Data Management and Volcano Plume Simulation with Parallel SPH Method and Dynamic Halo Domains

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Outline

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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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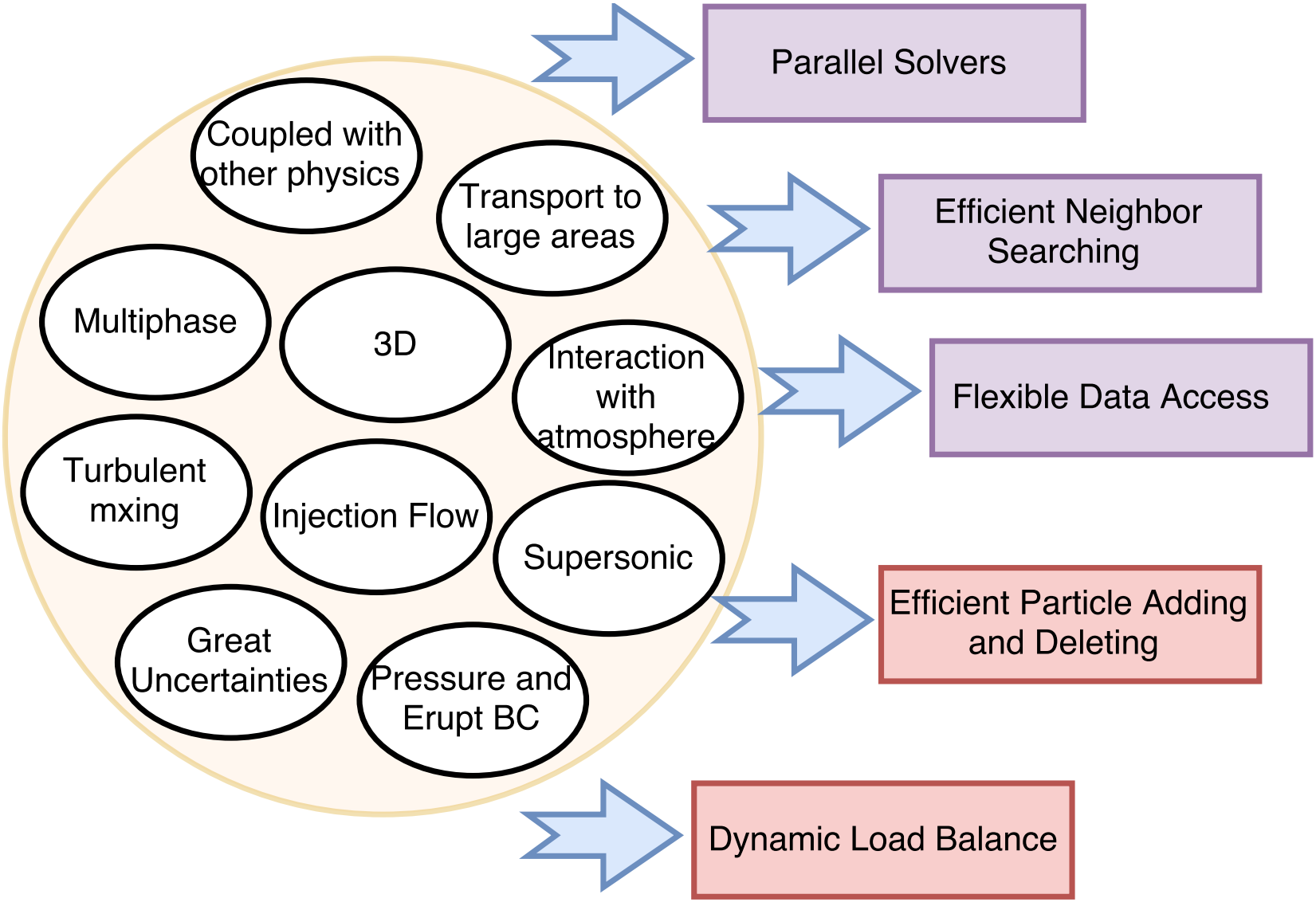
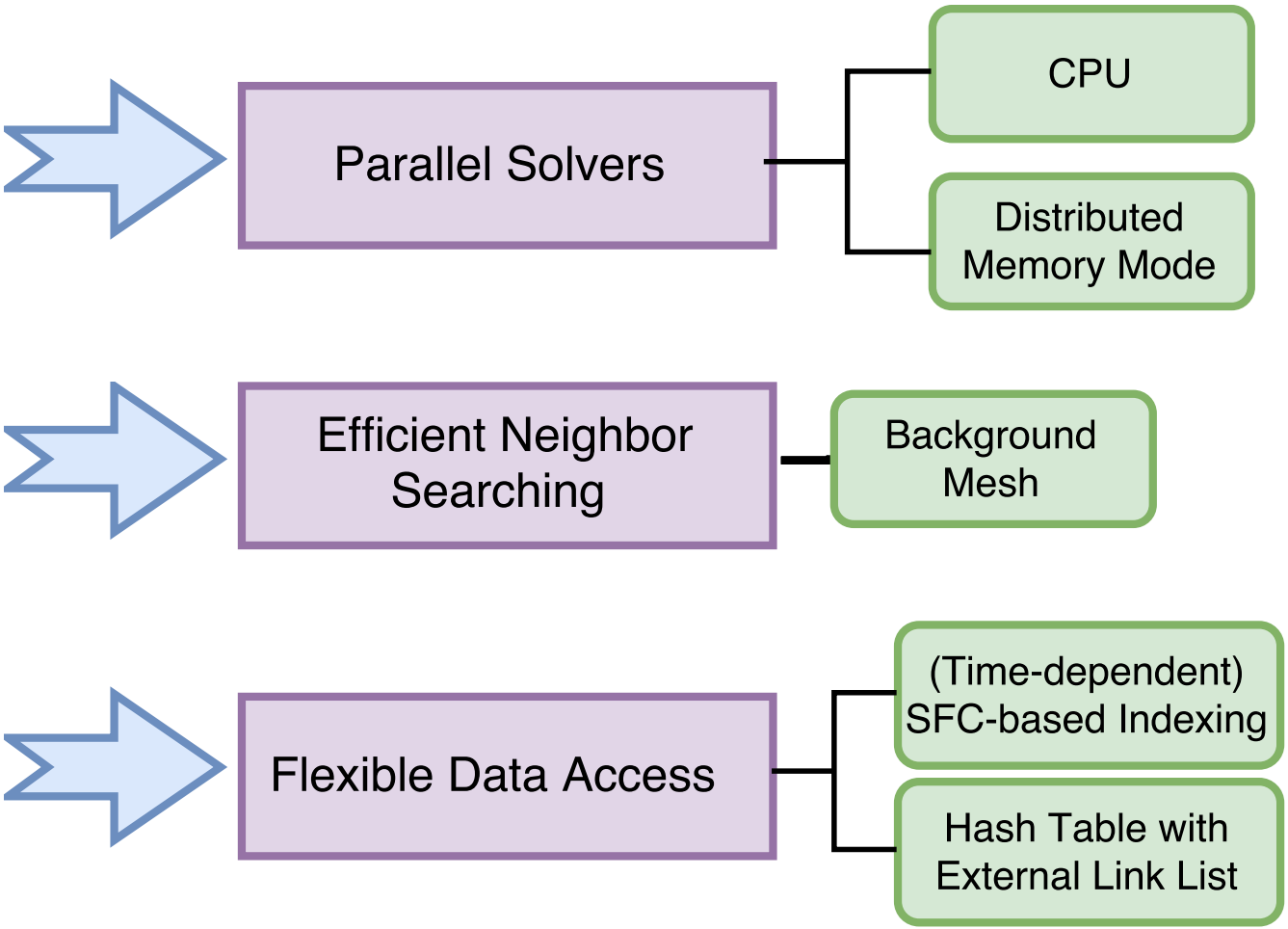
Requirements of the application



