Transactions of the Korean Nuclear Society Autumn Meeting
Changwon, Korea, October 30-31, 2025

High-Performance GPU Implementation of Decay Chain Models for Radioactive Dispersion Simulation

Jihyun Lee [a], Juryong Park [a], Hyung Jin Shim [a], Hiroshi Sagara [b], Eung Soo Kim [a*]
[a] *Nuclear Engr. Dept., Seoul National Univ., 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea*
[b] *Institute of Science Tokyo, 2 Chome-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan*
[*] *Corresponding author: kes7741@snu.ac.kr*

***Keywords :** Radioactive dispersion, CRAM, Lagrangian dispersion, GPU, High-performance computing

1. Introduction

Accurate simulation of radioactive decay chains is essential for nuclear safety and security, particularly in detecting and tracking unexpected radioactive materials and supporting emergency responses. Conventional time-stepping methods for decay calculations often suffer from high computational cost and numerical instability when handling large nuclide networks [1].

The Chebyshev Rational Approximation Method (CRAM) provides an efficient and stable alternative by enabling direct evaluation of the matrix exponential without requiring iterative time advancement [2]. This study implements a GPU-accelerated CRAM solver tailored for large-scale decay chain calculations within a Lagrangian dispersion framework. The proposed approach aims to significantly improve computational performance while maintaining high accuracy in predicting nuclide inventories, thereby enabling near real-time simulations for applications in nuclear safety, and emergency preparedness.

2. Methodology

2.1. Chebyshev Rational Approximation Method (CRAM)

For each particle, the nuclide inventory vector $\mathrm{n(t)} \in \mathbb{R}^N$ follows a liner system as

$$\boldsymbol{n}' = \boldsymbol{A}\boldsymbol{n} \ , \qquad \boldsymbol{n}(t) = e^{\boldsymbol{A}t}\boldsymbol{n}(0) \ , \tag{1}$$

where $\boldsymbol{A}$ includes decay constants on the diagonal and branching ratios off-diagonal.

CRAM evaluates the matrix exponential by a near-minimax rational approximation on the negative real axis:

$$e^{\boldsymbol{A}t}\boldsymbol{n}(0) = \alpha_0\boldsymbol{n}_0 + 2Re\left(\sum_{j=1}^{k/2}\alpha_j\left(\boldsymbol{A}t - \theta_j\boldsymbol{I}\right)^{-1}\boldsymbol{n}_0\right). \tag{2}$$

We employ standard orders—CRAM16 with $m = 8$ conjugate pairs for fast, engineering-grade accuracy, and CRAM48 with $m = 24$ pairs when near–machine-precision is required.

This formulation has several properties that make it well suited to large decay networks embedded in dispersion simulations [3]. Because the spectrum of $\boldsymbol{A}$ for pure decay lies on $(-\infty, 0]$, CRAM is unconditionally stable and allows large Δt without step-size restrictions, avoiding the error accumulation and stiffness limitations of explicit time stepping. The conjugate structure of the poles and weights guarantees a real final inventory even though intermediate solves are complex.

Computationally, the method is highly parallel. Each time step consists of independent shifted solves with the same sparsity pattern, so factorization/preconditioners can be reused when Δt is fixed, and many right-hand sides (particles) can be batched on the GPU to achieve high throughput.

2.2. Lagrangian Dispersion Model (LDM)

The Lagrangian Dispersion Model (LDM) is a particle-based approach that is extensively applied for the simulation of atmospheric transport of radionuclides.

In this framework, the motion of each particle is described by a combination of deterministic advection and stochastic turbulent diffusion [4]. The particle position at time t is updated as

$$\frac{dx(t)}{dt} = U(x,t) + u'(t) \tag{3}$$

where $x(t)$ is the particle position at time t, $U(x,t)$ denotes the mean wind velocity obtained from meteorological data, and $u'(t)$ is the turbulent velocity fluctuation.

The turbulent velocity component is generally modeled through a Langevin-type stochastic differential equation:

$$du_i'(t) = -\frac{u_i'(t)}{\tau_L}dt + \sqrt{\frac{2\sigma_i^2}{\tau_L}}dW_i(t) \tag{4}$$

where τ_L is the Lagrangian turbulence timescale, σ_i is the standard deviation of turbulent fluctuations in the i-th direction, and $dW_i(t)$ is the increment of a Wiener process describing Gaussian white noise. This stochastic formulation enables realistic representation of turbulent mixing and ensures physically consistent dispersion of particles in the atmosphere.

In practical applications, LDM also accounts for other environmental processes, such as gravitational settling and dry or wet deposition [5,6].

2.3. GPU-Accelerated Coupling of CRAM with LDM

To incorporate radioactive decay chains into the Lagrangian Dispersion Model (LDM), the CRAM solver was parted to GPU and tightly coupled with the particle-based transport framework. In this structure, each Lagrangian particle carries a nuclide inventory vector that evolves through both atmospheric process and nuclear transmutation.

