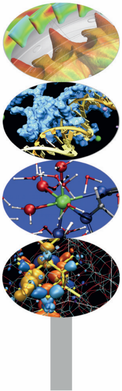
Cineca
TRAINING
High Performance
Computing 2016

HPC enabling of OpenFOAM® for CFD applications

HPC simulation of volcanic ash plumes and application of OpenFOAM to CFD volcanological problems



06-08 April 2016, Casalecchio di Reno, BOLOGNA.

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Effusive and explosive eruptions:

The example of Etna volcano

effusive (lava flows)

(2006)

(lava fountains)

(2014)

explosive (ash plumes)

(2015)

Explosivity is mostly controlled by multiphase processes in the magma (melt+gas+crystals):

- Gas phase transitions (gas exsolution, bubble nucleation and expansion).
- Non-linear magma rheology (brittle transition = fragmentation).

Challenges in magma ascent modeling with OpenFOAM

Effusive regime

- Introduce multicomponent physics and phase transitions
- Bubble nucleation
- Manage phase separation and degassing

Explosive regime

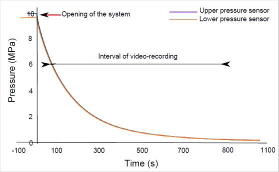
- Wave propagation
- Fragmentation conditions
- Manage different domains (below/above fragmentation)

TwoPhaseChangeEulerFoam

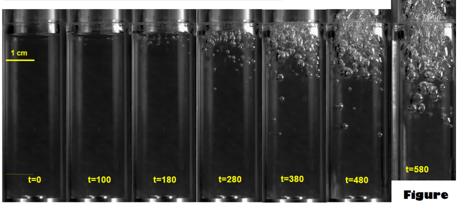
A new multiphase multicomponent model with phase change has been developed. Each phase is the mixture of several components and exsolution/evaporation laws can be defined for each component.

Test 1 (decompression experiment):

- validation through comparisons with decompression experiments performed at LMU, Munich.
- silicon oil chosen as analogue for magmatic melt, and saturated with Argon at 10MPA
- slow decompression to atmospheric conditions



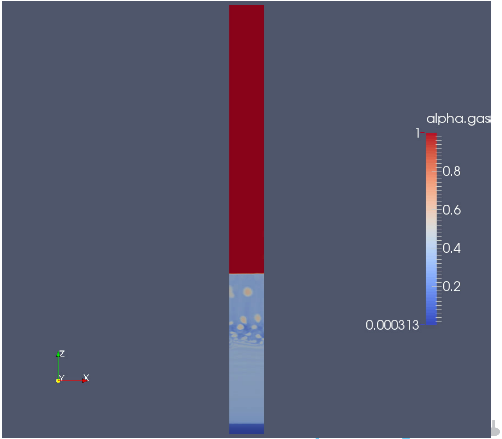
Snapshot from a decompression experiment performed using silicon oil with a viscosity of 100 Pa s. Gas exsolution, and the consequent nucleation of bubbles, are visible at the top of the liquid column roughly 100s after the beginning of the decompression.



Figure

TwoPhaseChangeEulerFoam

A new multiphase multicomponent model with phase change has been developed. Each phase is the mixture of several components and exsolution/evaporation laws can be defined for each component.



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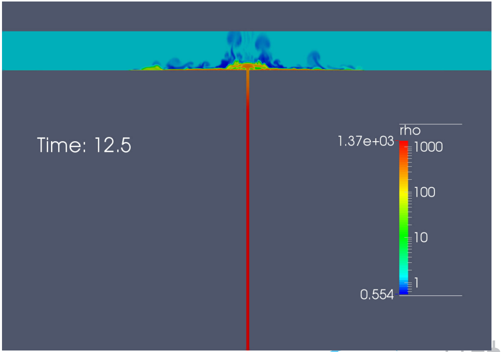
TwoPhaseChangeEulerFoam

A new multiphase multicomponent model with phase change has been developed. Each phase is the mixture of several components and exsolution/evaporation laws can be defined for each component.

Test 2 (gas-driven effusive eruption):

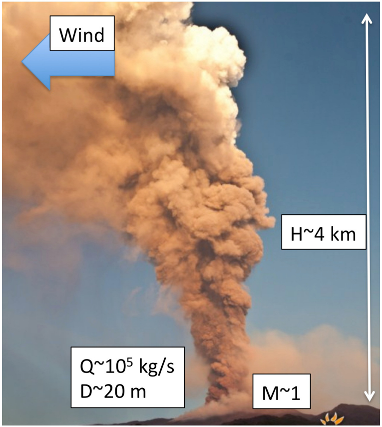
- rise of hot and high-viscosity magmatic mixture:
    - liquid phase: melt, dissolved H_2O, dissolved CO_2;
    - gas phase: exsolved H_2O, exsolved CO_2, air;



Explosive eruptions:

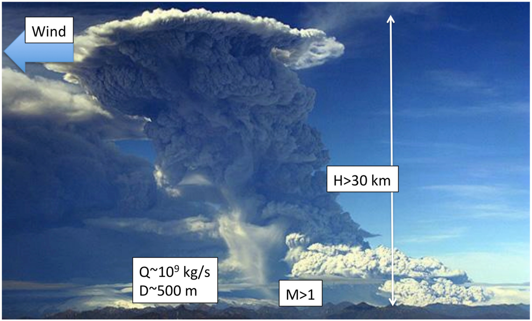
Volcanic plumes

Weak Plume



(Etna, 2011)

Strong Plume



(Chaitén, 2008)

Multiscale dynamics

Spatial and temporal scales

- Mass flow rate: $Q \sim UD^2$
- Reynolds number: $\mathrm{Re} = \frac{UD}{\mu} \sim 10^9$
- Typical Large-Eddy Scale: $L \sim (\mathrm{Str})D$
- Kolmogorov' length: $\eta \sim L^{-3/4} \sim L \times 10^{-7}$
- Integral length scale (plume height): $H \sim F^{1/4} S^{-3/4}$ $(F = g' UD^2 = g' Q;\ S = -g/\rho \frac{d\rho}{dz})$
- Integral time scale: $\tau \sim \sqrt{\frac{T_v}{(1+n)\Gamma g}} \sim 1 - 5 \times 10^2$ s

Number of degrees of freedom

- Minimum grid size: $\Delta x \sim L$
- Minimum number of cells: $N \sim (H/L)^3 \sim Q^{-1/4}$
- Minimum time-step $\Delta t \sim \Delta x / U$
- $N_{tot}(\mathrm{Weak}) \sim 10^{14}$; $N_{tot}(\mathrm{Strong}) \sim 10^{11}$

Challenges in volcanic plume modeling with OpenFOAM

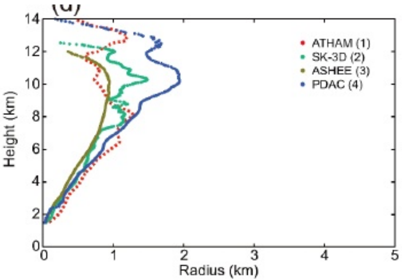
Multiphase flow

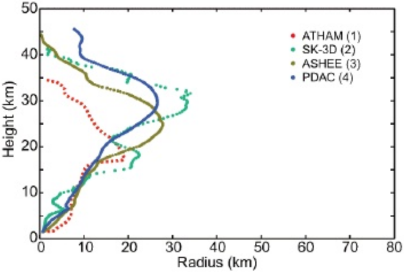
- Describe non-equilibrium gas–particle dynamics
- Manage compressibility, turbulence, heat exchange
- Model subgrid turbulence

Numerical solution

- Time-step constrained by vent conditions
- Compressible turbulence needs appropriate discretization schemes
- Number of cells is necessarily large! Effective parallelism.

Model-related uncertainty


Weak Plume


Strong Plume

Does uncertainty *blur* accuracy?

- A "blind" intercomparison test (4 models)
- Model-related uncertainty is still much larger than
  - Error associated with grid size
  - Error associated with SGS model
- Measurement uncertainty is within the model error

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Eulerian fields

A new model ASHEE (Ash Equilibrium Eulerian) has been developed taking advantage of the OpenFOAM infrastructure

- it models a mixture of I gas species and J solid particle species, each with diameter d_j
- the ith gas species is characterized by the following fields in each point $(\mathbf{x}, t)$
    - bulk density ρ_i
    - velocity $\mathbf{u}_\mathrm{g}$
    - temperature T_g
- the jth solid species is characterized by the following fields in each point $(\mathbf{x}, t)$
    - bulk density ρ_j
    - velocity $\mathbf{u}_j$
    - temperature T_j

Mass averaged Eulerian fields

The conservation equations for mass, momentum and energy are written focusing on the mass averaged mixture properties:

Mass averaged field ψ_m

Firstly we define the mixture density as $\rho_\mathrm{m} = \sum_{i=1}^{I} \rho_i + \sum_{j=1}^{J} \rho_j$, so that the mass fractions of each phase are defined:

- $y_i = \rho_i / \rho_\mathrm{m}$
- $y_j = \rho_j / \rho_\mathrm{m}$.