Our Strategies



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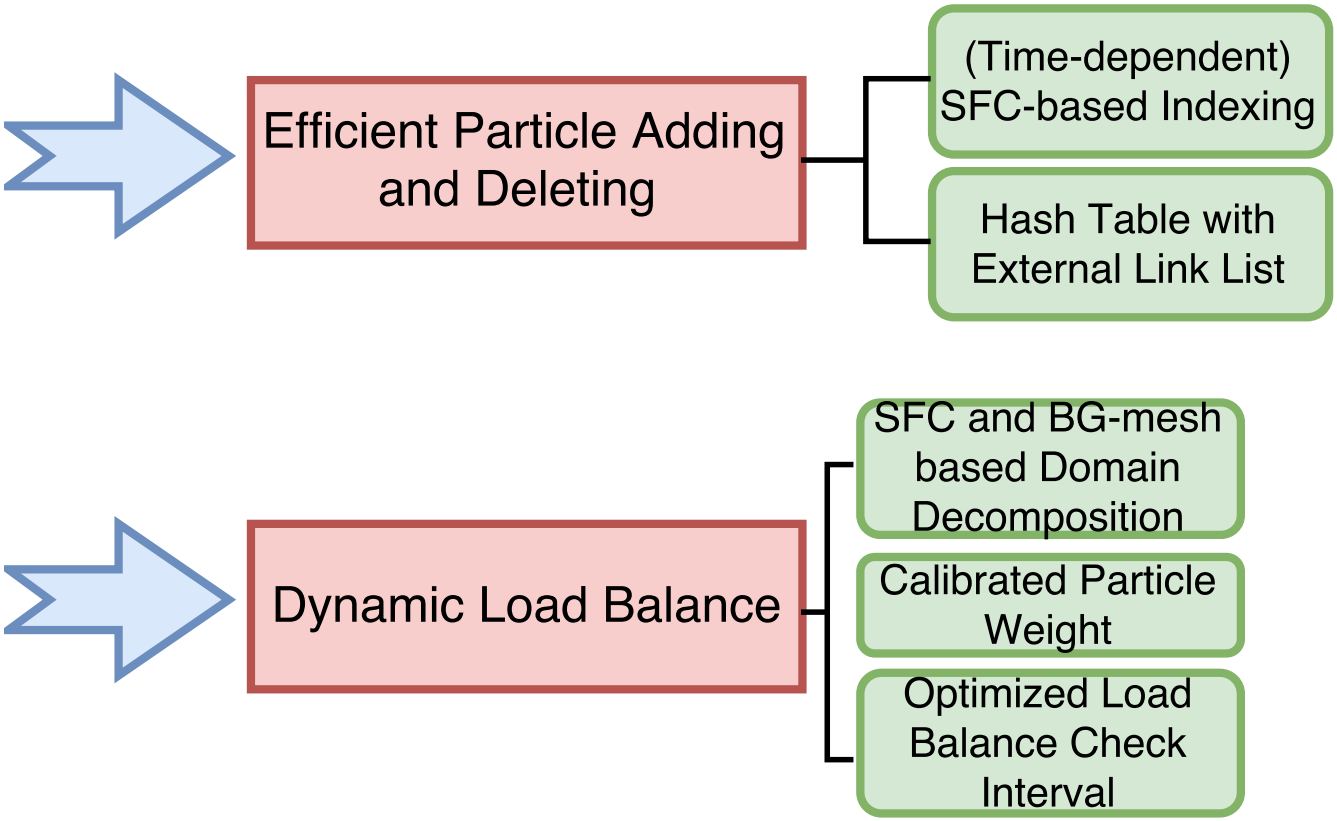

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Paricles and Bucket

The basic data structures used to support SPH are particles and buckets.