At each time step, the particle position and spread are updated according to wind fields and stability-dependent parameters, consistent with conventional Lagrangian particle formulations. Removal processes such as dry and wet deposition are applied multiplicatively, while the nuclide inventory is simultaneously advanced by the CRAM update. The CRAM method evaluates the matrix exponential through rational approximation, where each conjugate pole corresponds to an independent shifted linear system. These systems are mapped onto GPU threads, enabling concurrent solution across thousands of nuclides and particles.

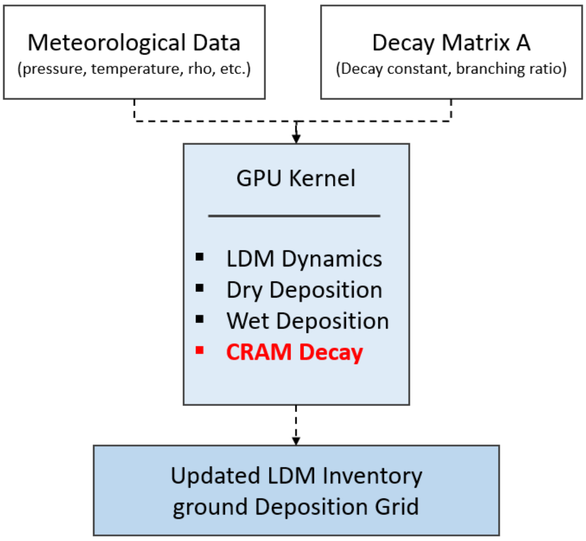

Fig. 1. CRAM-LDM workflow on GPU

The decay matrix ***A*** is stored in sparse CSR format and processed using GPU-optimized sparse kernels. Because all shifted systems share the same sparsity pattern, factorization and preconditioners can be reused, significantly reducing computational cost. Particle inventories are organized in a Structure-of-Arrays layout to ensure coalesced memory access, allowing batch processing of multiple particles in a single kernel launch.

By performing both transport and decay updates on the GPU, host-device data transfer is minimized, and the dispersion-decay coupling remains consistent. This design ensures scalability across three parallel dimensions (nuclides, particles, and meteorological datasets). As a result, the framework achieves high-throughput decay chain evaluation within LDM, extending the GPU acceleration strategies demonstrated for atmospheric dispersion to the domain of nuclear transmutation.

3. Results and Discussion

3.1. Verification of Standalone CRAM

Before coupling CRAM with the dispersion framework, the standalone GPU solver was verified against established references. A direct comparison with both a PETSc-based C++ solver and the MIT-CRPG OpenDeplete implementation confirmed that the maximum deviation in nuclide inventories was consistently within 10^{-16}, well within double-precision round-off. Importantly, the GPU implementation produced results that were indistinguishable from the CPU-based codes, with residual differences attributable only to summation order of floating-point arithmetic. This verification demonstrates that the accelerated solver maintains the stability and accuracy properties that make CRAM attractive for depletion problems, while enabling its use in high-throughput atmospheric transport simulations.

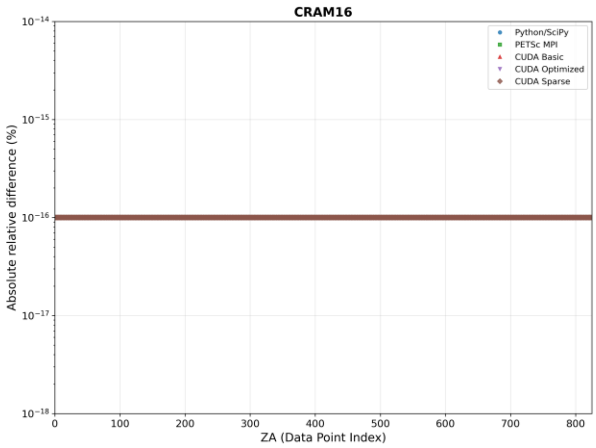

Fig. 2. Verification of CRAM16 implementation

3.2. Scenario Construction in the LDM Framework

Chain resolved radionuclide transport was simulated for 18 hours starting at 00:00 on 14 March 2011 using the LDM dispersion model. The setup used 30,000 Lagrangian particles, a fixed time step of 30 s, and a total duration of 64,800 s. A single continuous point source at longitude 129.48 and latitude 35.72 emitted a constant rate of each of the 60 nuclides throughout the period, and outputs were reported in normalized units so total release can be rescaled. Each particle carried a 60-dimensional inventory vector that was updated every time step by applying a precomputed CRAM transition matrix consistent with the 30 s step size, preserving all parent and daughter couplings during transport. Dry and wet deposition were enabled in their standard configurations and acted concurrently with advection and turbulent dispersion.

