

MUTAC Review April 28 - 29, 2005, LBNL

Target Simulation

Roman Samulyak, in collaboration with Yarema Prykarpatskyy, Tianshi Lu, Zhiliang Xu, Jian Du

Center for Data Intensive Computing Brookhaven National Laboratory U.S. Department of Energy

Brookhaven Science Associates U.S. Department of Energy

rosamu@bnl.gov





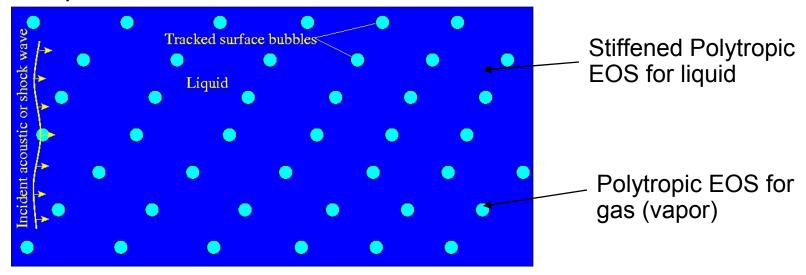
Talk Outline

- 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.

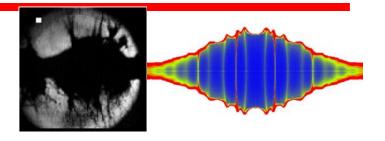


■ Homogeneous EOS model. Suitable average properties are determined and the mixture is treated as a pseudofluid that obeys an equation of single-component flow.

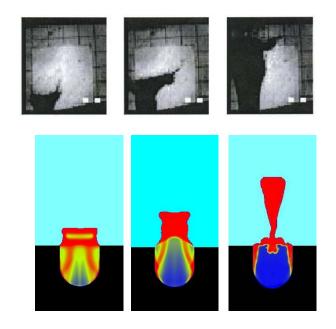


Homogeneous isentropic two phase EOS model (summary)

- 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.



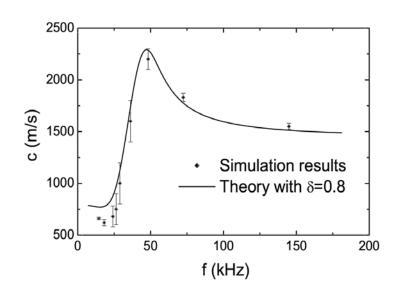
Potential features of the heterogeneous method

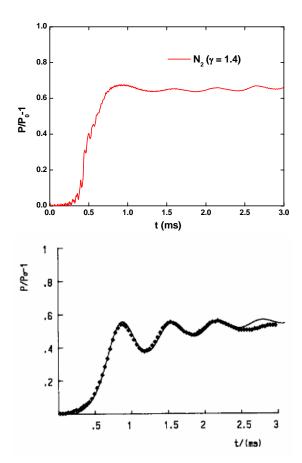
- Accurate description of multiphase systems limited only by numerical errors.
- Resolves small spatial scales of the multiphase system
- Accurate treatment of drag, surface tension, viscous, and thermal effects.
- Mass transfer due to phase transition (Riemann problem for the phase boundary)
- Models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



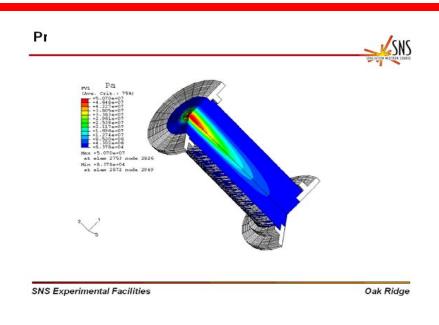
Validation of the direct method: linear waves and shock waves in bubbly fluids

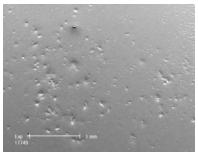
- Good agreement with experiments (Beylich & Gülhan, sound waves in bubbly water) and theoretical predictions of the dispersion and attenuations of sound waves in bubbly fluids
- Simulations were performed for small void fractions (difficult from numerical point of view)
- Very good agreement with experiments of the shock speed
- Correct dependence on the polytropic index

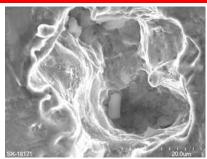




Application to SNS target problem





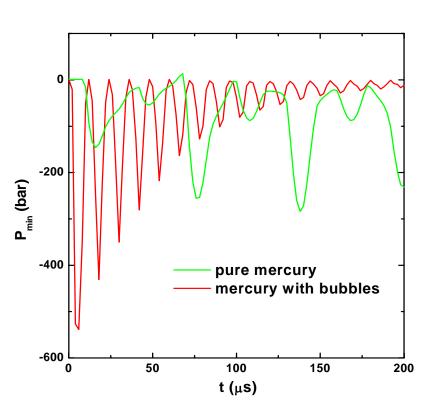


Left: pressure distribution in the SNS target prototype. Right: Cavitation induced pitting of the target flange (Los Alamos experiments)