Particle Class

Information that is contained in particle objects : Unique ID (key), affiliation, **primary variables, secondary variables**, flags and neighbor information.

Bucket Class

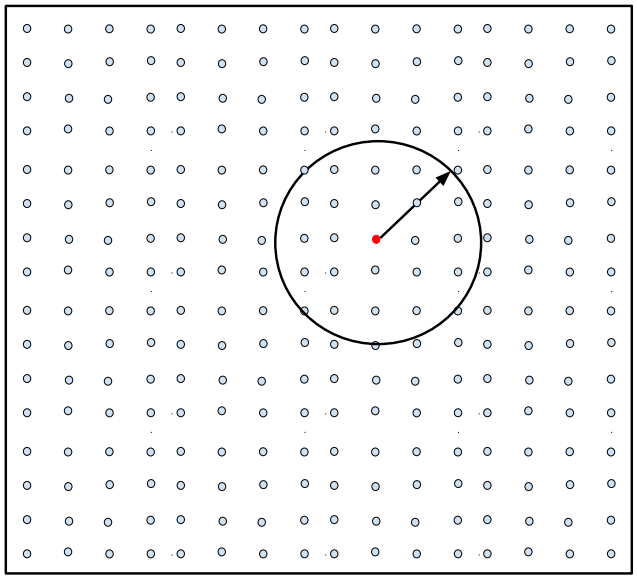
Information that is contained in bucket objects : Unique ID (key), affiliation, dimension information, flags, neighbor information and contained particles.

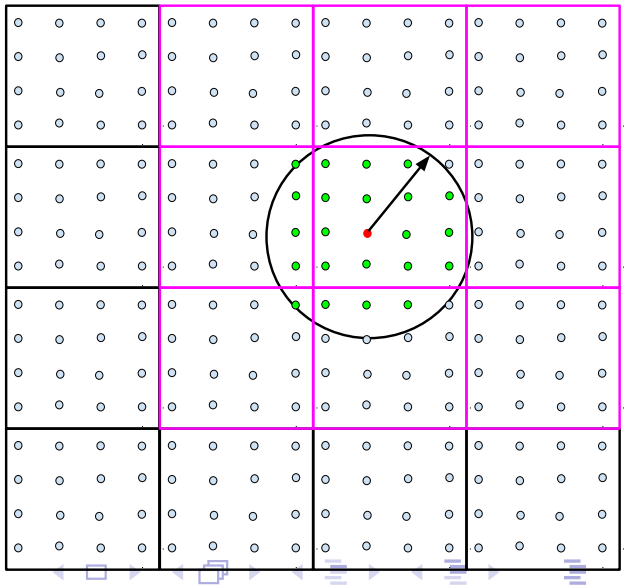
In SPH any function $A(\mathbf{x})$ and gradient of it can be approximated by.

$$< A(\mathbf{x}) > \approx \sum_b m_b \frac{A_b}{\rho_b} w(\mathbf{x} - \mathbf{x}_b, h) \tag{1}$$

$$< \nabla A(\mathbf{x}) > \approx \sum_b m_b \frac{A_b}{\rho_b} \nabla w(\mathbf{x} - \mathbf{x}_b, h) \tag{2}$$

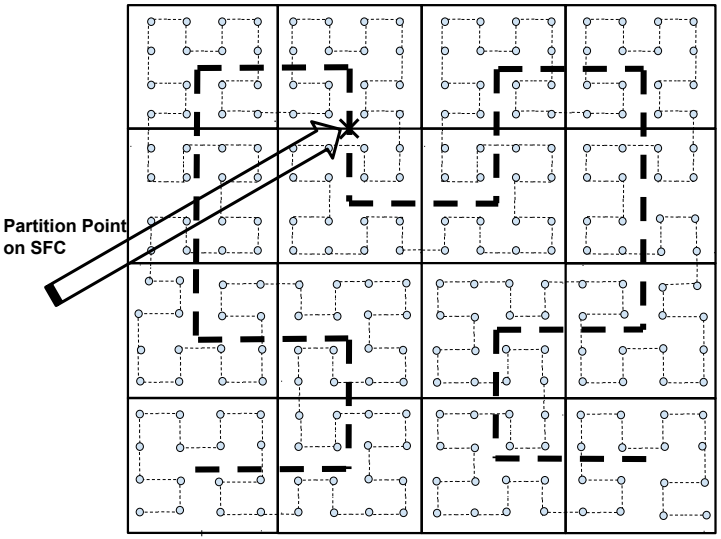
$b \in \{\text{particles with overlapping support}\} \subset \{\text{all particles}\}$

