Numerical Solution of Cahn-Hilliard System by Adaptive Least-Squares Spectral Element Method

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Abstract. There is a growing interest in the phase-field approach to numerically handle the interface dynamics in multiphase flow phenomena because of its accuracy. The numerical solution of phase-field models has difficulties in dealing with non-self-adjoint operators and the resolution of high gradients within thin interface regions. We present an h-adaptive mesh refinement technique for the least-squares spectral element method for the phase-field models. C^1 Hermite polynomials are used to give global differentiability in the approximated solution, and a space-time coupled formulation and the element-by-element technique are implemented. Two benchmark problems are presented in order to compare two refinement criteria based on the gradient of the solution and the local residual.

Keywords: adaptive, least-square, phase-field, Cahn-Hilliard, parallel computation

1 Introduction

A phase-field model can avoid the problems of interface smearing and of the inaccurate computation of surface tension, which arise in the interface tracking methods such as volume-of-fluids or level-set method. The phase-field models have been widely used to simulate the flow of two or more fluids [1; 2]. However, the phase-field method yields non-self-adjoint operators and the solution contains high gradients within thin interfacial regions. In this study, the Cahn-Hilliard equation is selected as a representative of the phase-field models.

The least-squares formulation with C^1 Hermite approximation is used in this study as a main setup. The advantage of this method in the phase-field methods is (1) it always provides a symmetric positive definite system, (2) the LBB condition is circumvented, and (3) the higher order global differentiability improves the approximation accuracy of the solution within the interface. Additionally, in our solver a space-time coupled formulation is used, and the element-by-element technique is implemented.

We also present a high-order h-adaptive mesh refinement technique. The adaptive mesh makes our solver more efficiently by assigning finer elements within narrow interfaces and coarser elements in pure phases. Dealing with drastic topological changes requires tracking the interface movements. We compare the performance of two refinement criteria based on the solution gradient and the local residual.

2 The Mathematical Formulation

2.1 The Cahn-Hilliard Equation

We define the space-time set $\Omega := \Omega_{\mathbf{x}} \times (0,T), T > 0$, for a two-dimensional open domain $\Omega_{\mathbf{x}} \in \mathbb{R}^2$. The boundary of Ω is denoted as $\Gamma := \partial\Omega_{\mathbf{x}} \times (0,T)$. For a flow of two immiscible fluids, the dimensionless Cahn-Hilliard equation is stated as follows: find the unknowns $C = C(\boldsymbol{x},t) : \Omega \to (0,1)$, $\omega = \omega(\boldsymbol{x},t) : \Omega \to \mathbb{R}$ such that

$$\frac{\partial C}{\partial t} - \frac{1}{Pe}\nabla^2\omega = 0 \qquad \text{in } \Omega, \tag{1}$$

$$\omega = C^3 - 1.5C^2 + 0.5C - Cn^2\nabla^2 C \qquad \text{in } \Omega, \tag{2}$$

$$C(\boldsymbol{x},0) = C_0(\boldsymbol{x}) \qquad \text{in } \Omega_{\mathbf{x}}, \tag{3}$$

$$\nabla C \cdot \mathbf{n} = 0, \quad \nabla\omega \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma. \tag{4}$$

Here C is the concentration, and w is the chemical potential. Peculet number $Pe = L_0U_0/M$ and Cahn number $Cn = \epsilon/L_0$ are used, where U_0 and L_0 are the reference velocity and length, M is the mobility, and ϵ is the interfacial parameter. The derivation and the physical meaning of the Cahn-Hilliard are explained in our previous study [3] in more detail.

2.2 Least-Squares Method

We use the Newton linearization method to handle with nonlinear terms. We use a subscript l to denote the terms from previous linearization step. For a two-dimensional spatial domain, the Cahn-Hilliard equation with the unknowns $\mathbf{u}^T = [C\ \omega]$ can be represented as

$$\frac{\partial}{\partial t}C - \frac{1}{Pe}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\omega = 0, \tag{5}$$

$$\left[3C_l^2 - 3C_l + 0.5 - Cn^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\right]C - \omega = 2C_l^3 - 1.5C_l^2. \tag{6}$$

