Application to SNS



Effect of the bubble injection:

- Peak pressure decreases within 100 µs
- Fast transient pressure oscillations. Minimum pressure (negative) has larger absolute value.
- Formation and collapse of cavitation bubbles in both cases have been performed.
- The average cavitation damage was estimated to be reduced by > 10 times in the case of the bubble injection

Dynamic cavitation

• A cavitation bubble is dynamically inserted in the center of a rarefaction wave of critical strength

• A bubbles is dynamically destroyed when the radius becomes smaller than critical. In simulations, critical radius is determined by the numerical resolution. With AMR, it is of the same order of magnitude as physical critical radius.

• There is no data on the distribution of nucleation centers for mercury at the given conditions. Some estimates within the homogeneous nucleation theory: $\frac{2S}{\Delta P_C}$

critical radius:
$$R_C = \frac{1}{2}$$

nucleation rate: $J = J_0 e^{-Gb}$, $J_0 = N \sqrt{\frac{2S}{\pi m}}$, $Gb = \frac{W_{CR}}{kT}$, $W_{CR} = \frac{16\pi S^3}{3(\Delta P_C)^2}$

$$P_c \cong -\left(\frac{16\pi S^3}{3kT\ln\left(J_0Vdt\right)}\right)$$

Critical pressure necessary to create a bubble in volume V during time dt

$$egin{aligned} &
ho_v(u_v-s)=
ho_l(u_l-s),\ &
ho_v(u_v-s)^2+p_v=
ho_l(u_l-s)^2+p_l,\ &(e_v+p_v)(u_v-s)-\kappa_vT_{v,x}=(e_l+p_l)(u_l-s)-\kappa_lT_{l,x} \end{aligned}$$

$$egin{aligned} M&=-rac{p_v-p_l}{u_v-u_l},\ M^2&=-rac{p_v-p_l}{ au_v- au_l},\quad au=rac{1}{
ho},\ (u_v-s)(u_l-s)&=rac{p_v-p_l}{
ho_v-
ho_l} \end{aligned}$$

$$arepsilon_l - arepsilon_v + rac{p_l + p_v}{2}(\eta - au_v) = rac{1}{M}(\kappa_v T_{v,x} - \kappa_l T_{l,x})$$

$$\left. rac{dp}{dT}
ight|_{egin{subarray}{c} ext{ Saturation conditions} \end{array}} = rac{Q_v}{T\left(rac{1}{
ho_v} - rac{1}{
ho_l}
ight)}$$

$$p_v = p_0 \exp\left[rac{Q_v \mathcal{M}}{R}\left(rac{1}{T_0}-rac{1}{T_s}
ight)
ight]$$



Riemann problem for the phase boundary: mathematical difficulties



- In the presence of heat diffusion, the system looses the hyperbolicity and self-similarity of solutions
- Mathematically, a set of elementary waves does not exist
- A set of constant states can only approximate the solution
- A simplified version (decoupled from acoustic waves) has been implemented in FronTier

• An iterative technique for more compex wave stucture is being implemented and tested



Adaptive Mesh Refinement

- Rectangular refined mesh patches are created in the location of high density gradients (interfaces, strong waves etc.)
- Interpolation of states from coarse to fine grids is performed
- Patches are sent to separate processors for maintaining a uniform load balance of a supercomputer
- Dynamic cavitation routines now work with AMR



Example of the AMR in FronTier: high speed fuel jet breakup.



Cavitation in the mercury jet interacting with the proton pulse

13





Other current and potential applications

• High speed liquid jet breakup and atomization

• Condensation and clustering of hydrogen in Laval nozzles which create highly collimated jets for tokamak refueling. This is an alternative technology to the pellet injection. Almost as efficient as the pellet injection, high energy density jet does not introduce transient density perturbations leading to plasma instabilities and the reduction of the energy confinement.

Mercury jet entering magnetic field. Schematic of the problem.