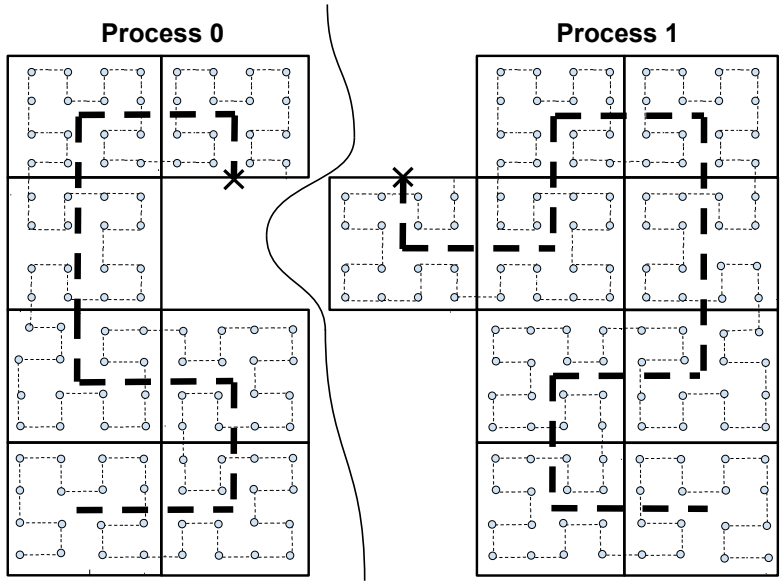




SFC-based Index & Domain Decomposition

SFC based key is defined as: $k = h_n(\mathbf{x})$, Where $h_n(\mathbf{x}) : [0,1]^n \rightarrow [0,1]$

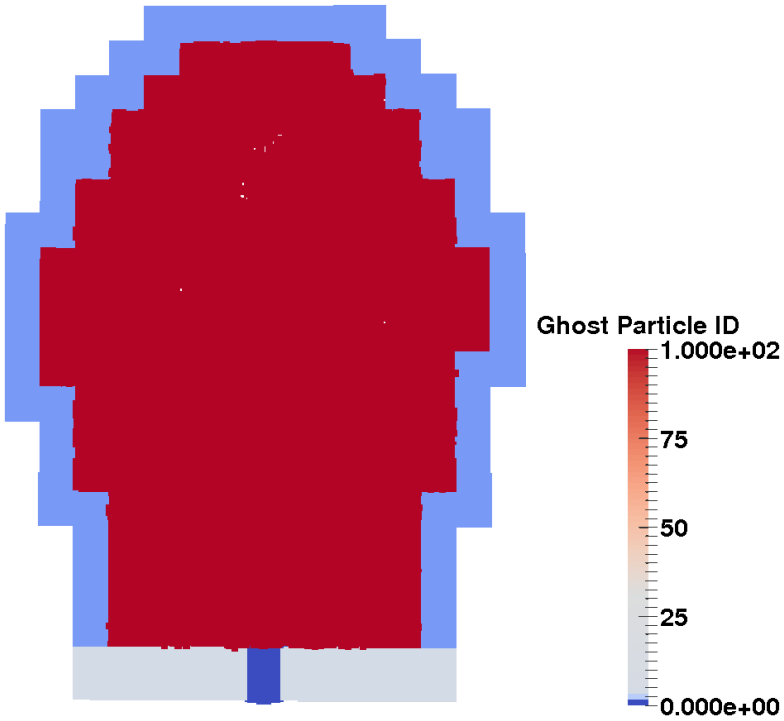


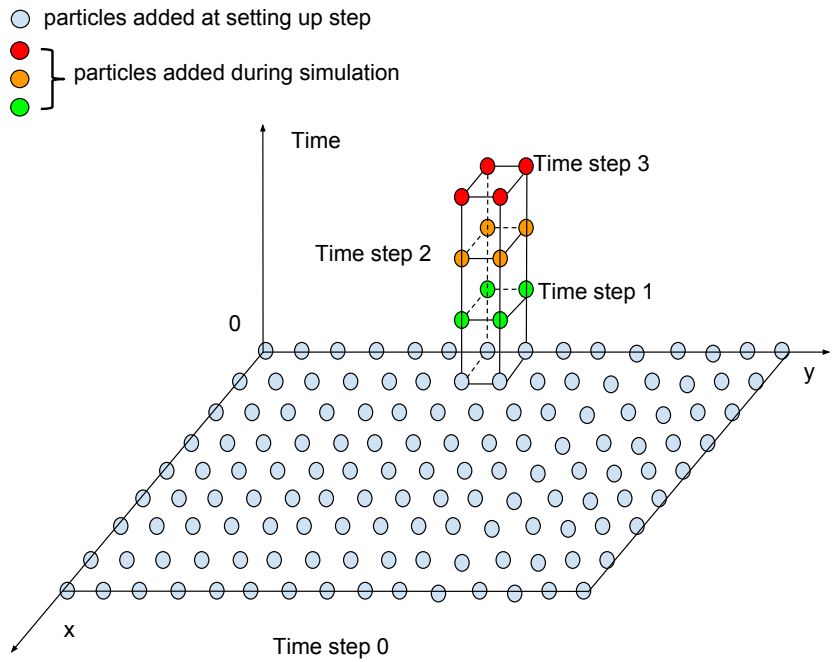


Features of SFC-based Index

- Guaranteed uniqueness of the indexing.
- Generating of indices are fast and independent
- Conserve spatial locality in ordering $\rightarrow$ promotes memory locality / **cache reuse**
- Global address space and ordering for use in domain decomposition

