MULTILEVEL CONTROL VARIATES FOR UNCERTAINTY QUANTIFICATION IN SIMULATIONS OF CLOUD CAVITATION*

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Abstract. We quantify uncertainties in the location and magnitude of extreme pressure spots revealed from large scale multiphase flow simulations of cloud cavitation collapse. We examine clouds containing 500 cavities and quantify uncertainties related to their initial spatial arrangement. The resulting 2,000-dimensional space is sampled using a nonintrusive and computationally efficient multilevel Monte Carlo (MLMC) methodology. We introduce novel empirically optimal control variate coefficients to enhance the variance reduction in MLMC. The proposed multilevel control variates Monte Carlo leads to more than two orders of magnitude speedup when compared to standard Monte Carlo methods. We identify large uncertainties in the location and magnitude of the peak pressure pulse and present its statistical correlations and joint probability density functions with the geometrical characteristics of the cloud. Characteristic properties of spatial cloud structure are identified as potential causes of significant uncertainties in exerted collapse pressures.

Key words. compressible multiphase flow, high performance computing, diffuse interface method, bubble collapse, cloud cavitation, uncertainty quantification, multilevel Monte Carlo, control variates, fault tolerance

AMS subject classifications. 76B10, 68W10, 65C05, 65C60, 68M15

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1. Introduction. Cloud cavitation collapse pertains to the inception of multiple gas cavities in a liquid, and their subsequent rapid collapse driven by an increase of the ambient pressure. Shock waves emanate from the cavities with pressure peaks up to two orders of magnitude larger than the ambient pressure [50, 13, 8]. When such shock waves impact on solid walls, they may cause material erosion, considerably reducing the performance and longevity of turbomachinery and fuel injection engines [69, 41]. On the other hand, the destructive potential of cavitation can be harnessed for noninvasive biomedical applications [18, 9] and efficient travel in military sub-surface applications [6]. Prevalent configurations of cavitation often involve

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FIG. 1. Surface view of a collapsing cloud containing 50,000 gas cavities (left) and pressure peak at the center of the cloud (right). Outer bubbles evolve into caplike shapes, forming an array of inwards directed velocity microjets. The resulting focused pressure peak amplifications of two orders of magnitude are exerted at the cloud center [31].

clouds of hundreds or thousands of bubbles [8]. The cloud collapse entails a location dependent, often nonspherical, collapse of each cavity that progresses from the surface to the center of the cloud. Pressure waves emanating from collapsing cavities located near the surface of the cloud act as amplifiers to the subsequent collapses at the center of the cloud. The interaction of these pressure waves increases the destructive potential as compared to the single bubble case. Cavitation, in particular, as it occurs in realistic conditions, presents a formidable challenge to experimental [7, 11, 84] and computational [1, 77] studies due to its geometric complexity and multitude of spatiotemporal scales. Blake et al. [5] studied the single bubble asymmetric collapse using a boundary integral method. Johnsen and Colonius [37] investigated the potential damage of single collapsing bubbles in both spherical and asymmetric regimes for a range of pulse peak pressures in shock-induced collapse. Lauer et al. [40] studied collapses of arrays of cavities under shock waves using the sharp interface technique of Hu et al. [34]. Recent numerical investigation of cloud cavitation involved a cluster of 125 vapor bubbles inside a pressurized liquid at 40 bar [19, 1], and a cluster of 2,500 gas bubbles with ambient liquid pressure of 100 bar [66]. Large scale numerical simulations of cloud cavitation collapse considered clouds containing 50,000 bubbles [31]. Visualizations of such a collapsing cloud and the resulting focused pressure peak at the center are reproduced in Figure 1. However, the computational demands of these simulations do not allow for further parametric studies.

A challenge in modeling and quantifying cloud cavitation collapse is the dependence of critical quantities of interest (QoIs), such as peak pressure or collapse time, on a particular (random) cloud configuration [77] (see also Figure 2). The systematic study of such dependencies can be addressed through an uncertainty quantification (UQ) framework, recently applied in [17, 6]. In [46, 47, 48], a mathematical framework was provided for uncertain solutions of hyperbolic equations. Popular probability space discretization methods include generalized polynomial chaos techniques (see [14, 42, 79, 63, 80, 27] and references therein). An alternative class of methods for quantifying uncertainty in PDEs are the stochastic collocation methods [83, 44, 82].

FIG. 2. Evolution of the normalized peak pressure versus normalized time in free-field collapse of two spherical clouds containing 1,000 bubbles. Two samples are drawn from the same uniform distribution (for the positions of the cavities) and log-normal distribution (for the radii of the cavities).

However, the lack of regularity of the solution with respect to the stochastic variables impedes efficient performance of both the stochastic Galerkin as well as the stochastic collocation methods, in particular, for high-dimensional parameter spaces. Here, we propose the development and implementation of nonintrusive Monte Carlo (MC) methods for UQ of cloud cavitation collapse. In MC methods, the governing equations are solved for a sequence of randomly generated samples, which are combined to ascertain statistical information. However, the robustness of MC methods with respect to solution regularity comes at the price of a low error convergence rate regarding the number of samples. Drawbacks of the aforementioned numerical UQ methods inspired the development of various multifidelity methods, such as Multi-Level MC (MLMC) [24]. Further developments include multifidelity Gaussian process regression based on cokriging [56], and purely data-driven algorithms for linear equations using Gaussian process priors to completely circumvent the use of numerical discretization schemes [65]. MLMC methods were introduced by Heinrich for numerical quadrature [32], then pioneered by Giles for Itô SPDEs [24], and have been lately applied to various stochastic PDEs [3, 15, 26, 53]. The MLMC algorithm was also extended to hyperbolic conservation laws and to massively parallel simulations of the random multidimensional Euler, magnetohydrodynamics, and shallow water equations [46, 47, 48, 49, 75, 72, 43]. Subsequent MLMC improvements include Bayesian inference for fusing knowledge on empirical statistical estimates and deterministic convergence rates [16], an alternative multifidelity setting for nonhierarchical structure of the resolution levels with jointly optimized control variate coefficients and the number of required MC samples (with a posteriori rounding to integers) [60, 61], multilevel control variates with a low-rank approximation to the solutions on coarser grids [22], and multilevel Markov chain MC posterior sampling in Bayesian inference problems [20, 21].

The ensemble uncertainty of the clouds is parametrized by means of probability distributions of cavity radii, positions, and initial internal pressures. Our goal is to perform simulations of cloud cavitation collapse with an unprecedented number of interacting cavities with full UQ on QoIs (peak pressure magnitudes, locations, and cloud collapse times) in terms of means, variances, confidence intervals, and even probability density functions. To the best of our knowledge, such extensive UQ analysis of (even small) clouds has not been accomplished before. We propose an improved non-intrusive MLMC method with novel empirically optimal control variate coefficients, termed MLCV. Design decisions in MLCV partially overlap with some of the MLMC improvements mentioned in the previous paragraph, with a specific focus of

MLCV being to achieve efficient UQ for black-box type deterministic models on large high performance computing (HPC) systems. We do our best to point out these similarities as well as highlight various differences throughout the manuscript; however, we acknowledge that a more elaborate comparison of these methodologies is beyond the scope of our work. MLCV is coupled with the state-of-the-art numerical solver for cloud cavitation collapse simulations and provides robust statistical estimates on relevant QoIs, emphasizing the importance of UQ in such problems.

The paper is structured as follows: section 2 introduces the governing multiphase equations and the finite volume method used for their solution. It also presents the empirically optimal control variate MLMC method for the statistical sampling of QoIs. Numerical experiments quantifying such uncertainties and identifying their relations to the geometric properties of the cloud by means of joint probability density function estimates are reported in section 3. We summarize our findings in section 4.

2. Computational methods. The governing system of equations for multiphase flows are discretized using a finite volume method (FVM) that is efficiently implemented so as to take advantage of supercomputer architectures. The sampling needed to estimate statistical properties from an ensemble of evolved QoIs is performed by a novel MLCV method. We introduce a Python implementation PyMLMC [74] of MLCV and its embedding in an open source UQ framework [29].

2.1. Governing equations. The dynamics of cavitating and collapsing clouds of bubbles are governed by the compressibility of the flow, with viscous dissipation and capillary effects taking place at orders of magnitude slower time scales. Hence, we describe cloud cavitation collapse through the Euler equations for inviscid, compressible, multiphase flows. The system of equations, derived from the Baer–Nunziato model [2], describes the evolution of density, momentum, and total energy of the multiphase flow in the domain $D \subset \mathbb{R}^3$ as in [54, 62]:

$$\begin{aligned}
 (1) \quad & \frac{\partial \alpha_1 \rho_1}{\partial t} + \nabla \cdot (\alpha_1 \rho_1 \mathbf{u}) = 0, \\
 (2) \quad & \frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot (\alpha_2 \rho_2 \mathbf{u}) = 0, \\
 (3) \quad & \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) = \mathbf{0}, \\
 (4) \quad & \frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) = 0, \\
 (5) \quad & \frac{\partial \alpha_2}{\partial t} + \mathbf{u} \cdot \nabla \alpha_2 = K \nabla \cdot \mathbf{u},
 \end{aligned}$$

where

$$(6) \quad K = \frac{\alpha_1 \alpha_2 (\rho_1 c_1^2 - \rho_2 c_2^2)}{\alpha_1 \rho_2 c_2^2 + \alpha_2 \rho_1 c_1^2}.$$

All quantities, unless otherwise stated, depend on spatial variable $\mathbf{x} \in D$ and time variable $t \geq 0$. This system comprises two mass conservation equations, one for each phase, conservation equations for momentum and total energy in single- or mixture-fluid formulation, as well as a transport equation for the volume fraction of one of the two phases with the source/sink term on the right-hand side. In (1)–(5), $\mathbf{u}$ denotes the velocity, p the pressure, $\mathbf{I}$ the identity tensor, ρ the (mixture) density, E the (mixture) total energy $E = \rho e + 1/2 \rho (\mathbf{u} \cdot \mathbf{u})$, where e is the (mixture) specific

internal energy. Moreover, ρ_k , α_k , and c_k with $k \in \{1, 2\}$ are density, volume fraction, and speed of sound of the two phases. For the mixture quantities, the following additional relations hold: $\alpha_1 + \alpha_2 = 1$, $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$, and $\rho e = \alpha_1 \rho_1 e_1 + \alpha_2 \rho_2 e_2$. We do not account for mass transfer between different phases (evaporation or condensation), so that the above equations describe a multicomponent flow. The source term in (5) for homogeneous mixtures [38] describes the reduction of the gas volume fraction in a mixture of gas and liquid when a compression wave travels across the mixing region and vice versa for an expansion wave. For a more detailed analysis on the positive influence of this term on the accuracy of the model equations, we refer to [66].