Thus, given a generic field $\psi(\mathbf{x}, t)$ for the ith gas species (ψ_i) or for the jth solid species (ψ_j), we define

$$\psi_\mathrm{m} = \sum_{i=1}^{I} y_i \psi_i + \sum_{j=1}^{J} y_j \psi_j$$

Physical configuration

The Eulerian model in “mixture” formulation

$$
\begin{aligned}
&\partial_t \rho_\mathrm{m} + \nabla \cdot (\rho_\mathrm{m} \mathbf{u}_\mathrm{m}) = \sum_{j \in \mathcal{J}} S_j ; \\
&\partial_t(\rho_\mathrm{m} y_i) + \nabla \cdot (\rho_\mathrm{m} \mathbf{u}_\mathrm{g} y_i) = 0, \quad i \in \mathcal{I} ; \\
&\partial_t(\rho_\mathrm{m} y_j) + \nabla \cdot (\rho_\mathrm{m} \mathbf{u}_j y_j) = S_j, \quad j \in \mathcal{J} ; \\
&\partial_t(\rho_\mathrm{m} \mathbf{u}_\mathrm{m}) + \nabla \cdot (\rho_\mathrm{m} \mathbf{u}_\mathrm{m} \otimes \mathbf{u}_\mathrm{m} + \rho_\mathrm{m} \mathbb{T}_\mathrm{r}) = \\
&\qquad\qquad = -\nabla p + \nabla \cdot \mathbb{T} + \rho_\mathrm{m} \mathbf{g} + \sum_{j \in \mathcal{J}} S_j \mathbf{u}_j ; \\
&\partial_t(\rho_\mathrm{m} h_\mathrm{m}) + \nabla \cdot [\rho_\mathrm{m} h_\mathrm{m} (\mathbf{u}_\mathrm{m} + \mathbf{v}_h)] + \\
&\qquad + \partial_t(\rho_\mathrm{m} K_\mathrm{m}) + -\nabla \cdot [\rho_\mathrm{m} K_\mathrm{m} (\mathbf{u}_\mathrm{m} + \mathbf{v}_K)] = \\
&\qquad\qquad = \partial_t p + \nabla \cdot (\mathbb{T} \cdot \mathbf{u}_\mathrm{g} - \mathbf{q}) + \rho_\mathrm{m} (\mathbf{g} \cdot \mathbf{u}_\mathrm{m}) + \sum_{j \in \mathcal{J}} S_j (h_j + K_j) .
\end{aligned}
$$

Physical configuration

- The “mixture” formulation is useful in *two-way* coupled multiphase systems, where the mass of the dispersed phase has a non-negligible effect on the dynamics.
- The problem is formulated in the dispersed regime $\epsilon_{\rm s} \lesssim 10^{-3}$, collisions between particles are disregarded
- It focuses the mathematical problem on the mass averaged fields: $\rho_{\rm m}\,,\ \mathbf{u}_{\rm m}\,,\ h_{\rm m}$ (improving stability).
- All the effects due to the kinematic decoupling are confined in the terms $\mathbb{T}_{\rm r}(y_j, \mathbf{v}_j)\,,\ \mathbf{v}_h(y_j, \mathbf{v}_j, h_j, h_{\rm m})\,,\ \mathbf{v}_K(y_j, \mathbf{v}_j, K_j, K_{\rm m})$, keeping into account the effect of the relative velocity $\mathbf{v}_j = \mathbf{u}_j - \mathbf{u}_{\rm g}$
- No explicit dependence on the drag functional expression is necessary at this level

Equilibrium Eulerian model

- if particles are perfectly coupled both thermally ($T_j = T_\mathrm{g} = T$) and kinematically ($\mathbf{u}_j = \mathbf{u}_\mathrm{g} = \mathbf{u}$) we recover the dusty gas model, where all the decoupling terms are zero
- in ASHEE we adopt the equilibrium-Eulerian model, where the system is thermally perfectly coupled while the kinematic decoupling is approximated via an asymptotic expansion relative to the Stokes time τ_j:

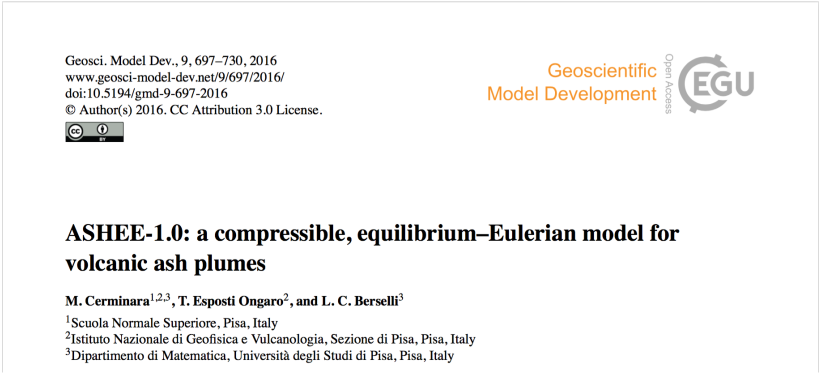
$$\mathbf{u}_j = \mathbf{u}_\mathrm{g} + \mathbf{w}_j - \tau_j(\mathbf{a}_\mathrm{g} + \mathbf{w}_j \cdot \nabla \mathbf{u}_\mathrm{g}) + O(\tau_j)$$

  where $\mathbf{w}_j = \tau_j \mathbf{g}$ is the settling velocity and $\mathbf{a}_\mathrm{g}$ is the gas phase acceleration