3.3. Lagrangian Particle Dispersion Result

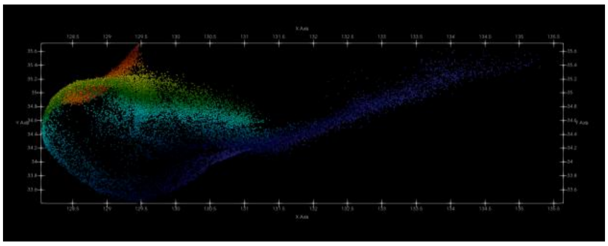

Fig. 3. Particle-based dispersion field with CRAM-enabled decay

Fig. 3 visualizes particle-based dispersion computed with a Lagrangian particle method. Colored markers denote the relative nuclide inventory carried by individual particles; spatial gradients reflect advection and turbulent diffusion, and the gradual coloring indicates removal by dry and wet deposition.

3.4. CRAM-Driven Nuclide Evolution in Lagrangian Dispersion (Work in Progress)

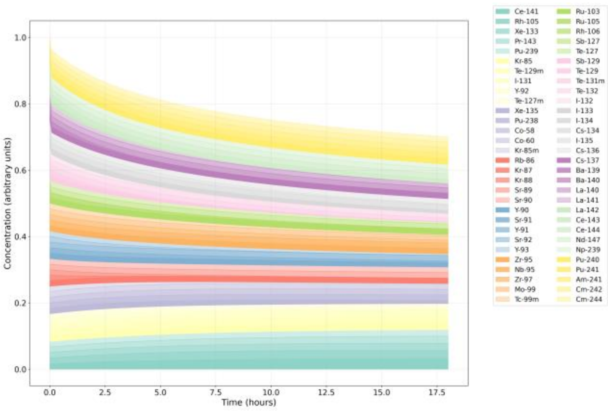

Fig. 4. CRAM-Coupled Concentration Profiles Over Time

Fig. 4 summarizes the chain-resolved concentration trajectories for all 60 nuclides using the CRAM-coupled dispersion solver. The stacked-area presentation highlights the relative contribution of each species to the total inventory while the aggregate mass monotonically declines due to decay and removal. Several short-lived daughters exhibit an initial rise followed by decay, whereas long-lived parents change only slowly over the 18-hour window. These patterns are consistent with expectations from chain kinetics, but the result should be regarded as preliminary. Independent validation and uncertainty analyses are ongoing, and these findings should be regarded as provisional until the coupling and parameter settings are verified.

4. Conclusion

This study presented a GPU-accelerated framework that integrates the Chebyshev Rational Approximation Method (CRAM) into a Lagrangian particle dispersion model for radioactive material transport. Unlike conventional dispersion codes that treat radioactive decay as simple exponential attenuation of parent nuclides, the proposed framework resolves full decay chains within each particle and time step, providing a more physically accurate representation of radionuclide concentration evolution in the atmosphere.

Verification confirmed that the GPU CRAM solver is numerically identical to established references, ensuring confidence in its accuracy. These findings underscore the necessity of including decay chain resolution in Level 3 PSA consequence analyses, especially for isotopes with half-lives on the order of hours.

On the performance side, the framework achieved an order-of-magnitude speedup relative to CPU implementations, making near real-time simulation feasible even for large multi-nuclide, multi- particle scenarios. CRAM16 was found sufficient for engineering-grade accuracy, while CRAM48 offers additional robustness for extreme time-step choices.

Overall, the GPU-accelerated CRAM-LDM system advances the state of the art in atmospheric dispersion modeling by improving both physical fidelity and computational efficiency. It provides a scalable and practical tool for supporting Level 3 PSA, emergency preparedness, and real-time decision support. Future extensions will incorporate nuclide-specific aerosol processes, precipitation effects, and integration with dynamic evacuation and dose modules to complete a fully coupled consequence assessment framework.

ACKNOWLEDGMENTS

This work was supported by the Nuclear Safety Research Program through the Korea Foundation Of Nuclear Safety (KoFONS) using the financial resources granted by the Nuclear Safety and Security Commission (NSSC) of the Republic of Korea. (No. RS-2021-KN063910) and the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. RS-2024-00436693).

REFERENCES

[1] J. Cetnar, General solution of Bateman equations for nuclear transmutations, Annals of Nuclear Energy, Vol. 33, No. 7, pp. 640–645, 2006.
[2] A. E. Isotalo, W. A. Wieselquist, A method for including external feed in depletion calculations with CRAM and implementation into ORIGEN, Annals of Nuclear Energy, Vol. 85, pp. 68–77, 2015.
[3] M. Pusa, Rational approximations to the matrix exponential in burnup calculations, Nuclear Science and Engineering, Vol. 169, No. 2, pp. 155–167, 2011.
[4] J. D. Wilson, B. L. Sawford, Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere,

Boundary-Layer Meteorology, Vol. 78, No. 1, pp. 191–210, 1996.
[5] H. Malá, P. Rulík, V. Bečková, J. Mihalík, M. Slezáková, Particle size distribution of radioactive aerosols after the Fukushima and the Chernobyl accidents, Journal of Environmental Radioactivity, Vol. 126, pp. 92–98, 2013.
[6] J. Park, S. Jang, S. Y. Kim, E. S. Kim, GPU-accelerated approaches for multi-unit level 3 PSA: Focusing on dispersion, evacuation, and dose assessment, Reliability Engineering & System Safety, Vol. 111268, 2025.