Eruption BC & Time-dependent SFC



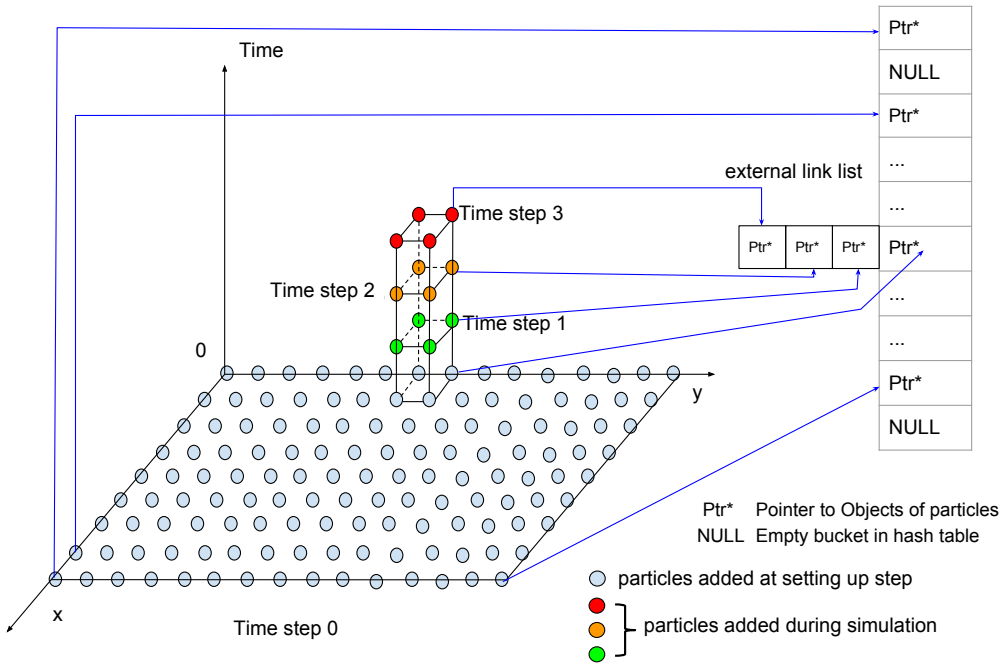


Time-dependent SFC

$$h_n : [0,1]^n \times \mathbf{T} \rightarrow [0,1] \times \mathbf{N} \tag{3}$$

Where $\mathbf{T} \subset [0, \infty)$ is the time dimension, and $\mathbf{N} = \{0, 1, 2, 3...\}$.
Then the time-dependent key can be expressed as: (k, n)

Hash Table with External Linked List



Hash Function

$$Index = \frac{Key - Min\,Key}{Max\,Key - Min\,Key} \times Hash\,Table\,Size \tag{4}$$

To avoid a non-uniform sparse hash table, only plug the first number, k, of the key, into Eq. (4). All particles with the same birth location will hash to the same index and be handled by external linked lists.

Dynamic Load Balance (Weighted particles)

The domain is decomposed by cutting SFC of buckets into pieces of equal work load. The work load of each bucket is calculated by summing up weights of all particles contained by that bucket. The work load associated to each particle is calibrated based on profilling data.

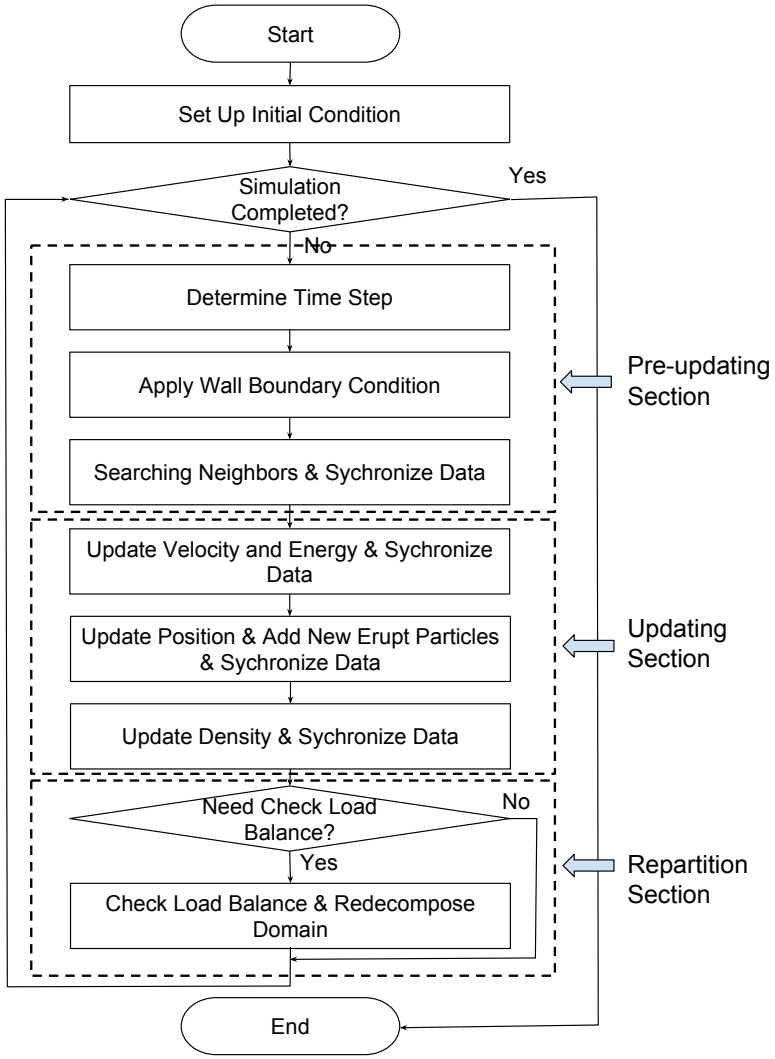
Step	Cost (ms)	Real	wall	eruption	pressure
neighbor search	0.41	Yes	No	No	No
update momentum and energy	0.70	Yes	No	No	No
update density	0.42	Yes	No	No	No
update position	0.01	Yes	No	Yes	No
velocity filtering	0.43	Yes	No	No	No
apply wall boundary condition	0.75	No	Yes	No	No
summation (ms)	-	1.97	0.75	0.01	0.00