Magnetic field of the 15 T solenoid is given in the tabular format



Equations of compressible MHD implemented in the FronTier code

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \mathbf{u} = -\nabla P + \mu \Delta \mathbf{u} + \frac{1}{c} (\mathbf{J} \times \mathbf{B})$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) e = -P \nabla \cdot \mathbf{u} + \frac{1}{\sigma} \mathbf{J}^{2}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) - \nabla \times \left(\frac{c^{2}}{4\pi\sigma} \nabla \times \mathbf{B}\right)$$

$$P = P(\rho, e), \quad \nabla \cdot \mathbf{B} = 0$$

$$\mathbf{J} = \sigma \left(-\nabla \phi + \frac{1}{c} \mathbf{u} \times \mathbf{B}\right)$$

$$\Delta \phi = \frac{1}{c} \nabla \cdot (\mathbf{u} \times \mathbf{B}),$$
with $\frac{\partial \phi}{\partial \mathbf{n}} \Big|_{\Gamma} = \frac{1}{c} (\mathbf{u} \times \mathbf{B}) \cdot \mathbf{n}$

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16



Limitations of DNS with the compressible MHD code

- Very stiff EOS. Low Mach number flow: $V_s = 1450$ m/s vs. $V_{iet} = 25$ m/s
- Large aspect ratio of the problem
- Simulation of long time evolution required (40 milliseconds). ~10⁵ time steps. Accumulation errors.
- Reduction of the EOS stiffness increases unphysical effects (volume changes due to increased compressibility)



Incompressible steady state formulation of the problem

$$\begin{split} \rho \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla P + \frac{1}{c} \left(\mathbf{J} \times \mathbf{B} \right) \\ \nabla \cdot \mathbf{u} &= 0 \\ \mathbf{J} &= \sigma \left(-\nabla \phi + \frac{1}{c} \mathbf{u} \times \mathbf{B} \right) \\ \nabla \cdot \mathbf{J} &= 0 \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{B} &= 0 \\ B.C.: \\ \nabla \times \mathbf{B} &= 0 \\ \frac{\partial \phi}{\partial \mathbf{n}} \bigg|_{\Gamma} &= \frac{1}{c} (\mathbf{u} \times \mathbf{B}) \cdot \mathbf{n} \\ p_{\Gamma} - p_{a} &= S \bigg(\frac{1}{r_{1}} + \frac{1}{r_{2}} \bigg) \\ \end{split}$$
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$$18 \qquad \mathbf{u}_{\Gamma} \cdot \mathbf{n} = 0 \qquad \mathbf{BROOKHAVEN}$$

Direct numerical simulation approach (FronTier):

- Construct an initial unperturbed jet along the B=0 trajectory
- Use the time dependent compressible code with a realistic EOS and evolve the jet into the steady state

Semi-analytical / semi-numerical approach:

- Seek for a solution of the incompressible steady state system of equations in form of expansion series
- Reduce the system to a series of ODE's for leading order terms
- Solve numerically ODE's

Ref.: S. Oshima, R. Yamane, Y. Mochimary, T. Matsuoka, JSME International Journal, Vol. 30, No. 261, 1987



Results: Aspect ratio of the jet cross-section



Results: Aspect ratio of the jet cross-section



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Deviation of the jet from the unperturbed axis



Influence of a mercury reservoir on the formation of the mercury jet. Jian Du, SUNY grad. student (work in progress)

Approach:

- Model turbulent flow in the reservoir inlet
- Observe the decay of turbulence in the reservoir and determine the optimal size of the reservoir.
- Currently we don't have a good agreement with classical experiments on the transition to turbueInce in a pipe. The numerically computed flow remains laminar at Reynolds numbers higher then critical
- There are several possible explanations:
 - Numerical resolution of the boundary layer
 - Compressible approximation limits the time step
 - Upwind type numerical schemes for hyperbolic conservation laws used by the FronTier code can also be responsible for the turbulence damping.





- New mathematical models for cavitation/phase transitions have been developed
 - Heterogeneous method (Direct Numerical Simulation)
 - Riemann problem for the phase boundary
 - Dynamic cavitation algorithms based on the homogeneous nucleation theory
 - Adaptive mesh refinement
 - Applications to mercury targets
- Deformation of the mercury jet entering a magnetic field has been calculated

Current study of role of the mercury reservoir in the formation of the jet will be continued

3D numerical simulations of the mercury jet interacting with a proton pulse in a magnetic field will be continued.