The equation system is closed by an appropriate equation of state for each of the phases. We employ the stiffened equation of state (see [45] for a review) to capture liquids and gases. This enables a simple, analytic approximation to arbitrary fluids and is expressed by

$$(7) \quad p = (\gamma_k - 1) \rho_k e_k - \gamma_k p_{c,k},$$

where isobaric closure is assumed [62]. Parameters γ_k and $p_{c,k}$ depend on the material. For $p_{c,k} = 0$, the equation of state for ideal gases is recovered. For the simulations in this manuscript, $\gamma_1 = 6.59$ and $p_{c,1} = 4.049 \cdot 10^8$ Pa are used for water and $\gamma_2 = 1.4$ and $p_{c,2} = 0$ Pa for air.

2.2. Numerical method. The governing system (1)–(5) can be recast into the quasi-conservative form

$$(8) \quad \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{Q})}{\partial x} + \frac{\partial \mathbf{G}(\mathbf{Q})}{\partial y} + \frac{\partial \mathbf{H}(\mathbf{Q})}{\partial z} = \mathbf{R}(\mathbf{Q}),$$

where $\mathbf{Q} = (\alpha_1 \rho_1, \alpha_2 \rho_2, \rho \mathbf{u}, E, \alpha_2)^T$ is the vector of conserved (except for α_2 which has a nonzero source term) variables and $\mathbf{F}(\mathbf{Q})$, $\mathbf{G}(\mathbf{Q})$, $\mathbf{H}(\mathbf{Q})$ are vectors of flux functions

$$\mathbf{F}(\mathbf{Q}) = \begin{pmatrix} \alpha_1 \rho_1 u_x \\ \alpha_2 \rho_2 u_x \\ \rho u_x^2 + p \\ \rho u_y u_x \\ \rho u_z u_x \\ (E + p) u_x \\ \alpha_2 u_x \end{pmatrix}, \quad \mathbf{G}(\mathbf{Q}) = \begin{pmatrix} \alpha_1 \rho_1 u_y \\ \alpha_2 \rho_2 u_y \\ \rho u_x u_y \\ \rho u_y^2 + p \\ \rho u_z u_y \\ (E + p) u_y \\ \alpha_2 u_y \end{pmatrix}, \quad \mathbf{H}(\mathbf{Q}) = \begin{pmatrix} \alpha_1 \rho_1 u_z \\ \alpha_2 \rho_2 u_z \\ \rho u_x u_z \\ \rho u_y u_z \\ \rho u_z^2 + p \\ (E + p) u_z \\ \alpha_2 u_z \end{pmatrix}.$$

The source term $\mathbf{R}(\mathbf{Q})$ has all elements equal to zero except the last one,

$$\mathbf{R}(\mathbf{Q})_7 = \alpha_2 (\nabla \cdot \mathbf{u}) + K \nabla \cdot \mathbf{u},$$

which appears due to rewriting (5) in conservative form [36] and incorporating the present source term. For the system (8), initial condition $\mathbf{Q}(\mathbf{x}, t = 0) = \mathbf{Q}_0(\mathbf{x})$ over the entire domain $\mathbf{x} \in D$ as well as boundary conditions at $\mathbf{x} \in \partial D$ for all times $t \geq 0$ need to be provided to complete the full specification of the multiphase flow problem. The method of lines is applied to obtain a semidiscrete representation of (8), where space continuous operators are approximated using the FVM for uniform structured grids. The approach yields a system of ordinary differential equations

$$(9) \quad \frac{d\mathbf{V}(t)}{dt} = \mathcal{L}(\mathbf{V}(t)),$$

where $\mathbf{V}$ is a vector of cell average values and $\mathcal{L}(\cdot)$ is a discrete operator that approx-

imates the convective fluxes and the given sources in the governing system. The temporal discretization of (9) is obtained by an explicit third-order low-storage Runge–Kutta scheme [81]. The computation of the numerical fluxes is based on a Godunov-type scheme using the approximate HLLC Riemann solver originally introduced for single-phase flow problems in [78]. The Riemann initial states are determined by a shock capturing third- or fifth-order accurate WENO reconstruction (see [35]). Following [36], the reconstruction is carried out using primitive variables, and the HLLC Riemann solver is adapted to (5) to prevent oscillations at interface. The solution is advanced with a time step size that satisfies the Courant–Friedrichs–Lewy (CFL) condition. For the coefficient weights in the Runge–Kutta stages, the values suggested in [28] are used, resulting in a total variation diminishing scheme.

2.3. Cubism-MPCF. The FVM used for the spatiotemporal numerical discretization of the nonlinear system of conservation laws in (8) is implemented in the open source software Cubism-MPCF [68, 30, 31, 66]. The applied scheme entails three computational kernels: computation of CFL-limited time-step size Δt based on a global reduction, evaluation of the approximate Riemann problem corresponding to the evaluation of the right-hand side $\mathcal{L}$ in (9) for each time step, and appropriate Runge–Kutta update steps. The solver is parallelized with a hybrid paradigm using the MPI and OpenMP programming models. The software is split into three abstraction layers: cluster, node, and core [30]. The realization of the Cartesian domain decomposition and the interranks MPI communication is accomplished on the cluster layer. On the node layer, the thread level parallelism exploits the OpenMP standard using dynamic work scheduling. Spatial blocking techniques are used to increase locality of the data, with intrarank ghost cells obtained from loading fractions of the surrounding blocks, and interranks ghost cells obtained from a global buffer provided by the cluster layer. On the core layer, the actual computational kernels are executed, exploiting data level parallelism and instruction level parallelism, which are enabled by the conversion from an array-of-structures to a structure-of-arrays layout. For the simulations reported here, the main parts of the computations were executed in mixed precision arithmetic. More details on software design regarding the parallelization and optimization strategies used in Cubism-MPCF can be found in [30, 31, 68, 66]. Cubism-MPCF has demonstrated state-of-the-art performance in terms of floating point operations, memory traffic, and storage, exhibiting almost perfect overlap of communication and computation [30, 66]. The software has been optimized to take advantage of the IBM BlueGene/Q (BGQ) and Cray XC30 platforms to simulate cavitation collapse dynamics using up to 13 trillion computational cells with very efficient strong and weak scaling up to the full size of the MIRA (Argonne National Laboratory) and Piz Daint (Swiss Supercomputing Center) supercomputers [68, 31, 66].

2.4. MLMC method. In this section, we introduce the MLMC framework for UQ. We also present a novel and improved numerical sampling method for approximating the statistical QoI.

This study is grounded on the theoretical probabilistic framework for nonlinear systems of conservation laws introduced in [47, 73]. Uncertainties in the system of conservation laws (8), such as uncertain initial data at time $t = 0$ for the vector of conserved quantities $\mathbf{Q}$, are modeled as *random fields* [47, 73]. They depend on the spatial and temporal variables $\mathbf{x}$ and t , as well as on the stochastic parameter $\omega \in \Omega$, which represents variability in the cloud configuration. For instance, for uncertain

initial data, we assume

$$(10) \quad \mathbf{Q}_0(\mathbf{x}, \omega) = \mathbf{Q}(\mathbf{x}, 0, \omega) \in \mathbb{R}^7, \quad \mathbf{x} \in D, \quad \omega \in \Omega,$$

i.e., at every spatial coordinate $\mathbf{x}$, initial data $\mathbf{Q}_0(\mathbf{x}, \omega)$ are a random vector containing 7 values, one for each equation in (8). We further assume that $\mathbf{Q}_0$ is such that at every spatial point $\mathbf{x}$ the statistical moments such as expectation and variance exist and are defined by

$$(11) \quad \mathbb{E}[\mathbf{Q}_0](\mathbf{x}) = \int_{\Omega} \mathbf{Q}_0(\mathbf{x}, \omega) d\omega$$

and

$$(12) \quad \mathbb{V}[\mathbf{Q}_0](\mathbf{x}) = \int_{\Omega} \left(\mathbf{Q}_0(\mathbf{x}, \omega) - \mathbb{E}[\mathbf{Q}_0](\mathbf{x}) \right)^2 d\omega.$$

Such uncertainties, for instance in initial data $\mathbf{Q}_0$, are propagated according to the dynamics governed by (8). Hence, the resulting evolved solution $\mathbf{Q}(\mathbf{x}, t, \omega)$ for $t > 0$ is also a random field, called the *random entropy solution*; see [47, 73, 46] for precise formulation and details.

2.4.1. The classical MLMC. The statistical moments of the QoIs, such as expectation $\mathbb{E}[q]$, are obtained through sampling by the MLMC methodology. Multilevel methods employ a hierarchy of spatial discretizations of the computational domain D or, equivalently, a hierarchy of numerical deterministic solvers as described in subsection 2.2, ordered by increasing “level of accuracy” $\ell = 0, \dots, L$. In many applications, increasing level resolutions inevitably lead to increasing computational requirements, which is especially relevant for flow problems in multidimensional spatial domains. On each such discretization level ℓ , and for a given statistical realization (a “sample”) $\omega \in \Omega$, a numerical approximation of the QoI $q(\omega)$ using the applied FVM will be denoted by $q_{\ell}(\omega)$.