Equilibrium Eulerian model

- The contribution of the particle inertia can be accurately taken into account by using standard Navier-Stokes numerical algorithm, without needing to implicitly solve the drag term
- Particle decoupling and preferential concentration well modeled up to $St \lesssim 0.2$, keeping the advantages of the dusty gas model
- Total number of equation highly reduced for a polydispersed mixture ($4J$ PDEs less):
  - Eulerian: $I + 3 + 5J$
  - Equilibrium-Eulerian: $I + 3 + J$.
- Allows to solve efficiently the multiphase dynamics at geophysical scale for particles of size up to $\simeq 1$ mm.

Paper on the ASHEE model



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www.geosci-model-dev.net/9/697/2016/
doi:10.5194/gmd-9-697-2016

Geoscientific Model Development
Open Access

ASHEE-1.0: a compressible, equilibrium–Eulerian model for volcanic ash plumes

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[2]Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa, Pisa, Italy
[3]Dipartimento di Matematica, Università degli Studi di Pisa, Pisa, Italy

Numerical configuration

We implemented the following *subgrid-scale* LES models for the subgrid terms of the compressible equilibrium-Eulerian model:

- Compressible Smagorinsky (static and dynamic)
- Turbulent Kinetic Energy model (static and dynamic)
- WALE model (static and dynamic)

Numerical configuration

We modified the compressible monophase PISO-PIMPLE algorithm:

- predictor for the mixture density ρ_{m}
- PIMPLE loop
  - solve for the mass fractions $y_{i,j}$
  - predictor for the mixture velocity $\mathbf{u}_{\mathrm{m}}$
  - solve for the enthalpy h_{m}, fixing the compressibility
  - PISO loop
    - solve the decoupling
    - solve for pressure p
    - correct velocity and fluxes
  - solve LES models
- correct mixture density

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DHIT

Decaying Homogeneous and Isotropic Turbulence (256^3 cells)

The solver is able to simulate accurately the turbulence.

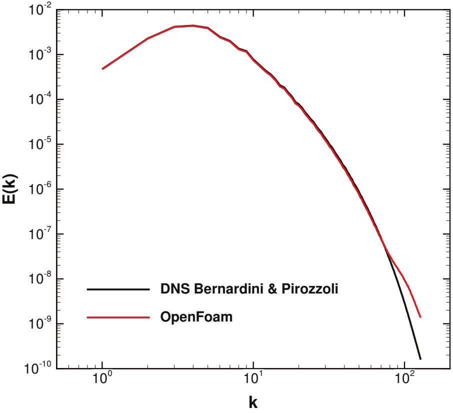


Figure: Test case validation: comparison with an eight order DNS after one large-eddy turnover time (10000 time steps).

Scalability

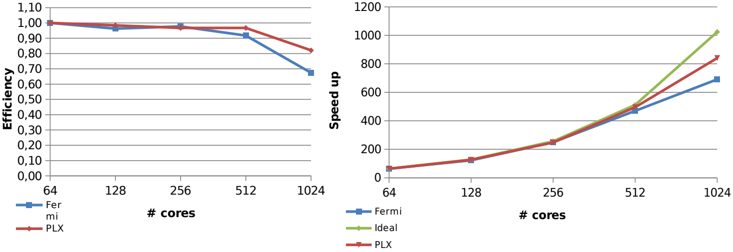


Figure: Scalability test on PLX and FERMI environments (with little output work). Collaboration between us and *Paride Dagna*.

In order to fix ideas, the solver reach a velocity in the range 1÷10 Mcells/s on 1024 cores (multiphase÷monophase) .