The final system with the boundary conditions is expressed in general as

$$\mathcal{L}\mathbf{u} = \mathcal{G} \qquad \text{in } \Omega, \tag{7}$$

$$\mathcal{B}\mathbf{u} = \mathbf{u}_\Gamma \qquad \text{on } \Gamma, \tag{8}$$

where $\mathcal{L}$ represents the partial differential operator, $\mathcal{G}$ is the corresponding source term, $\mathcal{B}$ is the boundary conditions operator, and $\mathbf{u}_\Gamma$ is the specified value on the boundaries. In this work, the boundary conditions are incorporated into the least-squares functional so that they are also a part of the minimization problem, namely

$$\mathcal{J}(\mathbf{u}) = \frac{1}{2}\left\|\mathcal{L}\mathbf{u} - \mathcal{G}\right\|_{0,\Omega}^2 + \frac{1}{2}\left\|\mathcal{B}\mathbf{u} - \mathbf{u}_\Gamma\right\|_{0,\Gamma}^2, \tag{9}$$

or equivalently,

Find $\mathbf{u} \in X(\Omega)$ such that

$$\mathcal{A}(\mathbf{u}, \mathbf{v}) = \mathcal{F}(\mathbf{v}) \qquad \forall \mathbf{v} \in X(\Omega), \tag{10}$$

with

$$\mathcal{A}(\mathbf{u}, \mathbf{v}) = (\mathcal{L}\mathbf{u}, \mathcal{L}\mathbf{v})_{0,\Omega} + (\mathcal{B}\mathbf{u}, \mathcal{B}\mathbf{v})_{0,\Gamma}, \tag{11}$$

$$\mathcal{F}(\mathbf{v}) = (\mathcal{G}, \mathcal{L}\mathbf{v})_{0,\Omega} + (\mathbf{u}_\Gamma, \mathcal{B}\mathbf{v})_{0,\Gamma}, \tag{12}$$

where $\mathcal{A} : X \times X \to \mathbb{R}$ is a symmetric, positive definite bilinear form, $\mathcal{F} : X \to \mathbb{R}$ a continuous linear form, and $X(\Omega)$ is a solution space.

2.3 Spectral Element Discretization

The computational domain Ω is divided into Ne subdomains Ω_e such that

$$\Omega = \sum_{e=1}^{Ne} \Omega_e, \qquad \Omega_i \cap \Omega_j = \emptyset, \quad i \neq j. \tag{13}$$

The discretization is based on a space-time coupled formulation. Space-time strips are consecutively aligned, and a strip is composed of only one element in time, $\Omega_e = \Omega_e^{\mathbf{x}} \times \Omega_e^t = (\mathbf{x}_e, \mathbf{x}_{e+1}) \times (t_n, t_{n+1})$ with the time step size $\Delta t = t_{n+1} - t_n$. Each subdomain is mapped onto the unit cube $(\xi, \sigma, \eta) \in [-1, 1]^3$ for a two-dimensional spatial domain, by an invertible mapping.

The transition region in the phase-field model is preferred to be close to a sharp interface, with the consequent impact on the numerical solution and need for higher spatial resolution. In this article, the local solution in each element Ω_e, $\mathbf{u}_e^h$, is approximated by C^1 p-version hierarchical approximation functions, so-called Hermite polynomials. A basis function for a two-dimensional space and time domain can be written as the tensor product of one-dimensional basis functions with same order, i.e., $\mathbf{\Phi}_m(\xi, \varsigma, \eta) = \phi_i(\xi) \otimes \phi_j(\varsigma) \otimes \phi_k(\eta)$, with $m =$

$i + j(p+1) + k(p+1)^2$ where $0 \leq i, j, k \leq p$. Thus, the local approximation $\mathbf{u}_e^h$ is expanded in $\mathbf{\Phi}$ continuous basis functions as

$$\mathbf{u}_e^h = \sum_{m=1}^{(p+1)^3} \mathbf{U}_e^m \mathbf{\Phi}_e^m. \tag{14}$$

The same basis functions and construction approach have been used in our previous study [4]. For more details we also refer to [5] and [6].

Together with integration by the Gaussian quadrature based on the GLL-roots, the discretization of the least-squares formulation (10) can be expressed on an element-level as

$$\mathbf{L}_e^T \mathbf{W}_e \mathbf{L}_e \mathbf{U}_e = \mathbf{L}_e^T \mathbf{W}_e \mathbf{F}_e, \tag{15}$$

where $\mathbf{L}$ is a matrix whose components are the evaluation of $\mathcal{L}$ with the Hermite polynomials at the quadrature points, and $\mathbf{F}$ is a vector of the evaluation of $\mathcal{G}$. $\mathbf{W}$ is a diagonal matrix of the quadrature weights, and in this article, the number of quadrature points Q are fixed at the same number of polynomials of one dimensional basis function as $Q = p + 1$.