The classical MLMC estimator [24] aims at providing accurate and computationally efficient estimates for statistical moments [47, 4] of q in terms of the telescoping sum of numerical approximations $q_{\ell}(\omega)$ over all levels. In particular, an approximation $E^{\text{MLMC}}[q_L]$ of the expected value $\mathbb{E}[q]$ is constructed from the approximate telescoping sum (neglecting the bias $\mathbb{E}[q - q_L]$)

$$(13) \quad \mathbb{E}[q] \approx \mathbb{E}[q_L] = \mathbb{E}[q_0] + \sum_{\ell=1}^L \left(\mathbb{E}[q_{\ell}] - \mathbb{E}[q_{\ell-1}] \right)$$

by additionally approximating all exact expectations using Monte Carlo sampling with *level-dependent* number M_{ℓ} of samples for QoIs q_{ℓ}^i , leading to

$$(14) \quad \mathbb{E}[q_L] \approx E^{\text{MLMC}}[q_L] = \frac{1}{M_0} \sum_{i=1}^{M_0} q_0^i + \sum_{\ell=1}^L \frac{1}{M_{\ell}} \sum_{i=1}^{M_{\ell}} \left(q_{\ell}^i - q_{\ell-1}^i \right).$$

We note that each sample q_{ℓ}^i is obtained by solving the governing system (8) using the FVM method from subsection 2.2 with discretization (number of mesh cells and time steps) corresponding to level ℓ . Assuming that samples for q_0^i and differences $q_{\ell}^i - q_{\ell-1}^i$ are drawn independently (however, sample pairs q_{ℓ}^i and $q_{\ell-1}^i$ are statistically dependent), the statistical mean square error of the (neglecting error due to the bias

term $\mathbb{E}[q - q_L]$, estimates of which for nonlinear hyperbolic systems are available only in special cases; see [47]) standard MLMC estimator is given by the sum of sample-reduced variances of differences between every two consecutive levels,

$$(15) \quad \varepsilon^2 = \mathbb{E} \left[\left(E^{\text{MLMC}}[q_L] - \mathbb{E}[q_L] \right)^2 \right] = \frac{\mathbb{V}[q_0]}{M_0} + \sum_{\ell=1}^L \frac{\mathbb{V}[q_\ell - q_{\ell-1}]}{M_\ell}.$$

An intuitive insight into the workings of the key MLMC advantage over standard MC is obtained by assuming that $\mathbb{V}[q_\ell] \approx \mathbb{V}[q]$ and observing that the MLMC sampling error in (15) can be approximated in terms of correlation coefficients of every two consecutive levels, i.e.,

$$(16) \quad \varepsilon^2 \approx \mathbb{V}[q] \left(\frac{1}{M_0} + 2 \sum_{\ell=1}^L \frac{1 - \text{Cor}[q_\ell, q_{\ell-1}]}{M_\ell} \right).$$

Note, that strongly correlated QoIs on two consecutive levels lead to a significant reduction in the required number of samples on levels $\ell > 0$. The optimal number of samples M_ℓ for each level $\ell = 0, \dots, L$ can be obtained using empirical or approximate asymptotic estimates on $\mathbb{V}[q_0]$ and $\mathbb{V}[q_\ell - q_{\ell-1}]$ by minimizing the amount of total computational work $M_0 \mathbb{W}_0 + \dots + M_L \mathbb{W}_L$ for a prescribed error tolerance τ such that $\varepsilon \leq \tau$ in (15), as described in [24], or in order to avoid empirical rounding, as suggested in [57]; see also the forthcoming subsection 2.5 for additional remarks. Here, $\mathbb{W}_0$ denotes the amount of computational work needed to compute a single sample (statistical realization) on a given resolution level 0. For levels $\ell > 0$, $\mathbb{W}_\ell$ denotes the amount of computational work needed to compute a pair of such samples on resolution levels ℓ and $\ell - 1$. The number of samples M_ℓ was shown to decrease exponentially with increasing level ℓ , and hence such reduction directly translates into large computational savings over single-level MC sampling methods, as reported in [46, 47, 48, 75, 72].

The proceeding generalization of a classical MLMC method builds upon an observation that the telescoping sum in (13) is not unique, i.e., there are many different ways to write such a telescoping sum involving approximations q_ℓ of QoI q and coarser resolutions levels ℓ . In particular, some applications of a well-established control variate theory has been already explored in recent works, including [55, 59, 61]. We present a novel method for reducing the variance using control variates and further increasing the efficiency of the classical MLMC method.

2.4.2. MLCV: Examples with two levels. For illustrative purposes and clear exposure of several motivational concerns, we first introduce the main underlying concepts of our approach by considering a significantly simplified example. In particular, we consider only two levels, a coarser level $\ell - 1$ and a finer level ℓ . The backbone of MLMC is the hierarchical variance reduction technique, where statistical moments at level ℓ use simulations from coarser discretization level $q_{\ell-1}$ as a *control variate* with “known” $\mathbb{E}[q_{\ell-1}]$ and the *predetermined* coupling coefficient $\alpha_\ell = 1$. The coupled statistical QoI q_ℓ^* with the same expected value as q_ℓ is given by

$$(17) \quad q_\ell^* = q_\ell + \alpha \left(\mathbb{E}[q_{\ell-1}] - q_{\ell-1} \right).$$

The variance reduction that is achieved in (17) by considering random variable q_ℓ^* instead of q_ℓ depends on the correlation between q_ℓ and $q_{\ell-1}$,

$$(18) \quad \mathbb{V}[q_\ell^*] = \mathbb{V} \left[q_\ell + \alpha \left(\mathbb{E}[q_{\ell-1}] - q_{\ell-1} \right) \right] = \mathbb{V}[q_\ell] + \alpha^2 \mathbb{V}[q_{\ell-1}] - 2\alpha \text{Cov}[q_\ell, q_{\ell-1}].$$

Statistical expectation estimators $E_{M_\ell}[\cdot]$ using M_ℓ samples are applied to q_ℓ^* instead of q_ℓ , leading to the building block of the MLMC estimator:

$$(19) \quad \mathbb{E}[q_\ell] = \mathbb{E}[q_\ell^*] \approx E_{M_\ell, M_{\ell-1}}[q_\ell^*] = E_{M_\ell}[q_\ell] + \alpha \left(\mathbb{E}[q_{\ell-1}] - E_{M_\ell}[q_{\ell-1}] \right).$$

In standard MLMC, the expectation $\mathbb{E}[q_{\ell-1}]$ is further approximated independently by the estimate $E_{M_{\ell-1}}[q_{\ell-1}]$ with a different number of MC samples $M_{\ell-1}$, and the coefficient α in (17)–(19) is set to unity; see [24, 23]. This constraint on coefficient α could potentially, but not necessarily, limit the efficiency of the variance reduction technique. For instance, under the assumption (to expose the role of level correlation) that variances at both levels are comparable, i.e., $\mathbb{V}[q_\ell] \approx \mathbb{V}[q_{\ell-1}]$, the variance of (19) would *increase* provided the correlation coefficient $\text{Cor}[q_\ell, q_{\ell-1}]$ drops below a threshold of $1/2$,

$$(20) \quad \mathbb{V}[q_\ell^*] \approx 2\mathbb{V}[q_\ell] - 2\text{Cor}[q_\ell, q_{\ell-1}]\mathbb{V}[q_\ell] \geq 2\mathbb{V}[q_\ell] - 2\frac{1}{2}\mathbb{V}[q_\ell] = \mathbb{V}[q_\ell].$$

To avoid this, the optimal α minimizing the variance of q_ℓ^* as in (18) can be used:

$$(21) \quad \alpha = \frac{\text{Cov}[q_\ell, q_{\ell-1}]}{\mathbb{V}[q_{\ell-1}]} \approx \text{Cor}[q_\ell, q_{\ell-1}].$$

A consequence of (21) is that the predetermined choice of $\alpha = 1$ in (17) is optimal *only* under very restrictive conditions: perfectly correlated levels with correlation coefficient $\text{Cor}[q_\ell, q_{\ell-1}] = 1$ and the assumption that coarser level estimates $\mathbb{E}[q_{\ell-1}]$ are already available (hence no computation is needed, i.e., $\mathbb{W}_{\ell-1} = 0$). Note, that for optimal α as in (21), variance is *always* reduced in (18), even for $0 < \text{Cor}[q_\ell, q_{\ell-1}] < 1/2$,

$$(22) \quad \mathbb{V}[q_\ell^*] = \left(1 - \text{Cor}[q_\ell, q_{\ell-1}]\right)^2 \mathbb{V}[q_\ell] < \mathbb{V}[q_\ell].$$

For $\mathbb{W}_{\ell-1} \neq 0$, it is necessary to obtain an estimate for $\mathbb{E}[q_{\ell-1}]$ in (17) as well. In such case, using the independence of estimators E_{M_ℓ} and $E_{M_{\ell-1}}$ and the central limit theorem, the variance of the two-level estimator $E_{M_\ell, M_{\ell-1}}[q_\ell^*]$ as in (19) with additional coarse-level approximation $E_{M_{\ell-1}}[q_{\ell-1}]$ is given by

$$(23) \quad \mathbb{V}[E_{M_\ell, M_{\ell-1}}[q_\ell^*]] = \frac{\mathbb{V}[q_\ell - \alpha q_{\ell-1}]}{M_\ell} + \frac{\mathbb{V}[\alpha q_{\ell-1}]}{M_{\ell-1}}.$$

Minimizing the variance of the estimator $E_{M_\ell, M_{\ell-1}}[q_\ell^*]$ in (23), i.e., finding jointly optimal unknown parameters $\alpha, M_\ell, M_{\ell-1}$, is a particularly challenging problem (even for this simple two-level example), since α is a real number and $M_\ell, M_{\ell-1}$ are integers. Several existing results address this optimization problem by introducing empirical simplifications, such as performing a joint real-valued optimization of α and $M_\ell, M_{\ell-1}$ together and then rounding down $M_\ell, M_{\ell-1}$ to integers [60, 61], or performing only-integer optimization on $M_\ell, M_{\ell-1}$ while disregarding α by using standard MLMC only [57]. On the other hand, even solving such a mixed optimization problem would result in an overall empirical sampling algorithm, since level variances and covariances required in (23) are not known and need to be estimated empirically. Motivated by these considerations, we instead propose a simple empirical optimization procedure for (23), which only partially relies on the conventional Lagrange multiplier methodologies used for the standard MLMC in [24]. That is, instead of performing Lagrange

multiplier optimization (over reals) jointly on α and $M_\ell, M_{\ell-1}$, we first optimize α independently of $M_\ell, M_{\ell-1}$ by introducing an auxiliary empirical variance reduction cost functional, and only then estimate $M_\ell, M_{\ell-1}$ using (also partially empirical due to rounding) Lagrange multipliers. To optimize α independently of $M_\ell, M_{\ell-1}$, we employ the level-specific inverse relation between the number of samples M_ℓ and the required computational cost per sample $\mathbb{W}_\ell$:

$$(24) \quad \frac{1}{M_\ell} \sim \mathbb{W}_\ell.$$

Using (24), we transform the variance estimate in (23) into an empirical total computational cost for variance reduction in $E_{M_\ell, M_{\ell-1}}[q_\ell^*]$,

$$(25) \quad C[q_\ell^*] = \mathbb{V}[\alpha q_{\ell-1}] \mathbb{W}_{\ell-1} + \mathbb{V}[q_\ell - \alpha q_{\ell-1}] \mathbb{W}_\ell,$$