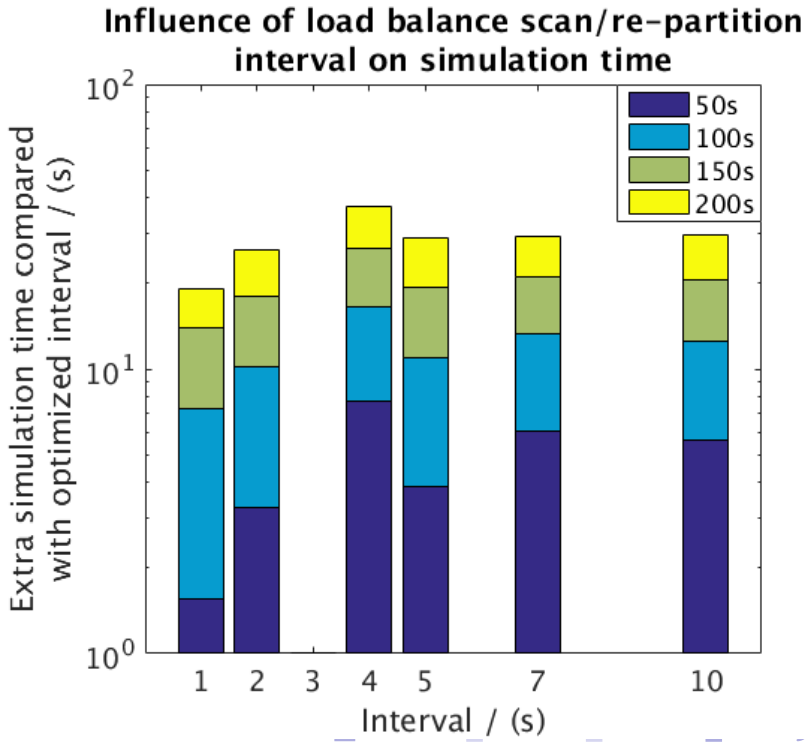
Compared with uniform particle weight, calibrated particle weights is computationally more efficient.

Physical time	10 s	20s	30 s	40 s
Same weight	1141.7	4119.4	10371.0	12453.7
Calibrated weights	1108.2	4057.0	10281.5	12166.3

Dynamic Load Balance (Load check interval)

The movement of particles and expansion of computational domain can lead to large load imbalance.





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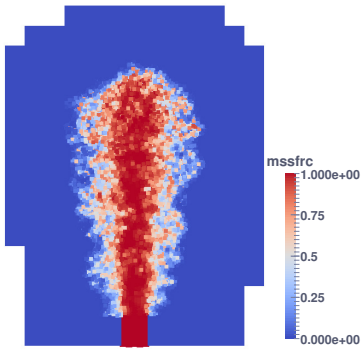
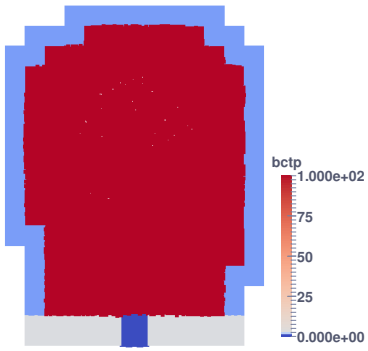
Dynamic Halo Domain

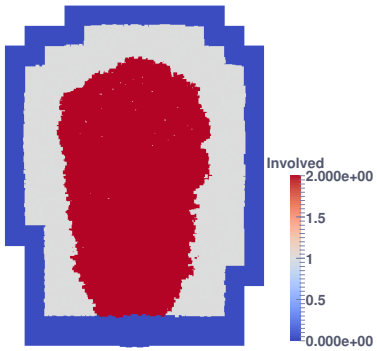
A lot of CPU time will be spent on computing associated with these stationary particles. The computational cost will be greatly reduced if the computational domain changes adaptively during simulation.