SGS LES models

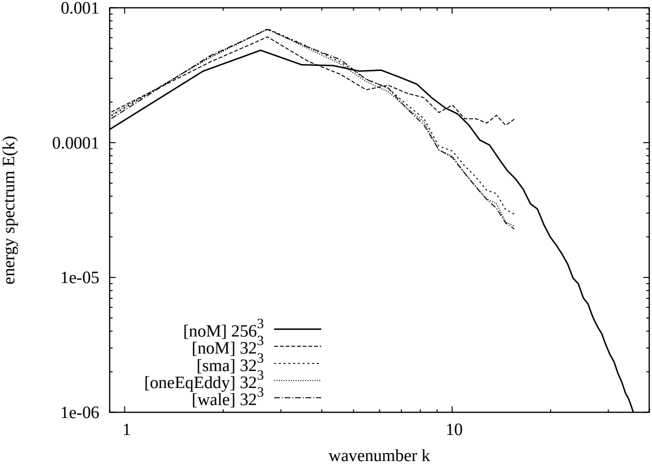


Figure: DHIT using static SGS LES models in a box with 32^3 cells

SGS LES models

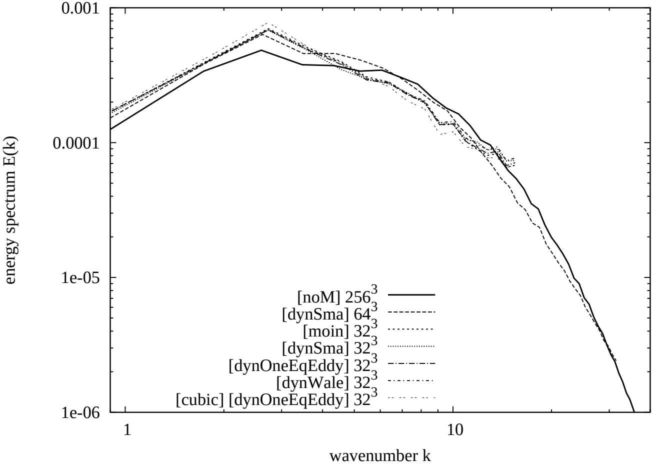
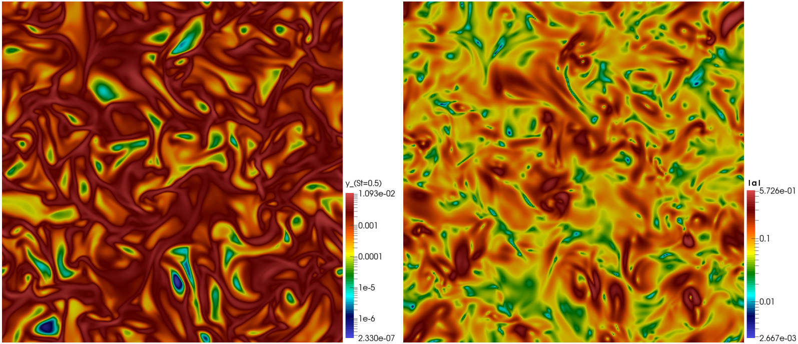


Figure: DHIT using dynamic SGS LES models in a box with 32^3 cells

Kinematic decoupling

Slice of the turbulent box at $t/\tau_{\mathrm{e}} \simeq 2.2$. The two panels represent respectively a logarithmic color map of $y_{j=2}$ (Stmax $= 0.5$) and of $|\mathbf{a}_{\mathrm{g}}|$



Kinematic decoupling

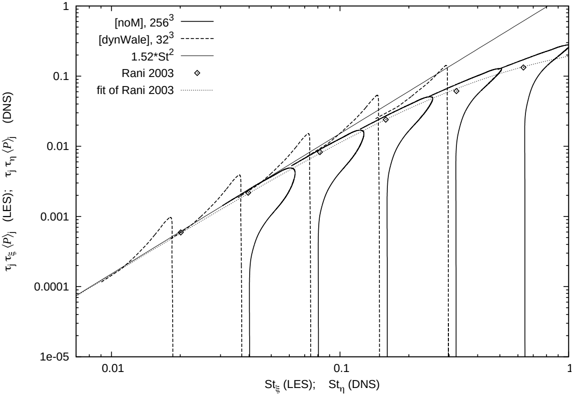


Figure: Evolution of the degree of preferential concentration with St_ξ (LES) or St_η (DNS). We obtain a good agreement between equilibriumEulerian LES/DNS and Lagrangian DNS simulations.