where variances of $\alpha q_{\ell-1}$ and $q_\ell - \alpha q_{\ell-1}$ are weighted by the corresponding computational costs $\mathbb{W}_{\ell-1}$ and $\mathbb{W}_\ell$, respectively. In order to find the empirically optimal α , the computational variance reduction cost $C[q_\ell^*]$ in (25) is minimized instead of $\mathbb{V}[q_\ell^*]$ in (18). The resulting empirically optimal coefficient α can be obtained by solving the linear equation resulting from setting the derivative of the total computational cost for the variance reduction $C[q_\ell^*]$ with respect to α to zero:

$$(26) \quad \begin{aligned} \frac{dC[q_\ell^*]}{d\alpha} &= \frac{d}{d\alpha} \left(\alpha^2 \mathbb{V}[q_{\ell-1}] \mathbb{W}_{\ell-1} + (\mathbb{V}[q_\ell] + \alpha^2 \mathbb{V}[q_{\ell-1}] - 2\alpha \text{Cov}[q_\ell, q_{\ell-1}]) \mathbb{W}_\ell \right) = 0 \\ &\Leftrightarrow 2\alpha \mathbb{V}[q_{\ell-1}] \mathbb{W}_{\ell-1} + 2\alpha \mathbb{V}[q_{\ell-1}] \mathbb{W}_\ell - 2 \text{Cov}[q_\ell, q_{\ell-1}] \mathbb{W}_\ell = 0 \\ &\Leftrightarrow \alpha \mathbb{V}[q_{\ell-1}] (\mathbb{W}_{\ell-1} + \mathbb{W}_\ell) - \text{Cov}[q_\ell, q_{\ell-1}] \mathbb{W}_\ell = 0. \end{aligned}$$

The resulting linear equation (26) is then solved for the empirically optimal α (and its approximation provided $\mathbb{V}[q_\ell] \approx \mathbb{V}[q_{\ell-1}]$):

$$(27) \quad \alpha = \frac{\mathbb{W}_\ell}{\mathbb{W}_\ell + \mathbb{W}_{\ell-1}} \frac{\text{Cov}[q_\ell, q_{\ell-1}]}{\mathbb{V}[q_{\ell-1}]} \approx \frac{\mathbb{W}_\ell}{\mathbb{W}_\ell + \mathbb{W}_{\ell-1}} \text{Cor}[q_\ell, q_{\ell-1}].$$

We note, that (27) reduces to the standard control variate coefficient (21) if $\mathbb{W}_{\ell-1} = 0$.

2.4.3. MLCV: Control variates for MLMC. We generalize the concept of empirically optimal control variate coefficients from subsection 2.4.2 to an arbitrary number of levels in the MLMC estimator. In particular, control variate contributions from multiple levels can be used,

$$(28) \quad q_L^* = \left(q_L - \alpha_{L-1} q_{L-1} \right) + \left(\alpha_{L-1} q_{L-1} - \alpha_{L-2} q_{L-2} \right) + \cdots + \left(\alpha_1 q_1 - \alpha_0 q_0 \right) + \alpha_0 q_0,$$

allowing for a generalization of the telescoping sum in (13) to the control variate setting introduced in (17), where the coefficient for the finest level $\ell = L$ is fixed to $\alpha_L = 1$:

$$(29) \quad \mathbb{E}[q_L] = \mathbb{E}[q_L^*] = \alpha_0 \mathbb{E}[q_0] + \sum_{\ell=1}^L \left(\alpha_\ell \mathbb{E}[q_\ell] - \alpha_{\ell-1} \mathbb{E}[q_{\ell-1}] \right).$$

Using the mutual statistical independence of $\alpha_0 q_0$ and differences $\alpha_\ell q_\ell - \alpha_{\ell-1} q_{\ell-1}$ together with the central limit theorem analogously to subsection 2.4.2, the empirical total computational variance reduction cost employing (24) and generalizing

(25) for q_L^* over all levels as in (28), is given by

$$(30) \quad \begin{aligned} C[q_L^*] &= \mathbb{V}[\alpha_0 q_0] \mathbb{W}_0 + \sum_{\ell=1}^L \mathbb{V}[\alpha_\ell q_\ell - \alpha_{\ell-1} q_{\ell-1}] \mathbb{W}_\ell \\ &= \alpha_0^2 \mathbb{V}[q_0] \mathbb{W}_0 + \sum_{\ell=1}^L \left(\alpha_\ell^2 \mathbb{V}[q_\ell] + \alpha_{\ell-1}^2 \mathbb{V}[q_{\ell-1}] - 2\alpha_\ell \alpha_{\ell-1} \text{Cov}[q_\ell, q_{\ell-1}] \right) \mathbb{W}_\ell. \end{aligned}$$

Minimization of $C[q_L^*]$ pertains to solving a linear system of equations,

$$(31) \quad \frac{\partial}{\partial \alpha_\ell} C[q_L^*] = 0, \quad \ell = 0, \dots, L-1.$$

Using the following abbreviations,

$$(32) \quad \begin{aligned} \sigma_\ell^2 &= \mathbb{V}[q_\ell], \\ \mathbb{W}_{\ell, \ell-1} &= \mathbb{W}_\ell + \mathbb{W}_{\ell-1}, \\ \sigma_{\ell, \ell-1}^2 &= \text{Cov}[q_\ell, q_{\ell-1}], \\ \mathbf{a} &= (\alpha_0, \dots, \alpha_{L-1})^\top \in \mathbb{R}^L, \end{aligned}$$

the linear system in (31) can be written in the tridiagonal matrix form

$$(33) \quad \mathbf{M} \mathbf{a} = \mathbf{b},$$

with the load vector given by

$$(34) \quad \mathbf{b} = \left(\underbrace{0, \dots, 0}_{L-1}, \sigma_{L, L-1}^2 \mathbb{W}_L \right)^\top \in \mathbb{R}^L$$

and the tridiagonal matrix $\mathbf{M} \in \mathbb{R}^{L \times L}$ given by

$$(35) \quad \mathbf{M} = \begin{bmatrix} \sigma_0^2 \mathbb{W}_{1,0} & -\sigma_{1,0}^2 \mathbb{W}_1 & & & \\ -\sigma_{1,0}^2 \mathbb{W}_1 & \ddots & & \ddots & \\ & \ddots & \ddots & & -\sigma_{L-1, L-2}^2 \mathbb{W}_{L-1} \\ & & -\sigma_{L-1, L-2}^2 \mathbb{W}_{L-1} & \sigma_{L-1}^2 \mathbb{W}_{L, L-1} & \end{bmatrix}.$$

For a special case of two levels with $L = 1$, the solution of (33) reduces to (27). In the general multilevel setting with $L \geq 2$, the well-posedness (existence and uniqueness of the solution) of the system (33) is guaranteed by the following theorem.

THEOREM 2.1 (well-posedness of the control variate coefficients). *If $\mathbb{W}_\ell, \sigma_\ell^2 > 0$ for every level $\ell = 0, \dots, L$ then matrix $\mathbf{M}$ in (35) is positive-definite and hence the system (33) can be solved uniquely for the control variate coefficients vector $\mathbf{a}$.*

Proof. First, we verify that $\mathbf{M}$ in (35) is positive-definite, i.e., that $\mathbf{a}^\top \mathbf{M} \mathbf{a} > 0$ for all $\mathbf{a} \neq 0$. In particular, the matrix-vector multiplications expand to

$$\begin{aligned}
 \mathbf{a}^\top \mathbf{M} \mathbf{a} &= \alpha_0^2 \sigma_0^2 \mathbb{W}_1 + \alpha_0^2 \sigma_0^2 \mathbb{W}_0 - \alpha_1 \alpha_0 \sigma_{1,0}^2 \mathbb{W}_1 \\
 &\quad - \alpha_1 \alpha_0 \sigma_{1,0}^2 \mathbb{W}_1 + \alpha_1^2 \sigma_1^2 \mathbb{W}_2 + \alpha_1^2 \sigma_1^2 \mathbb{W}_1 - \alpha_2 \alpha_1 \sigma_{2,1}^2 \mathbb{W}_2 \\
 &\quad \dots \\
 &\quad - \alpha_\ell \alpha_{\ell-1} \sigma_{\ell,\ell-1}^2 \mathbb{W}_\ell + \alpha_\ell^2 \sigma_\ell^2 \mathbb{W}_{\ell+1} + \alpha_\ell^2 \sigma_\ell^2 \mathbb{W}_\ell - \alpha_{\ell+1} \alpha_\ell \sigma_{\ell+1,\ell}^2 \mathbb{W}_{\ell+1} \\
 &\quad \dots \\
 &\quad - \alpha_{L-2} \alpha_{L-3} \sigma_{L-2,L-3}^2 \mathbb{W}_{L-2} + \alpha_{L-2}^2 \sigma_{L-2}^2 \mathbb{W}_{L-1} + \alpha_{L-2}^2 \sigma_{L-2}^2 \mathbb{W}_{L-2} \\
 &\quad - \alpha_{L-1} \alpha_{L-2} \sigma_{L-1,L-2}^2 \mathbb{W}_{L-1} + \alpha_{L-1}^2 \sigma_{L-1}^2 \mathbb{W}_L + \alpha_{L-1}^2 \sigma_{L-1}^2 \mathbb{W}_{L-1}.
 \end{aligned} \tag{36}$$

In the expansion (36) of $\mathbf{a}^\top \mathbf{M} \mathbf{a}$, for every level $\ell = 1, \dots, L-1$, each group of terms with identical common factors $\mathbb{W}_\ell$ adds up to a nonnegative sum Σ_ℓ , defined by

$$\begin{aligned}
 \Sigma_\ell &= \alpha_{\ell-1}^2 \sigma_{\ell-1}^2 \mathbb{W}_\ell - \alpha_\ell \alpha_{\ell-1} \sigma_{\ell,\ell-1}^2 \mathbb{W}_\ell - \alpha_\ell \alpha_{\ell-1} \sigma_{\ell,\ell-1}^2 \mathbb{W}_\ell + \alpha_\ell^2 \sigma_\ell^2 \mathbb{W}_\ell \\
 &= \mathbb{W}_\ell (\alpha_{\ell-1}^2 \sigma_{\ell-1}^2 - 2\alpha_\ell \alpha_{\ell-1} \sigma_{\ell,\ell-1}^2 + \alpha_\ell^2 \sigma_\ell^2) \\
 &= \mathbb{W}_\ell (\alpha_{\ell-1}^2 \mathbb{V}[q_{\ell-1}] - 2\alpha_\ell \alpha_{\ell-1} \text{Cov}[q_\ell, q_{\ell-1}] + \alpha_\ell^2 \mathbb{V}[q_\ell]) \\
 &= \mathbb{W}_\ell \mathbb{V}[\alpha_{\ell-1} q_{\ell-1} - \alpha_\ell q_\ell] \geq 0.
 \end{aligned} \tag{37}$$