The discretized algebraic equation is solved element-by-element with the conjugated gradient method with the Jacobi preconditioner. Matlab code and Matlab MPI developed at our group are used. The local solutions in each elements $\mathbf{u}_e^h$, are glued to construct the global approximation of the solution $\mathbf{u}^h$, i.e.,

$$\mathbf{u}^h = \bigcup_{e=1}^{Ne} \mathbf{u}_e^h. \tag{16}$$

3 Adaptive Mesh Refinement

3.1 C^1 continuous h-refinement

When the refinement level of neighboring elements is different, among the nodal basis of the coarser element, ones which have non-zero values on the element interface are shared with the finer element. To ensure the global C^1 continuity over a non-conformal element interface, we introduce two L^2-norm least-squares functionals to be minimized for the value of solution, $\mathcal{J}_0^r$, and for the derivative of solution, $\mathcal{J}_1^r$, respectively, over the inter-element interface γ between the finer element F and the coarser element C:

$$\mathcal{J}_0^r \left(\mathbf{u}_b^F; \mathbf{u}_b^C\right) = \int_\gamma \left(\mathbf{u}_b^F - \mathbf{u}_b^C\right)^2 d\mathrm{s}, \tag{17}$$

$$\mathcal{J}_1^r \left(\mathbf{u}_b^F; \mathbf{u}_b^C\right) = \int_\gamma \left(\nabla \mathbf{u}_b^F \cdot \mathbf{n} - \nabla \mathbf{u}_b^C \cdot \mathbf{n}\right)^2 d\mathrm{s}, \tag{18}$$

where $\mathbf{u}_b$ is the solution on the inter-element interface. With the expansion coefficients related to the solution value on the inter-element interface $\mathbf{U}_{b,0}$, the

minimization statement of $\mathcal{J}_0^r$ can be written in an algebraic form as

$$\nabla \mathcal{J}_0^r = 0; \quad \mathbf{U}_{b,0}^F = \mathbf{H}_F^{-1} \mathbf{H}_C \mathbf{U}_{b,0}^C \equiv \widetilde{\mathbf{Z}}_0 \mathbf{U}_{b,0}^C, \tag{19}$$

where $\mathbf{H}$ is a matrix of Hermite polynomials at the quadrature points, and $\widetilde{\mathbf{Z}}_0$ is the projection matrix for the solution value. Similarly, with the expansion coefficients related to the derivative of solution on the inter-element interface $\mathbf{U}_{b,1}$, the minimization statement of $\mathcal{J}_1^r$ is expressed as

$$\nabla \mathcal{J}_1^r = 0; \quad \mathbf{U}_{b,1}^F = \mathbf{D}_F^{-1} \mathbf{D}_C \mathbf{U}_{b,1}^C \equiv \widetilde{\mathbf{Z}}_1 \mathbf{U}_{b,1}^C, \tag{20}$$

with $\mathbf{D}$ a matrix of derivative of Hermite polynomials at the quadrature points, and $\widetilde{\mathbf{Z}}_1$ is the projection matrix for the derivative of solution.

With the relations (19) and (20), we can express all unknowns of finer element $\mathbf{U}^F$ in terms of $\mathbf{U}^{F'}$ composed of the unknowns of coarser element on the boarder and inner element unknowns $\mathbf{U}_i^F$ only:

$$\mathbf{U}^F = \begin{bmatrix} \mathbf{U}_{b,0}^F \\ \mathbf{U}_{b,1}^F \\ \mathbf{U}_i^F \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{Z}}_0 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \widetilde{\mathbf{Z}}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{b,0}^C \\ \mathbf{U}_{b,1}^C \\ \mathbf{U}_i^F \end{bmatrix} = \mathbf{Z} \mathbf{U}^{F'}, \tag{21}$$

where $\mathbf{Z}$ is the total projection matrix.

These constraints are implemented into the least-squares method by replacing $\mathbf{U}$ as $\mathbf{U}^{'}$ using Equation (21). The formulation at an element-level becomes

$$\mathbf{Z}_e^T \mathbf{L}_e^T \mathbf{W}_e \mathbf{L}_e \mathbf{Z}_e \mathbf{U}_e^{'} = \mathbf{Z}_e^T \mathbf{L}_e^T \mathbf{W}_e \mathbf{F}_e. \tag{22}$$

$\mathbf{Z}_e^T$ is multiplied to maintain the symmetricity of the least-squares system.