Advection schemes

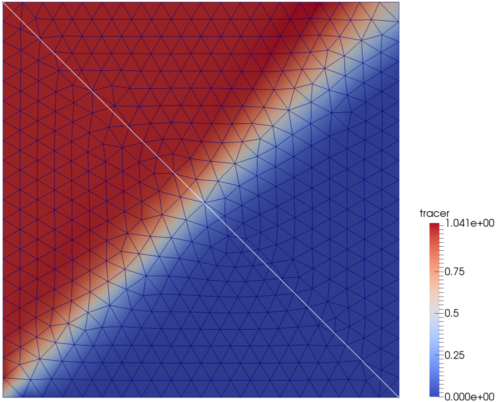


Figure: Advection test case from *Holzmann-cfd* solved with ASHEE

Advection schemes

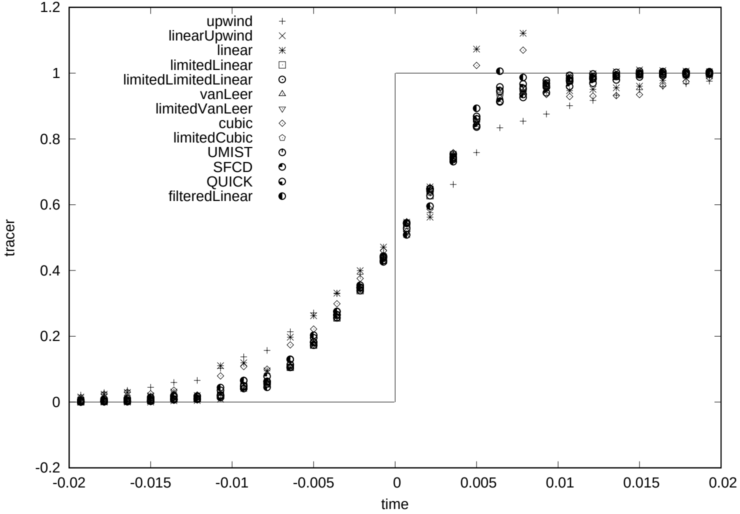


Figure: Tracer mass fraction along the cavity section.

Advection schemes

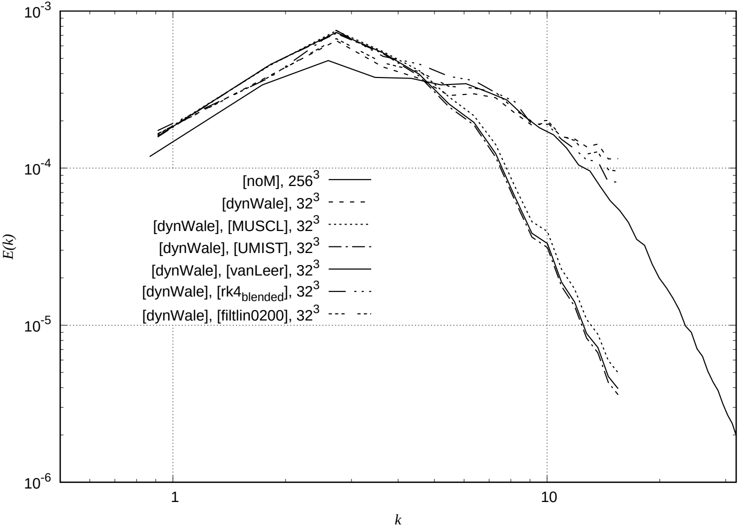
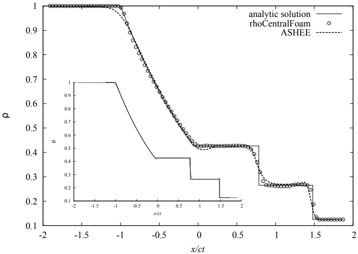
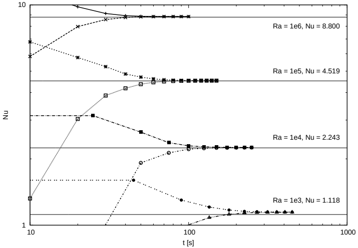


Figure: Performances of OpenFOAM schemes in DHIT LES

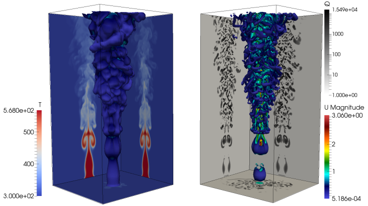
Other benchmarks



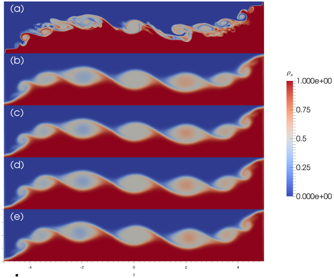
Sod's shock tube



Natural convection



Experimental plume



Mixing

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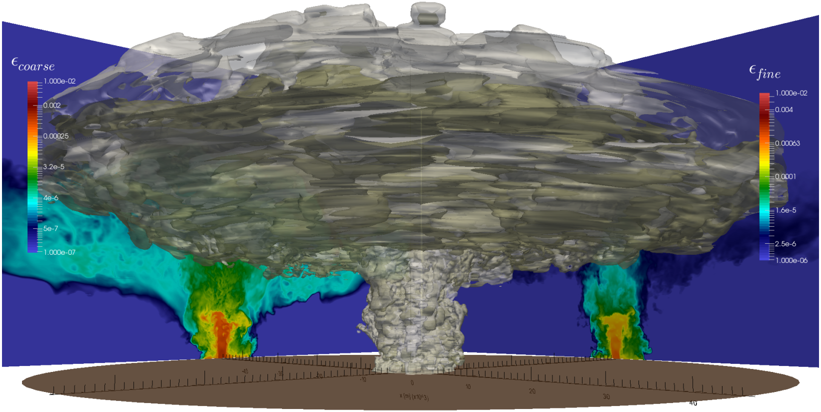
Plinian eruption

We have used ASHEE to simulate volcanic eruptions (scale ≈ 100 km) from the vent (mass eruption rate up to Mton/s) to the atmosphere