Employing inequality (37), the expansion of $\mathbf{a}^\top \mathbf{M} \mathbf{a}$ in (36) can be bounded from below by the remaining terms involving factors $\mathbb{W}_0$ and $\mathbb{W}_L$, which are both nonnegative, since $\mathbb{W}_0$ and $\mathbb{W}_L$ were both assumed to be positive:

$$\mathbf{a}^\top \mathbf{M} \mathbf{a} \geq \alpha_0^2 \sigma_0^2 \mathbb{W}_0 + \alpha_{L-1}^2 \sigma_{L-1}^2 \mathbb{W}_L \geq 0. \tag{38}$$

We note that strict equalities in (37) and (38) can be achieved if and only if all coefficients α_ℓ are zero, i.e., $\mathbf{a} = 0$. This proves that $\mathbf{a}^\top \mathbf{M} \mathbf{a} > 0$ for all $\mathbf{a} \neq 0$ and, hence, matrix $\mathbf{M}$ in (35) is positive-definite. Since positive-definite matrices are invertible, the system of equations (33) can be solved uniquely. $\square$

Generalizing (14), the unbiased MLCV estimator is then given by

$$\mathbb{E}[q_L] \approx E^{\text{MLCV}}[q_L] = \alpha_0 \frac{1}{M_0} \sum_{i=1}^{M_0} q_0^i + \sum_{\ell=1}^L \frac{1}{M_\ell} \sum_{i=1}^{M_\ell} (\alpha_\ell q_\ell^i - \alpha_{\ell-1} q_{\ell-1}^i) \tag{39}$$

with empirically optimal control variate coefficients α_ℓ given by (33). We assume that samples for $\alpha_0 q_0^i$ and differences $\alpha_\ell q_\ell^i - \alpha_{\ell-1} q_{\ell-1}^i$ are drawn independently (however, individual q_ℓ^i and $q_{\ell-1}^i$ are statistically dependent). The statistical mean square error $\varepsilon_{\text{MLCV}}^2$ of the MLCV estimator is given by the sum of sample-reduced variances of α_ℓ -weighted differences between every two consecutive levels,

$$\begin{aligned}
 \varepsilon_{\text{MLCV}}^2 &= \mathbb{E} \left[\left(E^{\text{MLCV}}[q_L] - \mathbb{E}[q_L] \right)^2 \right] = \frac{\mathbb{V}[\alpha_0 q_0]}{M_0} + \sum_{\ell=1}^L \frac{\mathbb{V}[\alpha_\ell q_\ell - \alpha_{\ell-1} q_{\ell-1}]}{M_\ell} \\
 &=: \frac{\tilde{\sigma}_0^2}{M_0} + \sum_{\ell=1}^L \frac{\tilde{\sigma}_\ell^2}{M_\ell}.
 \end{aligned} \tag{40}$$

Given computational costs $\mathbb{W}_\ell$ of evaluating a single approximation q_ℓ^i for each level $\ell = 0, \dots, L$ and a desired tolerance $\tau > 0$, the total computational cost of MLCV can be minimized under the constraint of $\varepsilon_{\text{MLCV}}^2 \leq \tau$ by choosing the optimal (up to rounding to integers) number of MC samples M_ℓ on each level according to [52], yielding

$$(41) \quad M_\ell = \left\lceil \frac{1}{\tau^2} \sqrt{\frac{\tilde{\sigma}_\ell^2}{\mathbb{W}_\ell}} \sum_{k=0}^L \sqrt{\tilde{\sigma}_k^2 \mathbb{W}_k} \right\rceil.$$

Alternatively, given the available total computational budget $\mathcal{B}$ instead of a desired tolerance τ , the MLCV error $\varepsilon_{\text{MLCV}}^2$ is minimized by choosing the optimal (up to rounding to integers) M_ℓ according to

$$(42) \quad M_\ell = \left\lceil \mathcal{B} \sqrt{\frac{\tilde{\sigma}_\ell^2}{\mathbb{W}_\ell}} / \sum_{k=0}^L \sqrt{\tilde{\sigma}_k^2 \mathbb{W}_k} \right\rceil.$$

A discrete optimization problem for (40) could be formulated, avoiding roundoff operations in (41) or (42), and providing a truly optimal *integer* M_ℓ , as suggested in [57]. We note, however, that even though such rounding does not influence the efficiency of the method on coarser levels, where the number of samples is large, and are most probably overshadowed by the used approximate estimators for $\tilde{\sigma}_\ell^2$, such empirical rounding could have detrimental effects on computational efficiency on the finest levels of resolution. In particular, the rounding of samples can be particularly detrimental to the optimal performance of MLMC coupled with very expensive HPC codes, since the largest impact of rounding is on the highest resolution levels, where the number of samples is expected to be very low (as observed in the numerical simulations in section 3), provided a sufficient number of levels is used [57].

2.4.4. Adaptive MLCV algorithm. The MLCV algorithm proceeds iteratively, with each iteration improving the accuracy of the estimated statistics for the QoIs, such as the expectation $\mathbb{E}[q]$. Each iteration improves the accuracy of auxiliary parameters, such as σ_ℓ^2 , $\sigma_{\ell,\ell-1}^2$, $\mathbb{W}_\ell$, $\tilde{\sigma}_\ell^2$ and, henceforth, also the optimality of the derived quantities, such as control variate coefficients α_ℓ and the number of samples M_ℓ , for each level $\ell = 0, \dots, L$.

A single iteration of the algorithm consists of the following 8 steps.

- (1) *Warm-up:* Begin with a level-dependent number of warm-up samples. The optimal choice is dependent on the specific application; we used a heuristic choice

$$(43) \quad M_\ell = \left\lceil \frac{\mathbb{W}_L}{\mathbb{W}_\ell} \frac{1}{2^{(L-\ell)}} \right\rceil, \quad \ell = L, L-1, \dots, 0.$$

The choice of M_ℓ as in (43) prevents efficiency deterioration of the final MLCV estimator by ensuring that the total computational budget for the warm-up iteration does not exceed $2\mathbb{W}_L$ (i.e., comparable to the computational work required for a single simulation on the finest resolution level); at the same time, it allows one to prescribe sufficiently many samples on the coarser levels, where $\tilde{\sigma}_\ell^2$ is expected to be large. In our particular application, computational work for each level scales as $\mathbb{W}_\ell = \mathcal{O}(2^{4\ell})$ and, hence, the number of required warm-up samples is given by $1, 8, \dots, 2^{3L}$ for $\ell = L, L-1, \dots, 0$. We note

that a constant (level-independent) number of warm-up samples can be very inefficient [52, 16].

- (2) *Solver*: Evaluate approximations q_ℓ^i for each level $\ell = 0, \dots, L$ and sample $i = 1, \dots, M_\ell$, which have not yet been evaluated in previous iterations.
- (3) *Indicators*: Using q_ℓ^i , estimate σ_ℓ^2 , $\sigma_{\ell,\ell-1}^2$, and $\mathbb{W}_\ell$ for $\ell = 0, \dots, L$. Optionally, empirical estimates of $\sigma_{\ell,\ell-1}^2$ could be used within a Bayesian inference framework to fit an exponential decay model for $\sigma_{\ell,\ell-1}^2$ w.r.t. levels $\ell = 1, \dots, L-1$. Assuming Gaussian errors, this reduces to a least-squares line fit to the natural logarithm of indicators $\sigma_{\ell,\ell-1}^2$.
- (4) *Coefficients*: Compute the control variate coefficients α_ℓ from estimated σ_ℓ^2 and $\sigma_{\ell,\ell-1}^2$ using (33).
- (5) *Errors*: Using q_ℓ^i and α_ℓ , estimate α_ℓ -weighted covariances $\tilde{\sigma}_\ell^2$ and total sampling error $\hat{\varepsilon}_{\text{MLCV}}^2 \approx \varepsilon_{\text{MLCV}}^2$ as in (40).
- (6) *Estimator*: If the required tolerance is reached, i.e., $\hat{\varepsilon}_{\text{MLCV}} \leq \tau$, or if the prescribed computational budget $\mathcal{B}$ is spent, then evaluate the MLCV estimator (39) and terminate the algorithm. Otherwise, proceed to the optimization step.
- (7) *Optimization*: Compute the optimal (up to rounding to integers) required number of samples $\hat{M}_\ell$ from $\tilde{\sigma}_\ell$ and $\mathbb{W}_\ell$ using either (41) or (42), respectively. *Remark.* If we obtain $\hat{M}_\ell < M_\ell$ for some level ℓ , we *keep* the already computed samples, i.e., we set $\hat{M}_\ell = M_\ell$. In order to adjust for such a constraint in the optimization problem, we subtract the corresponding sampling error $\tilde{\sigma}_\ell^2/M_\ell$ from the required tolerance τ^2 , or subtract the corresponding amount of computational budget $M_\ell \mathbb{W}_\ell$ from $\mathcal{B}$, respectively. Afterwards, the number of samples $\hat{M}_\ell$ for the *remaining* levels (where $\hat{M}_\ell = M_\ell$ was not enforced) are reoptimized according to either (41) or (42), respectively. We repeat this procedure until $\hat{M}_\ell \geq M_\ell$ is satisfied for all levels $\ell = 0, \dots, L$.
- (8) *Iterations*: Go back to step (2) and continue the algorithm with the updated number of samples $\hat{M}_\ell$.

If the empirical estimates in steps (3)–(5) of the above adaptive MLCV algorithm are sufficiently accurate, the algorithm will terminate after two iterations—the initial warm-up iteration and one additional iteration with already empirically optimal α_ℓ and M_ℓ . A more detailed discussion of the special cases within the MLCV algorithm, alternative approaches, related work, and possible extensions is provided in subsection 2.5. We would also like to note, that same samples are used to estimate both the indicators in step (3) and the MLMC estimator in step (6). This could potentially introduce correlations between the estimated MLMC expectation and the number of used samples on each level, leading to an additional bias in the MLMC estimator. One way to avoid this would be to use different samples for indicators and for MLMC estimates, incurring additional computational overhead.