3.2 Refinement Strategy

For a transient problem, the decision should be made on the elements in the original unrefined grid to be refined or retrieved at each time step. During the refinement, an element is split into four daughter elements. An element with the refinement level k can be made by k-th mesh refinements from the reference element. In this study, the maximum refinement level is set to 2, and we confine the irregularity up to 1-level, i.e., the difference in the refinement levels of neighboring elements is no larger than 1. In addition to the advantage of implementation, the 1-level irregularity can improve the accuracy in describing the interface [7].

Regarding the decision on refinement, we consider two refinement criteria. With the first criterion (gradient), the elements where the solution gradient exceed a certain tolerance are refined, and it requires that

$$\|\nabla \mathbf{C}\|_{0,\Omega_e}^2 \geq tol_g, \tag{23}$$

with tol_g the discretization tolerance for the gradient. The gradient criterion does not use any error estimator but it intensively targets to the interface.

The second criterion (residual) is based on the local residual in each element, and it is defined as

$$\|\mathcal{R}\|^2_{0,\Omega_e} = \int_{\Omega_e} \left(\mathcal{L}\mathbf{u}^h - \mathcal{G}\right)^2 d\Omega_e. \tag{24}$$

The conforming elements with top certain percent of local residual are refined.

4 Numerical Examples

4.1 Poisson problem

We first solve the Poisson problem with exact solution and compare two refinement criteria. Consider the equation

$$\nabla^2\mathbf{u} = \left(4r^2/\sigma^4 - 4/\sigma^2\right)\exp(-r^2/\sigma^2), \tag{25}$$

with the exact solution $\mathbf{u} = \exp(-r^2/\sigma^2)$, where $r^2 = x^2 + y^2$ and $\sigma = \sqrt{2}/5$.

The spatial domain is $\Omega = [-0.5, 0.5]^2$. In this example, tol_g is set to 2.8, and the percentage of refined elements with the residual criterion change by cases to have similar number of degrees of freedom (Ndofs) with the gradient criterion. Figure 1 shows the solution on the adaptive meshes by two refinement criteria with $Ne = 10 \times 10$ and $p = 4$. The hilltop area is refined into level 2 with the residual criterion, but in level 1 with the gradient criterion.

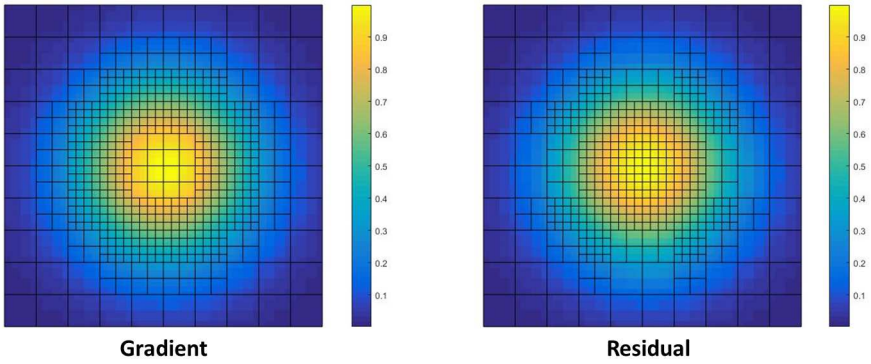

Fig. 1. Solution of Poisson problem and adaptive mesh with $Ne = 10 \times 10$ and $p = 4$ generated by gradient criterion (left) and by residual criterion (right).

The estimated error, defined as $\|\mathbf{u} - \mathbf{u}_{ex}\|^2_{0,\Omega}$, with respect to the Ndofs for both refinement criteria is illustrated in Figure 2. The error exponentially decays with increasing Ndofs for all expansion order cases. To compare the results from two refinement criteria, we define the following index, called refinement efficiency

R_{ef}, composed of ratios of the error and Ndofs from the conforming grid and non-conforming grid, denoted as subscript c and n, respectively:

$$R_{ef} = \frac{\|\mathbf{u}_c - \mathbf{u}_{c,ex}\|^2_{0,\Omega}}{\|\mathbf{u}_n - \mathbf{u}_{n,ex}\|^2_{0,\Omega}} \times \frac{Ndofs_c}{Ndofs_n}. \tag{26}$$