Volcanic plumes

We are participating to an international benchmark initiative involving two numerical simulations:

weakPlume

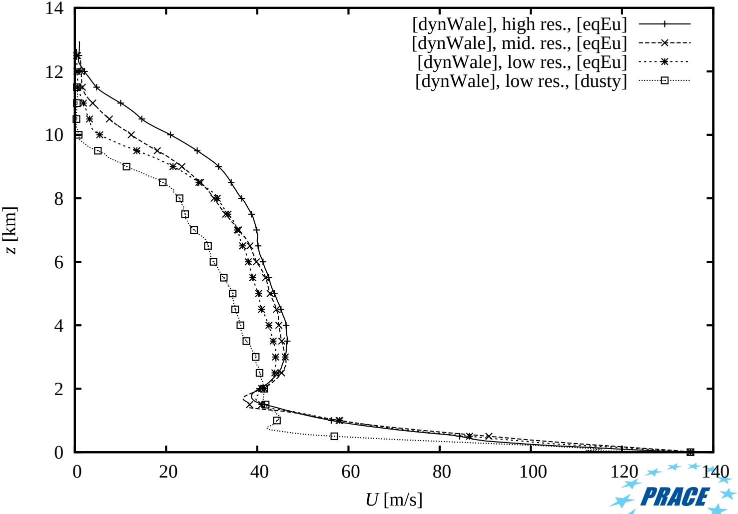
- duration: 0.2 hours
- Mass flow rate: $1.5 * 10^6$ kg/s
- Exit velocity: 135 m/s
- Exit temperature: 1273 K
- Exit gas fraction: 3 wt%
- Grain size distribution:
  - coarse: 1 mm
  - fine: 62.5 μm

strongPlume

- duration: 2.5 hours
- Mass flow rate: $1.5 * 10^9$ kg/s
- Exit velocity: 275 m/s
- Exit temperature: 1053 K
- Exit gas fraction: 5 wt%
- Grain size distribution:
  - coarse: 0.5 mm
  - fine: 15.6 μm

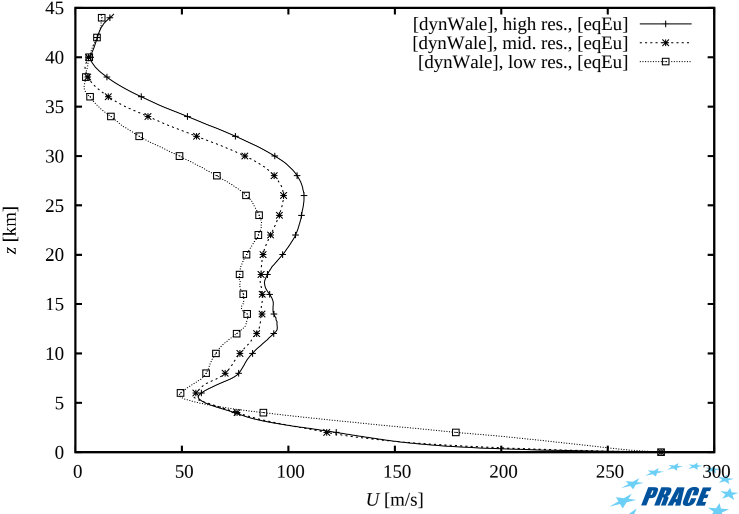
Effects of resolution and SGS model

Time and horizontal average of the velocity field, with 8, 16 and 32 cells in a vent diameter; with and without decoupling model (weakPlume)



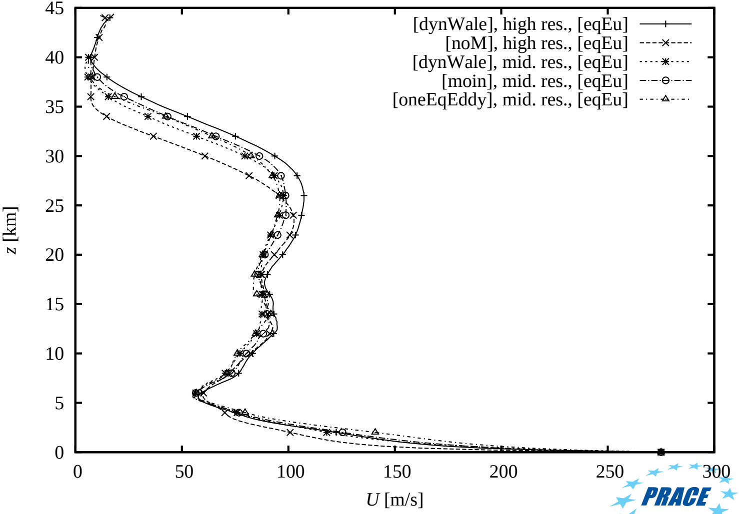
Effects of resolution

Time and horizontal average of the velocity field, with 8, 16 and 32 cells in a vent diameter (strongPlume)