Alternative optimal coefficients (jointly with empirically rounded M_ℓ to integers) for each level in the MLMC estimator was suggested in [59, 61], where a multifidelity MC method is described. There, some statistical realizations (samples) are *reused*, i.e., the same result is used in both estimates $E_{M_\ell}[\alpha_\ell q_\ell]$ and $-E_{M_{\ell+1}}[\alpha_\ell q_\ell]$, each contributing to a separate difference in the telescoping MLMC estimator (39). Such “recycling” strategy requires less sampling, however, error analysis complexity is highly increased due to additional statistical dependencies, absent in the MLCV method. On the other hand, for “recycled” sampling, the resulting error minimization problem is separable in terms of coefficients α_ℓ and number of samples M_ℓ and, hence, no linear system

(33) needs to be solved [59]. The linear system (33) is, however, very small, sparse, and needs to be solved only a few times, hence, is not a bottleneck of this algorithm.

We do not have at present a comparative study to evaluate which approach could provide better variance reduction (in particular when taking into account the required computational work). On one hand, we could have a joint optimization using Lagrange multipliers followed by the rounding of M_ℓ (analogous to the initial work in [25]) and, on the other, the proposed MLCV employing a simplified empirical variance reduction cost functional (30) taking into account different computational costs on different levels of resolution.

2.5. Technical considerations regarding iterations in the MLCV algorithm. In this section we briefly outline technicalities that are often encountered in practical use of the MLCV algorithm from subsection 2.4.4, namely, the strategies to avoid inefficient oversampling at the finest resolution level during the “warm-up” step 0 and to efficiently mitigate uncertainties due to possible inaccurate indicator estimates in the algorithm execution control at step 6.

2.5.1. The number of warm-up samples on the finest resolution level.

Notice, that in order to have *empirical* estimates of σ_ℓ^2 , $\sigma_{\ell,\ell-1}^2$, and $\hat{\sigma}_\ell^2$, at least *two* samples would be required on each level $\ell = 0, \dots, L$. Enforcing $M_L \geq 2$ might be very inefficient in the cases when only *one* sample is actually needed, since in presently considered applications the most computationally expensive samples are actually at the finest level $\ell = L$. To avoid this, initially only one warm-up sample on the finest mesh level $\ell = L$ could be computed, i.e., $M_L = 1$. For subsequent optimization steps of each M_ℓ , the variance of level difference $\sigma_{\ell,\ell-1}^2$ for level $\ell = L$ is inferred from available measurements on lower resolution levels using Bayesian inference, as described in step (3) of the MLCV algorithm. If more than one sample is actually required on the finest resolution level, optimization step (7) of the adaptive MLCV algorithm above will adjust M_L to the correct empirically optimal value and additional empirical estimates would be available for even more accurate inference.

2.5.2. Control of adaptive MLCV iterations for inaccurate indicators.

Final MLCV error $\varepsilon_{\text{MLCV}}$ could be underestimated by $\hat{\varepsilon}_{\text{MLCV}}$ in step 5 and be actually *larger* than the prescribed tolerance τ , since we only ensure the *estimated* total error $\hat{\varepsilon}_{\text{MLCV}} \leq \tau$. Since $\hat{\varepsilon}_{\text{MLCV}}$ is based on the *randomized* statistical estimators, it is also *random* and has a spread around its mean $\mathbb{E}[\hat{\varepsilon}_{\text{MLCV}}] = \varepsilon_{\text{MLCV}}$. We note that probability $\mathbb{P}[\varepsilon_{\text{MLCV}} > \hat{\varepsilon}_{\text{MLCV}}]$ of the resulting MLMC error $\varepsilon_{\text{MLCV}}$ being larger than the estimated error $\hat{\varepsilon}_{\text{MLCV}}$ (which is forced to be smaller than the prescribed tolerance τ) can be reduced by sufficiently *increasing* the number of samples $\hat{M}_\ell$ according to the estimates of the *fourth centered moment (kurtosis)* κ_ℓ^2 of the level differences. Such estimates would provide the *variance estimates* $\hat{\kappa}_\ell^2 \approx \mathbb{E}[(\hat{\sigma}_\ell^2)^2 - \mathbb{E}[\hat{\sigma}_\ell^2]^2]$ of the *empirical variance estimators* $\hat{\sigma}_\ell^2$. Then, increasing $\hat{M}_\ell$ by several standard deviations $\hat{\kappa}_\ell$ of $\hat{\sigma}_\ell^2$, the required percentile level α of the confidence interval $[\alpha/2, 1 - \alpha/2]$ of $\hat{\varepsilon}_{\text{MLCV}}$ can be reduced below the prescribed tolerance τ , this way *ensuring* the required high probability $\mathbb{P}[\varepsilon \leq \tau] \geq 1 - \alpha$ of true MLMC error ε *not exceeding* the prescribed tolerance τ . A continuation MLMC method incorporating similar techniques for estimation and control of error confidence intervals was already proposed in [16]. However, updating estimates after *each* computed sample could be very inefficient for large HPC applications, since such incremental techniques require heavy synchronization and would make efficient load balancing on distributed many-core systems very challenging. For such applications, only a small number of MLCV iterations is desired, which is the

FIG. 3. Scheme of the MLCV implementation library PyMLMC.

case if indicator estimates from the initial warm-up step 1 are sufficiently accurate and the termination criteria in step 6 are implemented only approximately (for instance, with a small allowed 5% deviation margin). Analogous considerations are valid when the optimization of samples is based on the total computational budget (i.e., (42)) rather than desired tolerance.

2.6. PyMLMC. The MLCV algorithm is distributed as an open source library PyMLMC [74]. A diagram of the software components is shown in Figure 3. PyMLMC provides a modular framework for native execution of deterministic solvers in their respective “sandbox” directories. This allows maximum flexibility for programming languages, distributed and/or shared memory architectures, and support for many-core accelerators. Due to the lack of communication among such sandboxed executions for each sample, the load balancing across samples can be relayed to the submission system (e.g., Slurm, LSF, LoadLeveler, Cobalt) of the compute cluster. Nested (across and within samples) parallelism is used, where few large parallel jobs are submitted for fine levels and, in parallel, many small (possibly even serial) jobs are submitted for coarse levels. To increase the efficiency and reduce the stress on submission systems, job batching (submitting a single job that computes multiple samples subsequently) and job merging (submitting a single job that computes multiple samples concurrently) or a combination of both is implemented. Once all samples (or at least some of them) are computed, statistical estimators are constructed as a postprocessing step using the NumPy and SciPy libraries. The “sandboxing” framework enables any additional required statistical estimates or QoIs to be evaluated at a later stage without the need to reexecute any of the computationally expensive sampling runs. The amount of required disk space in multilevel methods scales linearly w.r.t. the amount of the required computational budget. In particular, the total required disk space for all samples on all levels is of the same order as a *single* statistical estimator on the full three-dimensional domain. Hence, it is highly advantageous to keep all computed samples for the aforementioned postprocessing flexibility purposes.

In the present work (see section 3), we verified the efficiency of the (nested) parallelization of the MLCV coupled with the Cubism-MPCF solver on the entire MIRA supercomputer (Argonne National Laboratory) consisting of half a million cores. We note that large (exa)scale simulations on massively parallel computing

platforms are subject to processor failures at run-time [12]. Exploiting the natural fault tolerance in MLCV-FVM due to independent sampling, a fault tolerant (FT) MLMC (FT-MLMC) method was implemented in [58] and was shown to perform in agreement with theoretical analysis in the presence of simulated, compound Poisson distributed, random hard failures of compute cores. Such FT mechanisms are also available in PyMLMC, and have successfully excluded one corrupted sample on the coarsest level in the simulations reported in section 3.

3. Numerical simulations and analysis. The initialization of the cavities employs experimental findings indicating a log-normal distribution for their radii [51], whereas the position vectors are generated according to a uniform distribution as there is no prior knowledge.

3.1. Spherical cloud of 500 gas cavities with log-normally distributed radii. For a cubic domain $D = [0 \text{ mm}, 100 \text{ mm}]^3$, we consider a cloud of 500 bubbles located at the center $(50 \text{ mm}, 50 \text{ mm}, 50 \text{ mm})^T$ of the domain with a radius of $R_{\text{cloud}} = 20 \text{ mm}$. The log-normal distribution for the radii of the cavity is clipped so as to contain bubbles only within the range of $r_{\min} = 0.8 \text{ mm}$ to $r_{\max} = 1.2 \text{ mm}$. The resulting cloud gas volume content (w.r.t. to the volume of the sphere with radius R_{cloud}) is approximately 5% and the resulting cloud interaction parameter β is approximately 3, where $\beta = \alpha \left(\frac{R_{\text{cloud}}}{R_{\text{avg}}}\right)^2$ with cloud gas volume fraction α , cloud radius R_{cloud} , and average cavity radius R_{avg} (refer to [10] for a derivation). We note that both of these quantities depend on a statistical realization of the random cloud. An illustration of the cloud geometry is shown in Figure 4.

The cloud is initially at pressure equilibrium with the surrounding water phase at $p_{2,0} = 0.5 \text{ MPa}$. Throughout the entire domain, the density of the gas phase is set to $\rho_{2,0} = 5 \text{ kg/m}^3$ and the density of the liquid is set to $\rho_{1,0} = 1,000 \text{ kg/m}^3$. Starting 1 mm away from the surface of the cloud, there is a smooth pressure increase towards the prescribed ambient pressure of $p_{\infty} = 10 \text{ MPa}$, following the setup proposed in [76]. The resulting pressure ratio is $p_{\infty}/p_{2,0} = 20$. At the boundaries, nonreflecting, characteristic-based boundary conditions are applied, together with a penalty term for the prescribed far-field pressure of $p_{\infty} = 10 \text{ MPa}$ [64]. A single statistical realization

FIG. 4. Single statistical realization (sample) of the pressure field and cavity interfaces in the two-dimensional slice at $z = 50 \text{ mm}$ at the initial (left, $t = 0 \text{ μs}$) and at the collapse (right, $t = 46.4 \text{ μs}$) stages. Cavities collapse inwards, emitting pressure waves that focus near the center of the cloud. There is a two orders of magnitude difference in pressures at initial and collapse stages.

(sample) of the pressure field and cavity interfaces across the two-dimensional slice at $z = 50$ mm computed using Cubism-MPCF with resolution of 1024^3 mesh cells is depicted in Figure 4. Cavities are observed to collapse inwards, emitting pressure waves that focus near the center of the cloud at time $t = 46.4 \mu\text{s}$. We emphasize that each collapsing cavity emits a pressure shock wave (with propagating fronts depicted in Figure 4), leading to a low regularity (smoothness) of the approximated solution.