- 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

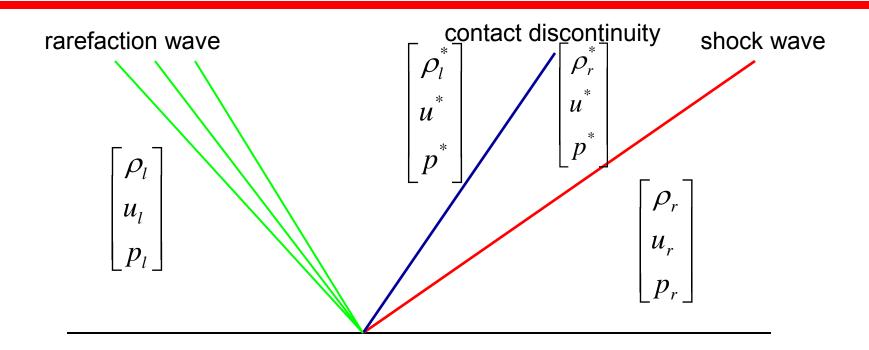
- A cavitation bubble is dynamically inserted in the center of a rarefaction wave of critical strength
- A bubbles is dynamically destroyed when the radius becomes smaller than critical. In simulations, critical radius is determined by the numerical resolution. With AMR, it is of the same order of magnitude 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:

critical radius: $R_C = \frac{2S}{\Delta P_C}$

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

$$P_c \simeq -\left(\frac{16\pi S^3}{3kT\ln(J_0Vdt)}\right)$$
 Critical pressure necessary to create a bubble in volume V during time dt

Riemann problem for the phase boundary: mathematical difficulties

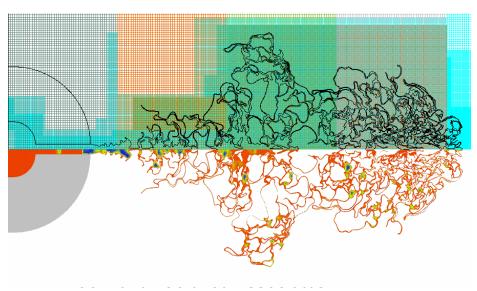


- In the presence of heat diffusion, the system looses the hyperbolicity and self-similarity of solutions
- Mathematically, a set of elementary waves does not exist
- A set of constant states can only approximate the solution
- A simplified version (decoupled from acoustic waves) has been implemented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

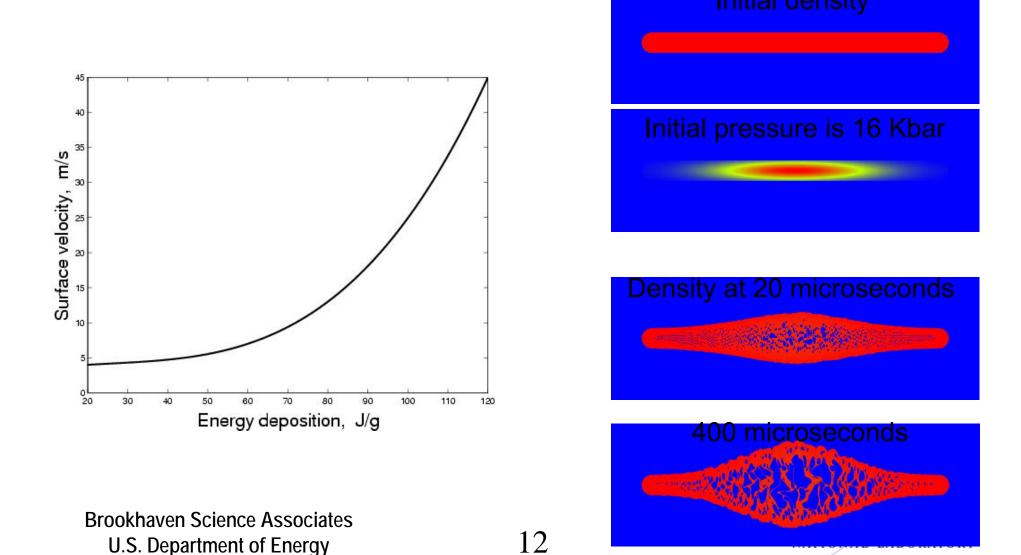


U.S. Department of Energy

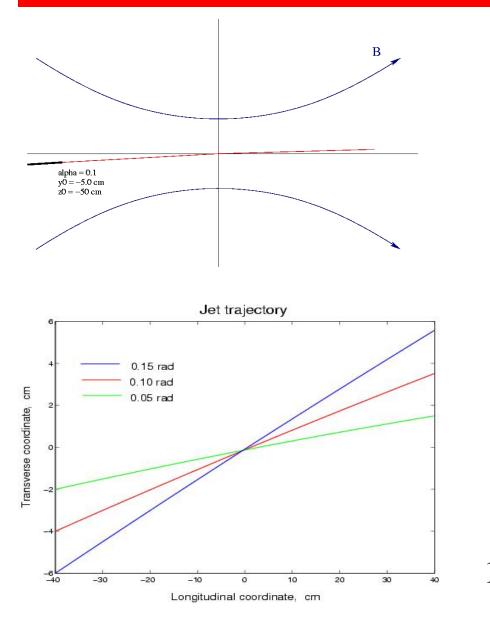
Example of the AMR in FronTier: high speed fuel jet breakup.



