Development of multiphase flow solvers based on OpenFOAM for volcanological research

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Outline

Conduit flow and the mechanism of magma fragmentation

- Multiphase compressible model
- Numerical solver based on OpenFOAM
- Benchmark: 2D bubble-shock wave interaction

Turbulent volcanic plumes

- Multiphase equilibrium Eulerian model
- Numerical solver based on OpenFOAM
- Benchmark: homogeneous, isotropic turbulence in compressible regime
Why OpenFOAM?

**Computational infrastructure**
- Modular structure and high level of abstraction
- Non-structured meshes: complex geometries, local mesh refinement, coupling subdomains
- Control of numerical accuracy and errors (?)
- High performances (?)
- High potential application to many fields of geophysics/volcanology

**Open source and free**
- Developers community (?)
- Users community
- No costs (?)
Controlling factors

- Rapid exsolution of volatiles (large pressure gradient)
- High volatile content (of magmatic or phreatic origin)
- High viscosity (evolved and crystalized magma)
- Highly non-linear dependency on temperature and water content
- A system of fractures from a deep reservoir to the surface

Figure: Scheme of volcanic conduit flow
Conduit flow model

Conservative approach

- The conduit flow model consists of a single temperature, two-phase (two velocities and two pressures) model for two compressible phases (magma+bubbles or gas+particles).
- Model equations are written in conservative form, to properly treat decompression and fragmentation waves and shocks.

The approach to multiphase modeling is based on the theory of the *thermodynamically compatible systems*. This allows modeling the bubbly-flow and the gas-particle regime with a single set of equations.

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Conservative Models and Numerical Methods for Compressible Two-Phase Flow

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Numerical resolution for a compressible two-phase flow model based on the theory of thermodynamically compatible systems

D. Zeidan
The numerical implementation is based on a Godunov-like, Riemann-solver-free approach, using central-upwind schemes (Kurganov, Noelle, Petrova, *SIAM J.*, 2001) for the integration of the hyperbolic terms.

- the KNP finite volume central scheme has been coupled with a second-order MUSCL-Hancock scheme, with the linear reconstruction of the predictor step done under a primitive variables formulation, to solve a conservative model for a two-phase compressible flow with two velocities and two pressures.

- The source/relaxation terms (e.g. pressure and/or velocity relaxations) are integrated analytically.
Experimental test case

- Interaction of a planar shock wave in air with a cylindrical volume of a gas with different density and sound speed (Haas and Sturtevant, 1987).
- A cylindrical bubble of fluorocarbon with diameter $d=50\text{mm}$ is located in the center of a tunnel with width $89\text{mm}$ and length $150\text{mm}$, filled with air at rest. At the initial time high pressure and high velocity generates a shock-wave (propagating from right to left).

Numerical solution

- The numerical solver has been implemented in OpenFOAM, starting from the $\text{rhoCentralFoam}$ compressible solver.
- For this test we used a grid of $1600\times400$ cells and the simulation has been done on the IBM PLX cluster at the High Performance Computing department of CINECA using 30 processors.
Comparison with the experiments

Esposti Ongaro et al.  OpenFOAM for volcanological research
The explosive volcano engine (2)

Figure: Scheme of volcanic conduit flow

Figure: Explosive eruption plume at Mount St. Helens (1980)
Factors controlling volcanic plume dynamics

- Initial Momentum and Buoyancy
- Grain size distribution
- Turbulent entrainment and heating of atmospheric air
- Buoyancy reversal
- Atmospheric stratification

Figure: Sketch of a volcanic plume (Woods, 1988)
The physical model should be able to treat polydisperse mixtures (with coarse particles) and compressibility.

Need for a "fast" numerical solver 1) accurate enough 2) non-diffusive.

Direct Numerical Simulation (DNS) not affordable (Reynolds’ number may exceed $10^9$, based on vent diameter and mixture parameters).
Numerical solver

- The numerical solver has been implemented in OpenFOAM taking as a basis the *sonicFoam* solver for compressible Navier-Stokes equations.
- Tests on the *rhoCentralFoam* solver (based on the central scheme by Kurganov and Tadmor, 2000) indicate excessive numerical diffusion for the simulation of turbulent flows.
- Variable time-stepping (based on initial residual threshold) has been implemented to accelerate the solution procedure, still maintaining a good accuracy.
Figure: Two dimensional gas-particles jet and its temporal spectrum in two different probes.

Boundary conditions

Some problems arise in the formulation of outflow boundary conditions, which must account for several, different physical phenomena:

- **Eddies** propagation
- Atmospheric **stratification**, due to gravity.
- **Sound and gravity waves**, due to compressibility effects.
Is OpenFOAM reliable for DNS and LES of compressible turbulent flows?
Numerical benchmark: compressible, homogeneous and isotropic turbulence

Decaying turbulence: initial conditions.

- Initial kinetic energy spectrum: \( E(k) \propto \left( \frac{k}{k_0} \right)^4 \exp \left( -2 \left( \frac{k}{k_0} \right)^2 \right) \)
- Solver: `sonicFoam` with a mixed second-fourth order central scheme

Figure: Compressible homogeneous and isotropic turbulence with r.m.s. Mach number \( Ma_{\text{rms}} = 0.2 \), compressibility factor \( \chi_0 = 0 \) and \( Re_\lambda = 210 \), in a box with \( 256^3 \) cells.
Numerical benchmark: compressible, homogeneous and isotropic turbulence

Figure: The effect of different resolutions on the kinetic energy spectrum.
Numerical benchmark: compressible, homogeneous and isotropic turbulence

(a) Evolution of the enstrophy. 
(b) Evolution of the kinetic energy. 
(c) Evolution of the energy dissipation. 
(d) Evolution of the Taylor microscale. 
(e) Evolution of the root-mean-square density fluctuations. 
(f) Evolution of the time step.
Numerical benchmark: compressible, homogeneous and isotropic turbulence

Figure: Scalability test on CINECA PLX and FERMI architectures.
Numerical benchmark: compressible, homogeneous and isotropic turbulence

Concluding remarks

- DNS of compressible turbulence with OpenFOAM gives results consistent with state-of-the-art spectral CFD codes.
- Non-diffusive fourth order central scheme for convective fluxes are required to well reproduce the energy spectrum.
- Our variable time-stepping method is robust and demonstrates good stability properties.
- HPC performance on this test case are satisfactory up to 1024 cores.