We consider four levels of spatial and temporal resolutions. The coarsest mesh consists of 512^3 cells with two intermediate meshes of $1,024^3$ and $2,048^3$ resolutions, and the finest mesh with $4,096^3$ cells. The time step size decreases according to a prescribed CFL condition with CFL number set to 0.3, resulting in approximately 2,250 and 20,000 time steps for the coarsest and finest levels, respectively. We note, that even on the coarsest resolution level, all cavities are resolved using at least approximately 5 mesh cells per radius. The convergence behavior of the Cubism-MPCF code for a single cavity analogous to cavities in these clouds was investigated in a recent work; see [66]. Based on this study, we expect strong bias in pressure sensors, whereas bias in vapor fraction sensors should be insignificant.

We note that the number of uncertainty sources in this simulation is very large: for each realization of a cloud, random three-dimensional spatial coordinates together with a random positive radius for all 500 cavities are needed, comprising in total 2,000 independent sources of uncertainty.

For each statistical sample of a collapsing cloud configuration and on each resolution level, simulations were performed for approximately $70 \mu\text{s}$ in physical time. Depending on the random configuration of the cloud, the main collapse occurred at approximately $40 - 50 \mu\text{s}$, followed by rebound and relaxation stages after $50 \mu\text{s}$. The obtained results are discussed in the following sections.

3.2. Performance of the MLCV. We quantify the computational gains of the MLCV method by comparing it to standard MLMC and plain MC sampling methods. The chosen quantity of interest q for (29) is the pressure as sampled by a sensor p_c placed at the center of the cloud and emulated as

$$(44) \quad p_c(t) = \frac{1}{|\mathcal{B}_r(\mathbf{c})|} \int_{\mathcal{B}_r(\mathbf{c})} p(\mathbf{x}, t) d\mathbf{x},$$

where pressure p is averaged over a sphere $\mathcal{B}_r(\mathbf{c})$ around the center of the cloud located at $\mathbf{c} = (50 \text{ mm}, 50 \text{ mm}, 50 \text{ mm})^\top$ with radius $r = 0.5 \text{ mm}$,

$$(45) \quad \mathcal{B}_r(\mathbf{c}) = \{\mathbf{x} \in D : \|\mathbf{x} - \mathbf{c}\|_2 \leq r\}.$$

For this particular choice of the QoI, $q = p_c$, estimated correlations between levels, implicitly used in (33), and the resulting empirically optimal control variate coefficients from (33) are depicted in Figure 5. Due to relatively high correlations between resolution levels, empirically optimal control variate coefficients exhibit only moderate deviations from unity, with the largest being at level 1 with deviation of 30%.

Estimated variances of level differences, required in (33), and sampling errors for each level, computed in (40), are depicted in Figure 6. Variances of differences are decreasing for finer levels of resolution, which requires a smaller number of MC samples M_ℓ in order to reduce the statistical error on finer resolution levels, where sampling entails computationally very expensive numerical simulations. Measurements of variances of differences $\sigma_{\ell, \ell-1}^2$ are plotted as circles, with the associated error bars,

FIG. 5. Estimated correlations between levels (left) and the resulting empirically optimal control variate coefficients (right) as in (33). In the left plot, circles depict measurements of correlations with the associated error bars, and the solid line depicts the resulting inferred values. Relatively high correlations and moderate deviations (up to 30%) in empirically optimal control variate coefficients are observed.

FIG. 6. Estimated variances of differences $\sigma_{\ell, \ell-1}^2$ (left) required in (33) and the resulting estimated sampling errors ε_ℓ (right) defined in (40) on each level. In the left plot, circles depict measurements $\sigma_{\ell, \ell-1}^2$ with the associated error bars, the solid line depicts the resulting inferred values, and the dashed line depicts the adjusted values $\tilde{\sigma}_{\ell, \ell-1}^2$ from (40), where empirically optimal control variate coefficients are applied. In the right plot, the brown line indicates estimated errors on each level after the initial MLMC warm-up iteration, whereas the orange line and the corresponding region indicate the estimated error improvements after the final MLMC iteration. The final total statistical error is estimated to be approximately $1.3 \cdot 10^{-2}$.

estimated from the variance of the estimator and the number of samples used in the warm-up stage. These measurements are used within a Bayesian inference framework to fit an exponential decay model for $\sigma_{\ell, \ell-1}^2$ w.r.t. “difference” levels $\ell = 1, 2, 3$. In particular, Gaussian error model and uniform prior are assumed, resulting in a simple weighted linear least squares regression on measured $\sigma_{\ell, \ell-1}^2$. The solid line depicts the resulting inferred values, which are later used in (33), whereas the dashed line depicts the adjusted values $\tilde{\sigma}_{\ell, \ell-1}^2$ from (40), where empirically optimal control variate coefficients are applied. The resulting statistical errors at both MLMC iterations (warm-up and final) are decreasing w.r.t. the increasing resolution level. At the final MLMC iteration, the errors are significantly decreased on all levels when compared to the warm-up iteration, resulting in the total statistical error estimate of approximately $1.3 \cdot 10^{-2}$.

For the optimization of sample numbers M_ℓ on each level, a prescribed budget of 16 million core hours was used and the optimal (up to rounding to integers) number of samples was determined by (42). Estimated number of samples M_ℓ for the warm-

FIG. 7. Estimated number of samples M_ℓ for the warm-up and final iterations of the MLCV algorithm (left) and the resulting estimated computational budget (right) on each level. Brown lines and the corresponding regions indicate number of samples and computational budget during the initial MLMC warmup iteration, whereas green lines indicate the total accounts of both quantities at the final MLMC iteration; green regions indicating the differences between these two iterations. We observe that despite thousand of samples required on coarser levels of resolution, the required corresponding computational budget is comparable among all levels.

TABLE 1

Comparison of MC, MLMC, and MLCV methods and estimated computational speedups over standard MC. MLCV is estimated to be more than two orders of magnitude faster than plain MC, and even more than three times faster than standard MLMC.

	$\{M_\ell\}_{\ell=0,\dots,L}$	Budget $\mathcal{B}$	Error ε	Speedup
MLCV	6400, 384, 40, 2	16.6 M CPU hours	$1.3 \cdot 10^{-2}$	176.8
MLMC	4352, 258, 32, 3	~ 50 M CPU hours	$1.3 \cdot 10^{-2}$	50.6
MC	~ 2 million	~ 2 B CPU hours	$1.3 \cdot 10^{-2}$	-

up and final iterations of the MLCV algorithm are depicted in Figure 7, together with the resulting estimated computational budget on each level. We observe that a significantly larger number of samples is required on the coarser levels of resolution owing to a strong reduction in level difference variances $\tilde{\sigma}_{\ell,\ell-1}^2$, which are also highest at the coarsest resolution levels. However, the required computational budget is comparable across all levels; such a multilevel approach achieves a significant (more than two orders of magnitude) reduction in statistical error (i.e., in the variance of the statistical estimators), while at the same time keeping the deterministic error (bias) small, which is controlled by the resolution of the finest level.

In Table 1, a comparison of MC, MLMC, and MLCV methods and estimated computational speedups is provided for a target statistical error of $1.3 \cdot 10^{-2}$. Note, that the number of samples on the same resolution as the finest level in both MLMC and MLCV and the resulting computational budget required for MC simulations are estimated by

$$(46) \quad M_{\text{MC}} = \left\lceil \frac{\sigma_L}{\varepsilon_{\text{MLCV}}} \right\rceil, \quad W_{\text{MC}} = M_{\text{MC}} W_L.$$

MLCV is estimated to be more than two orders of magnitude faster than the plain MC method, and even more than three times faster than standard MLMC method without optimized control variate coefficients. The overall computational budget of MLCV was only approximately 8 times larger than a single FVM solve on the finest resolution level.

FIG. 8. Uncertainties in the cloud gas volume (mean values with 50% and 90% confidence intervals, left) and global maximum pressure (scaled empirical histogram, right) within the cloud during the collapse. Since all initial cloud configurations contain the same number of equally sized cavities, very low uncertainties are observed in the evolution of the total gas volume. However, the statistical spread of the peak pressure is especially wide at its maximum value, implying a large uncertainty in the damage potential of the cavitation collapse.

FIG. 9. Uncertainties (mean values with 50% and 90% confidence intervals) in the gas volume (left) and pressure (right) sensor at the center of the cloud during the collapse. Notice that the statistical spread of the peak sensor pressure is especially wide at its maximum value and the post-collapse increase in the gas fraction during the rebound stage.

FIG. 10. Uncertainties (probability density functions) in the maximum speed of sound (left) and peak pressure location (right) during the collapse. The dashed line indicates the initial location of the cloud surface.

3.3. Statistics for temporal QOIs. MLMC statistical estimates are depicted in Figures 8, 9, and 10. The statistical spread of the maximum (in physical domain) pressure is especially wide at its peak (in time) value, implying a large uncertainty in the damage potential of the cavitation collapse. To the best of our knowledge, such

full probability density functions (PDFs) are reported here for the first time when using the MLMC methodology for nonlinear systems of conservation laws. To obtain such estimates, level-dependent kernel density estimators were used, with maximum bandwidth determined using a well-known “solve-the-equation” method [70, 66]. Such empirical PDFs are significantly more valuable in engineering, compared to less informative mean/median and deviations/percentiles estimators, especially for bimodal probability distributions often encountered in such nonlinear systems of conservation laws due to the presence of shocks [47]. In multilevel statistical quantiles and empirical PDFs, individual estimates on each resolution level are first obtained separately, and then all estimates are combined using a telescoping sum analogous to the definition provided in (32).

In Figure 8, uncertainties in the cloud gas volume (represented by the gas fraction sensor number 5, located at the center $\mathbf{c} = (50 \text{ mm}, 50 \text{ mm}, 50 \text{ mm})^\top$ with 20 mm radius (hence containing the entire cloud) and global maximum pressure within the cloud are measured during the entire collapse of 70 μs . As all initial cloud configurations contain the same number of equally sized cavities, very low uncertainties are observed in the evolution of the total cloud gas volume. However, the statistical spread of the peak pressure is especially wide at its maximum value, indicating a strong necessity for UQ in such complex multiphase flows.