Our strategy

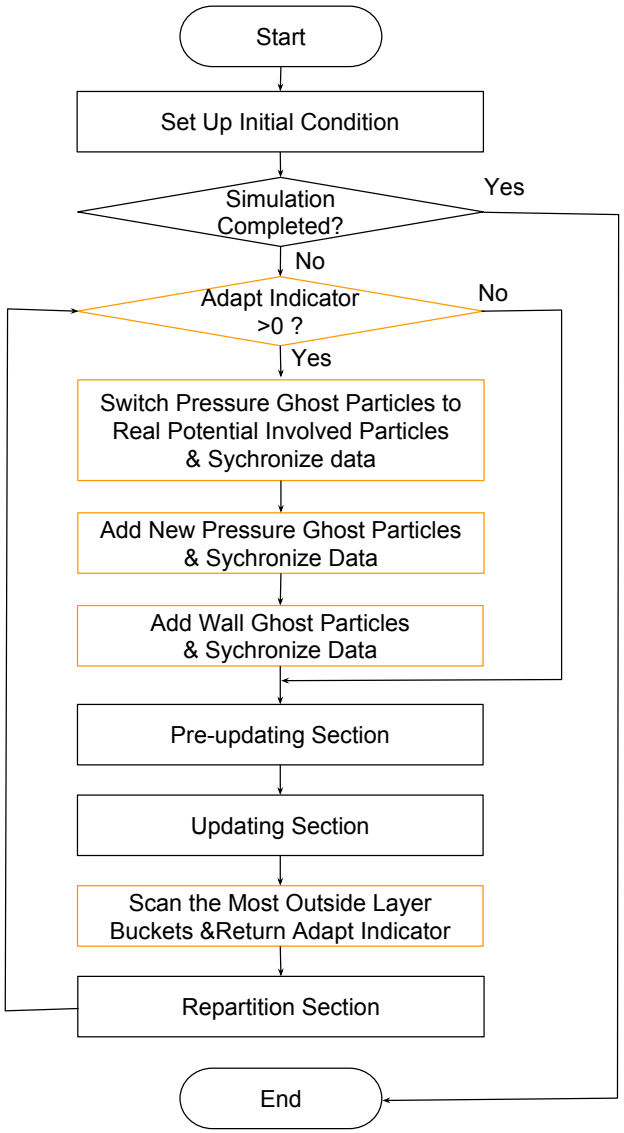
- An involvement flag to distinguish different states of involvement
- A scan function to monitor the outermost layer of the domain
- Shift pressure ghost particles into real particles when necessary





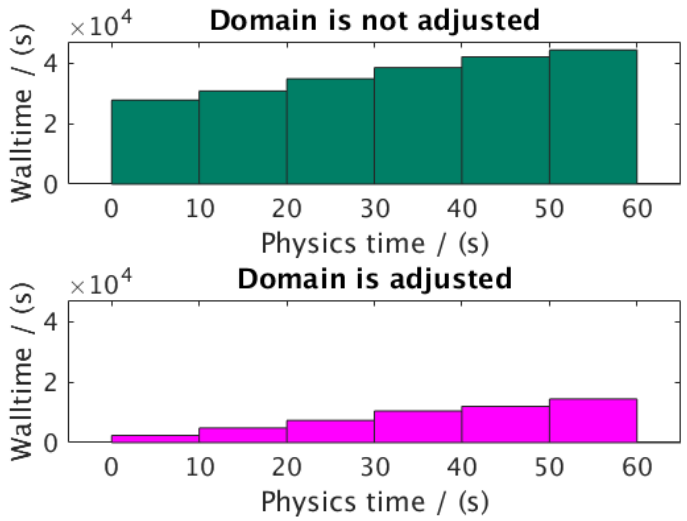


Dynamic Halo Domain



SWCH: switch pressure ghost particles to real. ADPP: add new pressure ghost particles. ADWP: add wall ghost particles. SCN: scann the outmost layer of the domain

Functions	Total time (s)	Called times
UPME	2954.8	201
UPP	38.55	201
ADPP	21.51	3
ADWP	8.88	3
SWCH	0.08	2
SCN	7.72	201



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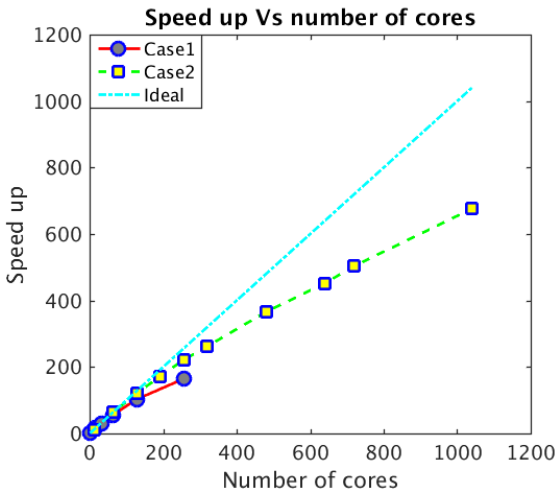
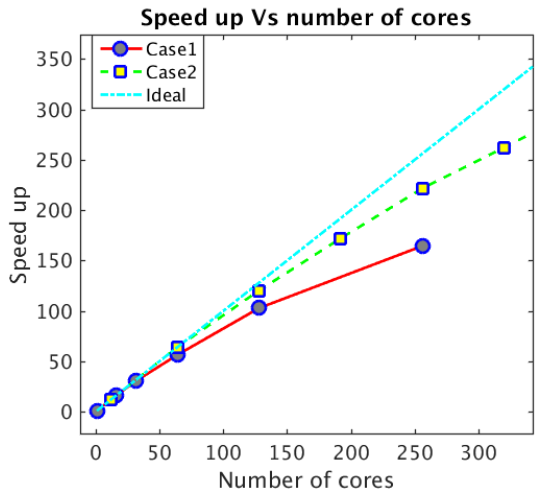
Scalability





