Developing SPH Based Modeling of Volcanic Plumes using Modified SPH Schemes

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1. Motivation for Choosing SPH
2. Physics Model
3. SPH Discretization
4. Verification and Validation
5. Data Structure and Parallelism

Motivation for Choosing SPH

Volcanic plume development is essentially a multi-phase, turbulent mixing process coupled with heat transfer and other microphysics processes without pre-defined boundaries. SPH (Smoothed particle hydrodynamics), as a mesh-less method, is suitable for such problems for several reasons:

- SPH is able to automatically construct the interface.
- Multiphase modeling is easily accomplished using SPH
- Adding of new physics and new phases is easier in terms of programming in SPH
- With very limited global communication requirements, SPH solvers can scale better for parallel computing than grid based ones.

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The governing equations and EOS for closing the system of equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{1}$$

$$\frac{\partial \rho \xi}{\partial t} + \nabla \cdot (\rho \xi \mathbf{v}) = 0 \tag{2}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v} + p\mathbf{I}) = \rho \mathbf{g} \tag{3}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p)\,\mathbf{v}] = \rho \mathbf{g} \cdot \mathbf{v} \tag{4}$$

$$p = (\gamma_m - 1)\,\rho e \tag{5}$$

Specific heat ratio γ_m is updated based on massfraction of erupted material:

$$\gamma_m = R_m / C_{vm} + 1 \tag{6}$$

$$R_m = \xi_g R_g + \xi_a R_a \tag{7}$$

$$C_{vm} = \xi_s C_{vs} + \xi_g C_{vg} + \xi_a C_{va} \tag{8}$$

$$\xi_a = 1 - \xi \tag{9}$$

$$\xi_g = \xi \cdot \xi_{g0} \tag{10}$$

$$\xi_s = \xi - \xi_g \tag{11}$$

Boundary Conditions

Eruption BC

$$\rho = const = p/\left(R_m T\right) \quad (12)$$

$$\xi = const = 1 \quad (13)$$

$$\mathbf{v} = const = \{u, v, w\}^T \quad (14)$$

$$\frac{\partial e}{\partial n} = \dot{M}e/\left(\pi r^2\right) \quad (15)$$

No-slip wall BC

$$\frac{\partial \rho}{\partial n} = const = 0 \quad (16)$$

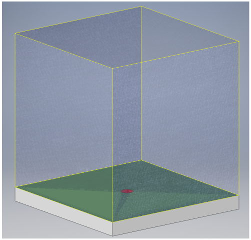
$$\frac{\partial \xi}{\partial n} = const = 0 \quad (17)$$

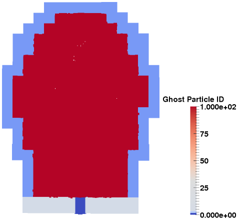
$$\mathbf{v} = const = \{0, 0, 0\}^T \quad (18)$$

$$\frac{\partial e}{\partial n} = 0 \quad (19)$$

Pressure outlet BC

$$p = p_a(z) \quad (20)$$





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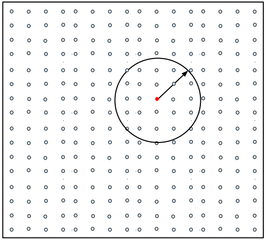
Any function A and its derivative can be approximated by:



$$< A(\mathbf{x}) > \approx \sum_b m_b \frac{A_b}{\rho_b} w(\mathbf{x} - \mathbf{x}_b, h) \quad (21)$$

$$< \nabla A(\mathbf{x}) > \approx \sum_b m_b \frac{A_b}{\rho_b} \nabla w(\mathbf{x} - \mathbf{x}_b, h) \quad (22)$$

Truncated Guassian kernel functions

$$w(\mathbf{x} - \mathbf{x}_b) = \begin{cases} \frac{1}{(h\sqrt{\pi})^d} exp\left[-\left(\frac{\mathbf{x} - \mathbf{x}\prime}{h} \right)^2 \right] & |\mathbf{x} - \mathbf{x}\prime| \leq 3h \\ 0 & \text{Otherwise} \end{cases} \quad (23)$$

We adopt the following artificial viscosity developed based on Riemann Solvers,:

$$\Pi_{ab}^{\beta} = \begin{cases} \dfrac{-\alpha\mu_{ab}\bar{c}_{ab} + \beta\mu_{ab}^2}{\bar{\rho}_{ab}} & \mathbf{v}_{ab}\cdot\mathbf{x}_{ab} < 0 \\ 0 & \mathbf{v}_{ab}\cdot\mathbf{x}_{ab} > 0 \end{cases} \tag{24}$$

Where

$$\mu_{ab} = \frac{h\mathbf{v}_{ab}\cdot\mathbf{x}_{ab}}{\mathbf{x}_{ab}^2 + (\eta h)^2} \tag{25}$$