In Figure 9, uncertainties are measured in the gas volume fraction sensor α_c and pressure sensor p_c at the center of the cloud as defined in (44). Similarly as for the observations of peak pressure behavior, the statistical spread of the peak sensor pressure is especially wide at its maximum value. The postcollapse increase in the gas fraction indicates the presence of a rebound stage. During this stage, the postcollapse gas fraction consistently (in terms of confidence intervals) exceeds precollapse values, indicating the presence of induced outgoing rarefaction waves.

In Figure 10, uncertainties in the maximum speed of sound and the peak pressure location distance from the center of the cloud are measured during the entire collapse of 70 μs . The uncertainty in the maximum speed of sound is a direct consequence of large uncertainties in the global peak pressure. However, on the contrary, the uncertainty in the distance of the peak pressure location from the cloud center is much smaller, i.e., the temporal-spatial profile of the pressure wave evolution as it travels from the surface of the cloud towards the center has a much lower uncertainty (when compared to the large observed uncertainties in the global maximum pressure estimates).

3.4. Statistics for spatial QoIs. In this section, we plot the statistical estimates of QoIs extracted along one-dimensional lines that are cut as a straight line through the center of the cloud in the three-dimensional computational domain. We note that radial symmetry is assumed in the statistical distribution of cavities within the cloud and, hence, such one-dimensional statistical estimates through the center of the cloud are sufficient to represent the global uncertainty in the entire three-dimensional domain. The objective of extracted one-dimensional line plots is to provide a better insight into uncertainty structures at the center of the cloud by plotting all statistical estimates in a single plot. The line is cut at a specific physical simulation time, when the peak pressure is observed and, hence, is slightly different for every sample. In order to reduce volatility in global maximum pressure measurements and, hence, the choice of the collapse time, we smoothen the observed peak pressure measurements with a Gaussian kernel of width 0.5 mm by means of a fast Fourier transform (refer to [71] for methodological details). Statistical estimates for such ex-

FIG. 11. MLMC-estimated uncertainties (PDFs) of the extracted pressure line at the pre-collapse time ($t = 43 \mu\text{s}$, left) and at the time of largest peak pressure ($\sim 46 \mu\text{s}$, right). The resulting uncertainty in encountered pressures increases significantly at the final collapse stage, with largest spreads observed near the epicenter of the cloud cavitation collapse.

tracted one-dimensional lines for pressure at different stages of the collapse process are provided in Figure 11.

The uncertainties are estimated using the MLMC methodology in the extracted pressure along the line in the x -direction (with coordinates $y = 50 \text{ mm}$ and $z = 50 \text{ mm}$ fixed) at the precollapse time $t = 43 \mu\text{s}$ and at the time of largest peak pressure, which occurs approximately at $46 \mu\text{s}$. The time of largest peak pressure depends on the initial cloud configuration and, hence, is a random variable, varying in each statistical realization. We observe that the resulting uncertainty in encountered pressures increases significantly at the final collapse stage, and the largest spreads are observed near the epicenter of the cloud cavitation collapse, where the damage potential is the highest.

3.5. Analysis of linear and nonlinear dependencies. Statistical estimates reported in the previous sections indicate that even though the initial cloud setup is very similar for all realizations, i.e., equal count of cavity bubbles, identical cloud radius, and cavity radii ranges (which resulted in very small uncertainties for the cloud volume reported in Figure 8), and equal initial gas and liquid pressures, the resulting peak pressure uncertainty is very large, as seen in Figures 9 and 11.

Hence, it is only the actual configuration (or distribution) of the cavities inside the cloud that can have such an amplifying (or attenuating) effect on the peak pressures. The main scope of this section is to investigate various QoIs that could potentially explain the cause of such nonlinear effects. The set of selected candidate metrics for the cloud configuration includes skewness (asymmetry) of the initial spatial cavity distribution inside the cloud, cloud interaction parameter β , and distance (from the center of the cloud) of the central cavity (i.e., the cavity closest to the center). Cloud skewness is a measure of asymmetry of the cloud and is estimated by a statistical centered third moment of the distribution of cavity locations along each of the three spatial axes. All quantities from this set of candidate metrics are tested for linear statistical correlations with the observed values of peak pressure, peak pressure distance from the center of the cloud, peak pressure at the sensor at the center of the domain, and collapse time (when largest peak pressure occurs). In addition, we have also tested for statistical correlations among QoIs themselves, such as peak pressure location and the location of the centermost cavity in the cloud. The results are provided as a Hinton diagram in Figure 12.

We observe multiple significant direct and inverse linear statistical correlations between candidate metrics and QoIs:

FIG. 12. Hinton diagram indicating pairwise linear statistical correlations between candidate metrics and selected QoIs. White squares indicate positive and black squares indicate negative correlations. The size of the square indicates the magnitude of the correlation in the interval $[0, 1]$. Cavities within the entire cloud and only in the core of the cloud are considered in the left and right plots, respectively.

- mild *inverse* correlation between *cloud skewness* and *pressure sensor* readings, mainly a consequence of the central sensor placement within the cloud;
- strong correlation between the *location of central cavity* and *location of peak pressure* (w.r.t. cloud center), confirming prior observations in [67] that peak pressures in the cloud are observed *within* cavities that are near the center of the cloud;
- strong *inverse* correlations between *peak pressure location* and *peak pressure magnitude*, indicating that highest peak pressures are most probable near the center of a cloud;
- moderate correlation between β and *collapse time*, since large β values can be a consequence of a large gas fraction in the cloud.

Despite numerous correlations explaining the statistical spread of observed pressures, the influence of cloud interaction parameter β remains undetermined. To this end, we consider cloud skewness and β only for the *core* of the cloud. We have identified the core of the cloud to be a region around the center of the cloud where uncertainties in peak pressure are largest, resulting in a spherical core with radius of 10 mm, based on results in Figure 11. In this case, correlations involving respective metrics such as cloud skewness and β for the core of the cloud, are observed to be more significant:

- mild *direct* correlation between β and pressure sensor readings, indicating stronger collapse for clouds with higher cloud interaction parameter β due to stronger pressure amplification;
- mild *inverse* correlation between cloud skewness and β .

Overall, such insight into statistical correlations provides a very informative description of interdependencies between cloud properties and observed collapse pressures, suggesting direct causal relations w.r.t. cloud nonskewness, interaction parameter β , and proximity of the central cavity to the cloud center. In particular, the polar symmetry of the cloud appears to be a critical component of the collapse dynamics. We did restrain, however, from restricting simulations to artificial “random yet completely symmetric” clouds, rarely observed in real world applications, in order to keep the UQ estimated unbiased with respect to bubble distributions.

FIG. 13. Joint PDFs of cloud interaction parameter β with collapse time (left) and the resulting pressure sensor reading (right). Higher values of cloud interaction parameter β are more likely to cause larger and more delayed collapse pressures.

FIG. 14. Joint PDFs of location of central cavity and location of peak pressure (left), and location of peak pressure and peak pressure magnitude (right). The location of the central cavity bubble correlates strongly with peak pressure location, which itself exhibits strong inverse correlations with the magnitude of the collapse pressures, explaining the wide confidence intervals observed in Figures 8 and 11.

Due to the nonlinear nature of the multiphase equations and the collapse process, nonlinear dependencies among candidate metrics and QoIs could be present, which might be inaccurately captured by the estimates of linear statistical correlations in Figure 12. We tested this hypothesis by estimating the full joint probability distribution for the pairs of significantly correlated candidate metrics and pressure behavior observations. In Figures 13 and 14, we provide results for a selected subset of tested correlation pairs, where the strongest and most relevant correlations were observed.

Joint probability distributions are consistent with linear correlation estimates obtained in Figure 12 and, additionally, provide valuable insight into nonlinear dependencies among QoIs. Obtained results provide a good global overview of causal links between cloud structure and collapse pressures and motivate further analysis to determine the complex mechanisms governing the dynamics of such large and complex cloud cavitation phenomena. We would also like to refer to an ongoing extensive (deterministic) parameter study [67] which investigates such causal links for a wider range of cloud sizes, cavity counts, and cloud interaction parameter β values.

4. Summary and conclusions. We have presented a nonintrusive multilevel MC methodology for UQ in multiphase cloud cavitation collapse flows, together with novel MLCV coefficients which maintain the efficiency of the algorithm even for weak correlations among resolution levels and deliver significant variance reduction improve-

ments. We have conducted numerical experiments for cavitating clouds containing 500 cloud cavities, which are randomly (uniformly) distributed within the specified 20 mm radius, and the radii of the cavity follow a log-normal distribution. The results of these numerical experiments have revealed significant uncertainties in the magnitude of the peak pressure pulse, emphasizing the relevance of UQ in cavitating flows. Furthermore, statistical correlation and joint PDF estimates have revealed potential underlying causes of this phenomenon. In particular, spatial arrangement characteristics of the cloud and its core, such as skewness, cloud interaction parameter β , and the position of the central cavity have been observed to have a significant influence on the resulting pressure amplification intensities during the collapse process.

All numerical experiments were performed by coupling an open source PyMLMC framework with Cubism-MPCF, a high performance petascale finite volume solver. The evolution of collapsing clouds has been simulated by explicit time stepping subject to a CFL stability constraint on a hierarchy of uniform, structured spatial meshes. Efficient MLMC sampling has been observed to exhibit more than two orders of magnitude in estimated computational speedup when compared to standard MC methods, with an additional factor 3 estimated speedup due to empirically optimal control variate coefficients. In the present work, we have observed the efficient scaling of the proposed hybrid MLCV-FVM method up to the entire MIRA supercomputer consisting of half a million cores. Considering that fault-tolerance mitigation mechanisms are implemented in PyMLMC and have been successfully used, we expect it to scale linearly and be suitable for the exascale era of numerical computing.

The proposed MLCV-FVM can deal with a very large number of sources of uncertainty. In the problems presented here, 2,000 sources of uncertainty are needed to fully describe the random initial configuration of the collapsing cloud. To the best of our knowledge, currently no other methods (particularly deterministic methods such as quasi-MC, stochastic Galerkin, stochastic collocation, PGD, ANOVA, or stochastic FVM) are able to handle this many sources of uncertainty, in particular, for nonlinear problems with solutions which exhibit pathwise low regularity and possibly nonsmooth dependence on random input fields. Furthermore, the proposed methodology is well suited for multilevel extensions of Markov chain MC methods for Bayesian inversion [33, 39].

The present multilevel methodology is a powerful general purpose technique for quantifying uncertainty in complex flows governed by hyperbolic systems of nonlinear conservation laws such as cloud cavitation flow problems.

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