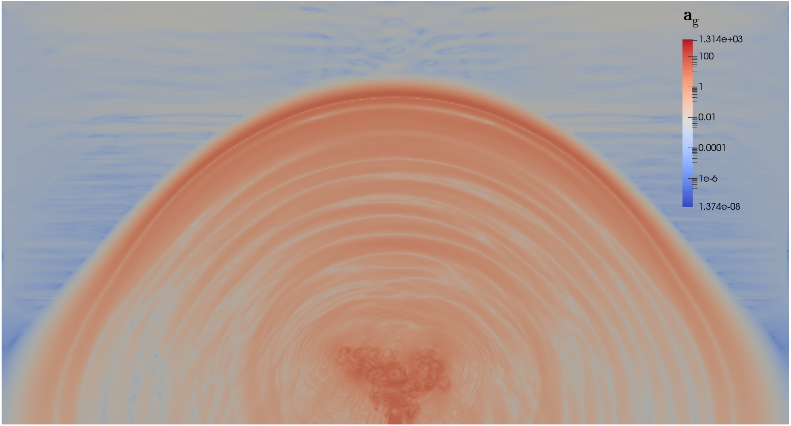
Effects of SGS model

Time and horizontal average of the velocity field, with 16 and 32 cells in a vent diameter; with different SGS models (strongPlume)



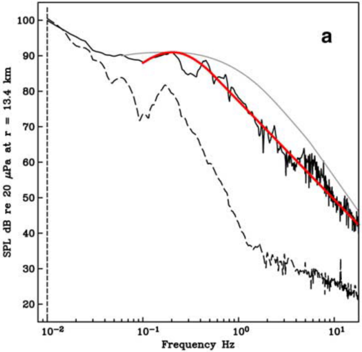
Volcanic infrasound

Compressibility and turbulence generate infrasound

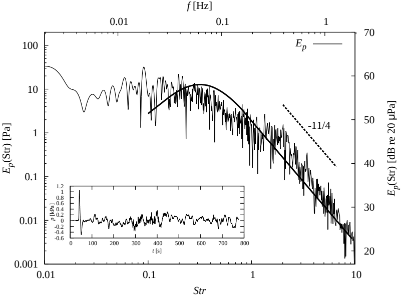


Observations & simulations

Observation of 8 March 2005 Mount St. Helens eruption (Matoza et al. 2009)



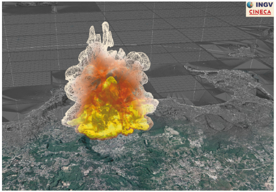
Simulation with ASHEE of the strongPlume eruption

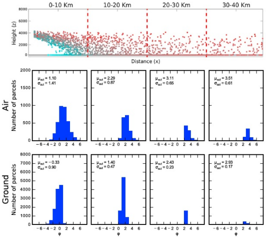


Summary of the second part

- We have developed the compressible version of the equilibrium-Eulerian model (ASHEE model)
- We have implemented it into the OpenFOAM infrastructure
- the solver has been tested up to 1024 cores. It shows a reasonable efficiency ($> 60\%$) on the Cineca Fermi infrastructure
- The numerical scheme has been tested and chosen to maximize accuracy and stability of dynamic LES simulations
- A number of different benchmarks have been performed satisfactorily
- The new solver is able to accurately and efficiently capture clustering, preferential concentration and settling up to 1 mm particles
- Applications to volcanological scale have been performed, comparing results with other models and with observations

Volcanic hazard assessment: an HPC/HTC challenge





Complex physics, multiscale dynamics

- Non-newtonian (non-linear) rheology
- Multiphase flows
- Broad range of spatial/temporal scales

Uncertainty on initial/boundary conditions

- Partial knowledge of the initial state
- Catastrophic dynamics
- Difficulty of measurements
- Repeatability issues

Future perspectives

Magma ascent modeling

- Implementation of fragmentation conditions
- More complex geometries
- Fluid-structure interaction

Volcanic plume modeling

- Add an arbitrary wind field
- Add volcano topography
- Add micro-physics, as water condensation, ash particles shape and aggregation

Future perspective

Numerical issues

- Non-reflecting boundary conditions
- Improve the advection scheme
- Implement a shock capturing correction
- Optimize parallel linear algebra in OpenFOAM

Volcanic hazard assessment

- Sensitivity and uncertainty analysis (coupled with Dakota).
- Coupling with meteorological solvers.
- "Nowcasting" of volcanic plume scenarios.

Thank You!

Contacts

- research web-page: *https://sites.google.com/site/matteocerminara*
- CFD movies: *https://www.youtube.com/user/MatteoCerminara*

Acknowledgments: we acknowledge CINECA for the availability of high-performance computing resources and technical support on porting OpenFOAM on HPC architectures in the framework of ISCRA projects: IsB06 VolcFOAM, IsC26 VolcAshP and IsC07 GEOFOAM.