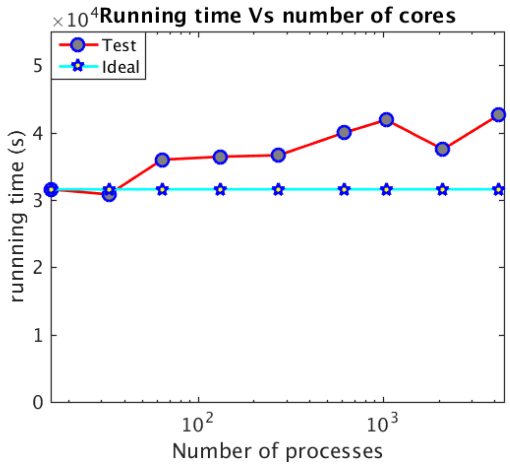


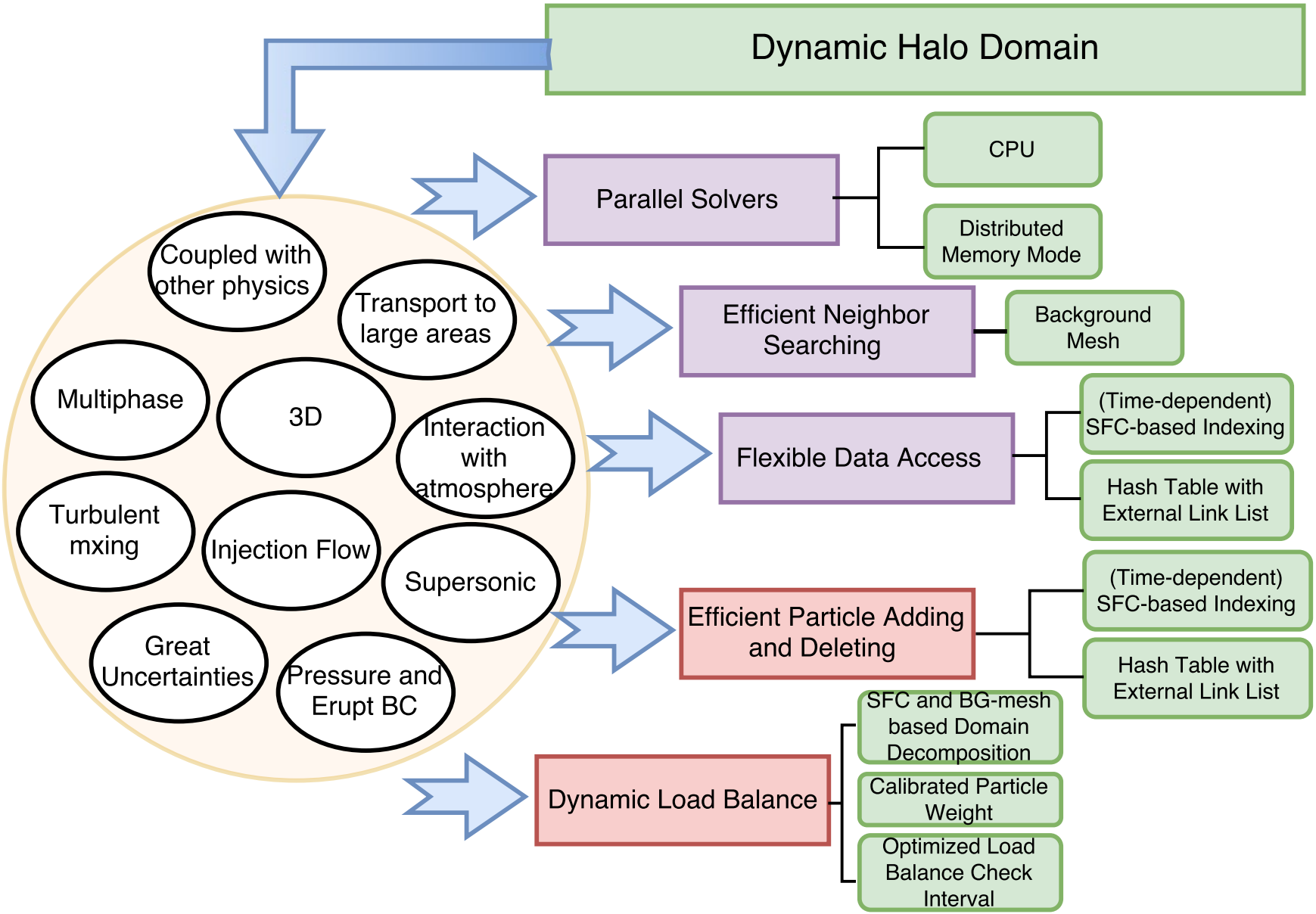
Figure: The left figure shows strong scalability tests result. middle figure is the zoomed view of first one. It is obviously shown that strong scalability is better when the problem size is larger. The right figure is weak scalability test results

A Typical Simulation Results

University at Buffalo
The State University of New York

Play/Pause

Requirements of the application



Summary

- We developed data management strategies for a MPI-parallel implementation of the SPH method to simulate volcanic plumes. Acceptable scalability was achieved.
- The flexibility of our data access methodology enables implementation of mesh-free methods for solving more complicated problems and using more advanced techniques, such as dynamic particle splitting techniques.
- The data structure, particle and bucket indexing strategies, domain decomposition, dynamic load balancing method and domain adjusting strategies in this paper can be adopted by other mesh-free methods (not just SPH).

- Current/Future
  - Better dynamic load balancing strategy.
  - Adaptive background grid and better domain decomposition algorithm.

Thank you!
Questions are welcome.