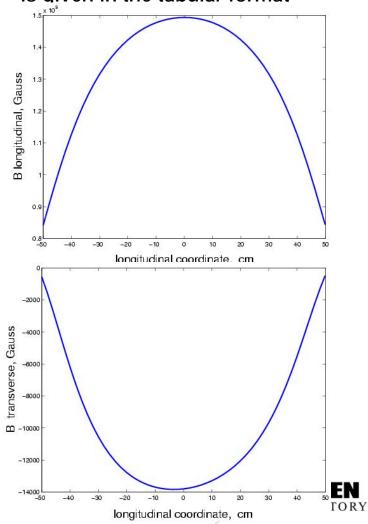
Cavitation in the mercury jet interacting with the proton pulse



Mercury jet entering magnetic field. Schematic of the problem.



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



13

Incompressible steady state formulation of the problem

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \frac{1}{c} (\mathbf{J} \times \mathbf{B})$$

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

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

$$\nabla \cdot \mathbf{J} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{B} = 0$$

$$\nabla \times \mathbf{B} = 0$$

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

$$p_{\Gamma} - p_{a} = S \left(\frac{1}{r_{1}} + \frac{1}{r_{2}} \right)$$

Brookhaven Science Associates U.S. Department of Energy



 $\mathbf{u}_{\Gamma} \cdot \mathbf{n} = 0$

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

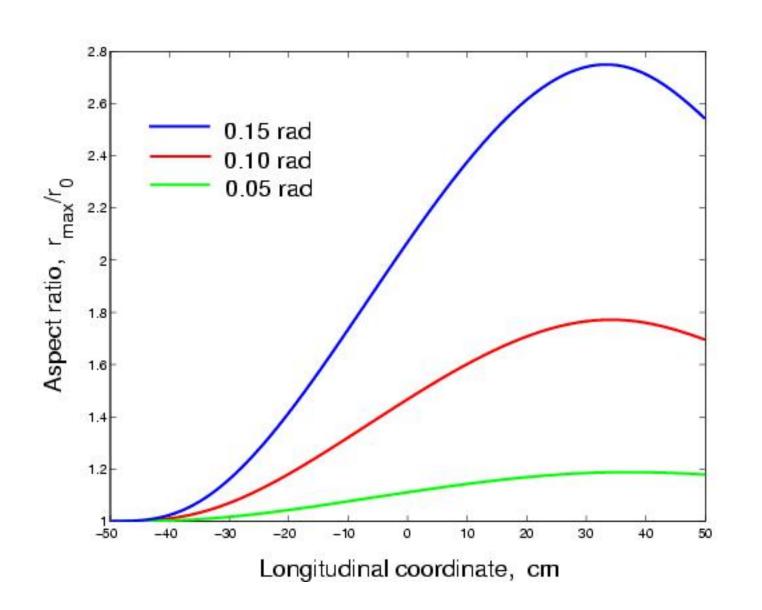
Semi-analytical / semi-numerical approach:

- 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



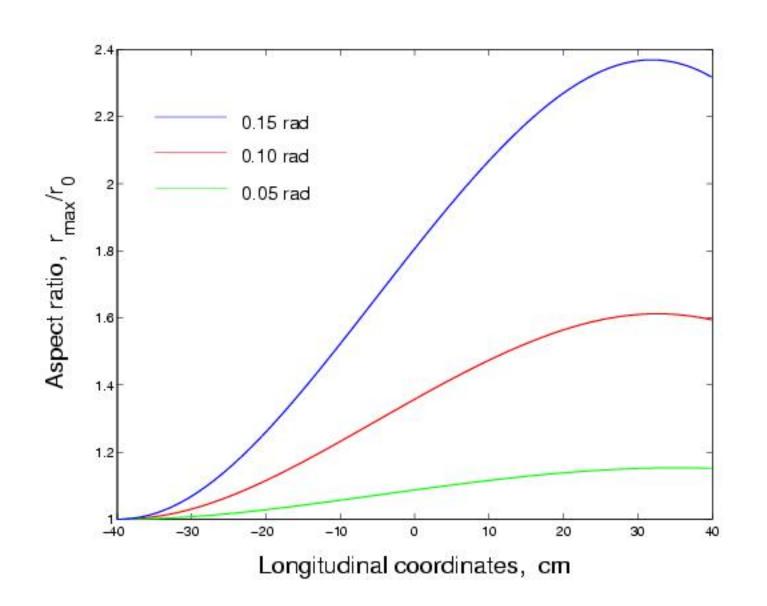
Results: Aspect ratio of the jet cross-section



B = 15 TV0 = 25 m/s



Results: Aspect ratio of the jet cross-section



B = 15 TV0 = 25 m/s





Conclusions and Future Plans

- 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.