Time step is constrained by CFL condition

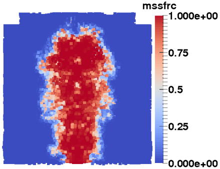
$$\Delta t = \mathrm{CFL}\min_a \left\{ \frac{\left[\frac{m_a}{\rho_a}\right]^{\frac{1}{d}}}{c_a} \right\} \tag{26}$$

The classical SPH method was known to suffer from tensile instability and boundary deficiency. To address these difficulties, we adopted a corrected SPH formulation.

$$A_a = \frac{\sum_b m_b \dfrac{A_b}{\rho_b} w\left(x_a - x_b, h\right)}{\sum_b m_b \dfrac{1}{\rho_b} w\left(x_a - x_b, h\right)} \tag{27}$$

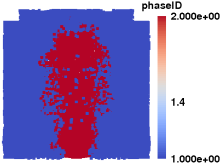
$$\nabla A_a = \frac{\sum_b m_b \dfrac{A_b - A_a}{\rho_b} \nabla_a w\left(x_a - x_b, h\right)}{\sum_b m_b \dfrac{x_b - x_a}{\rho_b} \nabla_a w\left(x_a - x_b, h\right)} \tag{28}$$

In our model, only density needs to be updated respectively for each phase:



$$< \rho_{\alpha}^{a} >= \frac{\sum m_b w_{\alpha b}(h)}{\sum \frac{m_b}{\rho_b} w_{\alpha b}(h) + \sum \frac{m_j}{\rho_j} w_{\alpha j}(h)} \quad (29)$$

$$< \rho_{\alpha}^{sg} >= \frac{\sum_j m_j w_{\alpha j}(h)}{\sum \frac{m_b}{\rho_b} w_{\alpha b}(h) + \sum \frac{m_j}{\rho_j} w_{\alpha j}(h)} \quad (30)$$



- The mass discontinuity and density discontinuity issues in traditional formulations of SPH is fixed by this new formulation
- In areas far away from the interface, updating of density is exactly the same as that for single phase flow

A LANS Type Turbulence Model

To capture sub-particle scale momentum and energy exchange due to turbulence, we adopt a LANS type turbulence model, the $SPH - \varepsilon$ turbulence model and extend it for compressible flow.
Velocity is smoothed (averaged) by

$$\widehat{\mathbf{v}}(\mathbf{x}) = \int \mathbf{v}(\mathbf{x}\prime)\, G(|\mathbf{x}\prime - \mathbf{x}|, l)\, d\mathbf{x}\prime \tag{31}$$

Where G satisfies:

$$\int G(|\mathbf{x}\prime - \mathbf{x}|, l)\, d\mathbf{x}\prime = 1 \tag{32}$$

$$\lim_{h \to 0} G(\mathbf{x}\prime - \mathbf{x}, h) = \delta(\mathbf{x}\prime - \mathbf{x}) \tag{33}$$

Averaging introduces an extra turbulence stress term:

$$\Phi_{ab} = \frac{\varepsilon}{2} \frac{\mathbf{v}_{ab} \cdot \mathbf{v}_{ab}}{\rho_b} \tag{34}$$

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Use Reynolds analogy to model the heat transfer due to turbulence.

$$\kappa = \frac{C_p \mu}{Pr} \tag{35}$$

Instead of an analytical expression, heat transfer coeffient is calculated for each pair of particles.

$$\kappa_{t,ab} = \begin{cases} 0 & \textit{if} \quad \mathbf{v}_{ab} \cdot \mathbf{x}_{ab} \leq 0 \\ \dfrac{\varepsilon \bar{C}_{p,ab} \bar{\rho}_{ab} x_{ab}^2 \mathbf{v}_{ab} \cdot \mathbf{v}_{ab}}{2SPr_t \bar{h}_{ab} \bar{c}_{ab} \mathbf{v}_{ab} \cdot \mathbf{x}_{ab}} & \text{otherwise} \end{cases} \tag{36}$$

Discretized Governing Equations

$$\left\langle \frac{d\mathbf{v}_\alpha}{dt} \right\rangle = -\sum_b \left[m_b \left(\frac{p_b}{\rho_b^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha b}^{\beta} - \Phi_{\alpha b} \right) \nabla_\alpha w_{\alpha b}(h) \right] - \sum_j \left[m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha j}^{\beta} - \Phi_{\alpha j} \right) \nabla_\alpha w_{\alpha j}(h) \right] + \mathbf{g} \tag{37}$$

$$\left\langle \frac{de_\alpha}{dt} \right\rangle = 0.5 \sum_b \left[m_b \widehat{\mathbf{v}_{\alpha b}} \left(\frac{p_b}{\rho_b^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha b}^{\beta} - \Phi_{\alpha b} \right) \nabla_\alpha w_{\alpha b}(h) \right] + 2 \sum_b \frac{m_b}{\rho_\alpha \rho_b} \kappa_{t,\alpha b} (T_\alpha - T_b) F_{\alpha b}(h) + 0.5 \sum_j \left[m_j \widehat{\mathbf{v}_{\alpha b}} \left(\frac{p_j}{\rho_j^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha j}^{\beta} - \Phi_{\alpha j} \right) \nabla_\alpha w_{\alpha j}(h) \right] + 2 \sum_j \frac{m_j}{\rho_\alpha \rho_j} \kappa_{t,\alpha j} (T_\alpha - T_j) F_{\alpha j}(h) \tag{38}$$

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Verification and Validation

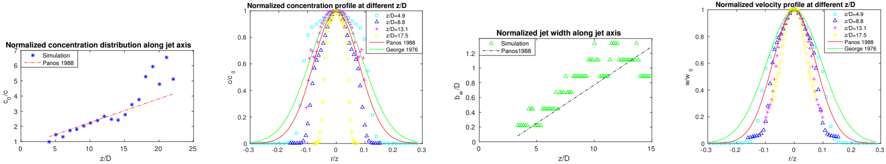

Figure: JPUE test verification: dimensionless velocity and concetration distribution along centraline and across the cross-section.

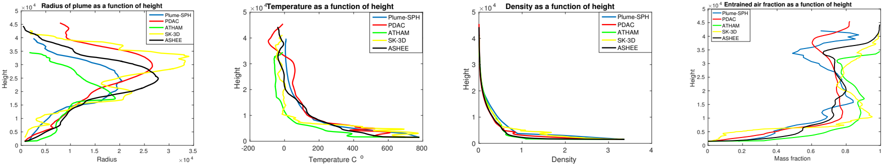

Figure: Simulation of Pinatubo (Philippines, 15 June 1991) : integrated are profiles compared with existing mesh-based models

Annimation of Pinatubo Eruption

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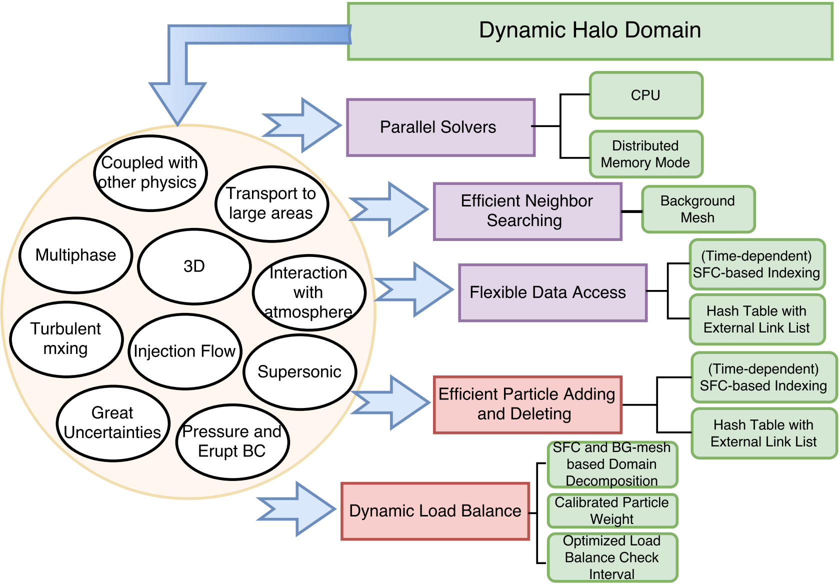
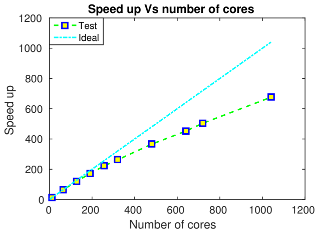
Eruption condition, atmosphere, material propertities are mimic Pinatubo eruption (Philippines, 15 June 1991).
Eruption conditions: vent velocity is 275 $m \cdot s^{-1}$, vent gas mass fraction is 0.05, vent temperature is 1053 K, vent height is 1500 km, mass discharge rate is $1.5 \times 10^9 kg \cdot s^{-1}$.

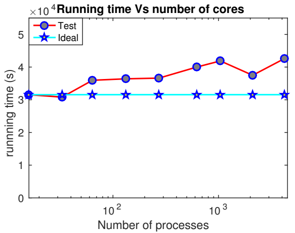
Play/Pause

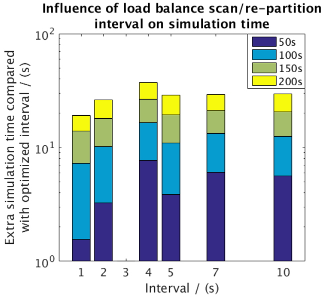
Requirement and Our Strategies

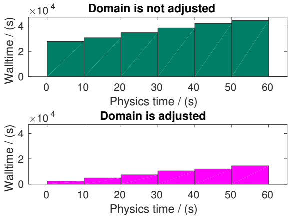


Scalability and Computational Permormance









Summary

- We present an initial effort and results towards developing a first principle based plume model with comprehensive physics, adopting proper numerical tools and high performance computing.
- More advanced numerical techniques, such as adaptive particle size, Godunov-SPH, semi-explicit time advancing scheme and better data management strategies and algorithms are on our list to exploit in the future.

Thank you!
Questions are welcome.

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