The refinement efficiency is presented in Figure 3. We can conclude that the

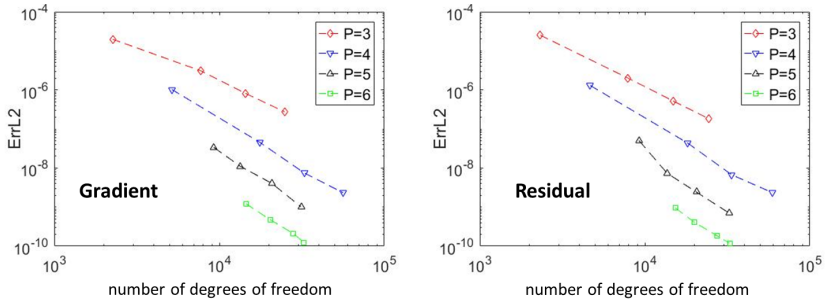

Fig. 2. Error with respect to Ndofs with gradient (left) and residual (right) criteria.

efficiency is higher with the gradient criterion in lower Ndofs, while the residual criterion is more efficient in higher Ndofs. With the gradient criterion the efficiency decreases more monotonously with respect to the Ndofs. This conclusion is also applicable to the solution from the phase-field method because of similar contour of solution - having a plateau on the hilltop with steep hill.

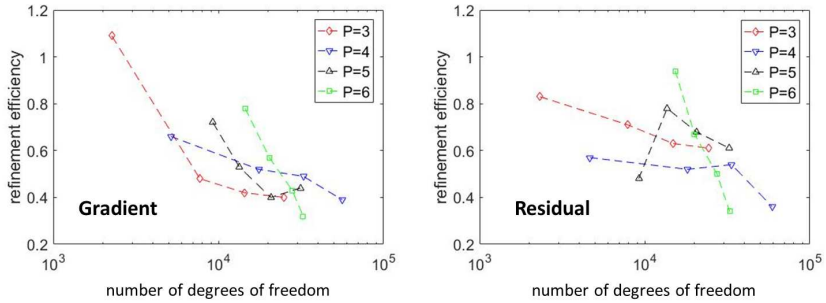

Fig. 3. Refinement efficiency with respect to Ndofs with gradient (left) and residual (right) criteria.

4.2 Benchmark Cross

The equilibrium state induced by the Cahn-Hilliard equation has the minimum local free energy and surface tension energy [8]. A cross-shaped droplet is initially located at the center of the domain $[0, 0.8]^2$, filled with another phase. The original unrefined grid in space is 10^2, and a single time-element of $\Delta t = 0.08$ is used. Polynomials with order of $p = 4$ are used to approximate the solution. The parameters used are $M = 1, Re = 1, Ca = 1, Pe = 100$ and $Cn = 0.01$. The tolerance in the gradient refinement criterion is set to 20, and for the residual refinement criterion 28% and 20% of elements in the initial coarse grid are refined, which correspond to the numbers of refined elements in the gradient criterion at the first and the last time step, respectively.

Among three cases, with the gradient criterion and with the residual criterion of 28% and 20%, no significant difference in the concentration is found. Figure 4 presents the evolution of the concentration and the local residuals of the three cases on the refined grids. With the gradient criterion, the only elements containing the interfaces are refined, so the distribution of the local residuals is symmetric. On the other hand, with the residual criterion, the refinement is performed rather assymetrically. Note that here the local residual from the Navier-Stokes equation is negligible, of order under 10^{-6}, compared with the one from the Cahn-Hilliard equation over the entire domain. Figure 5 shows the total residual and the Ndofs in time in log scale for the three cases. With the residual criterion of 28%, lower total residual can be achieved than the one with the gradient criterion, but it requires more Ndofs. Compared with the result from the residual criterion of 20%, the gradient criterion has a similar total residual and Ndofs at the final phase but yields more stable result in time. The total residual and Ndofs from the residual criterion have many fluctuation in time due to assymetric refinement of grid.

5 Concluding Remarks

We presented an adaptive least-squares spectral element scheme for the Cahn-Hilliard equation as a representative of the phase-field model. C^1 Hermite polynomials were used as basis functions to provide the global differentiability of solution, and the corresponding refinement scheme was provided. Two refinement criteria were considered, based on the solution gradient and the local residual. Steady-state Poisson problem with manufactured solution and the Cahn-Hilliard equation with a cross shaped initial solution were solved. Since the gradient criterion targets only interface elements, it gives us more stable and predictable error results. However, at the higher resolution case, the residual criteria becomes more efficient because the asymmetricity in refinement becomes subtle as the number of degrees of freedom increases. Therefore, we recommend to use the gradient criterion for the phase-field method, but it is worth considering the residual criterion if the initial grid already has a larger number of degrees of freedom.

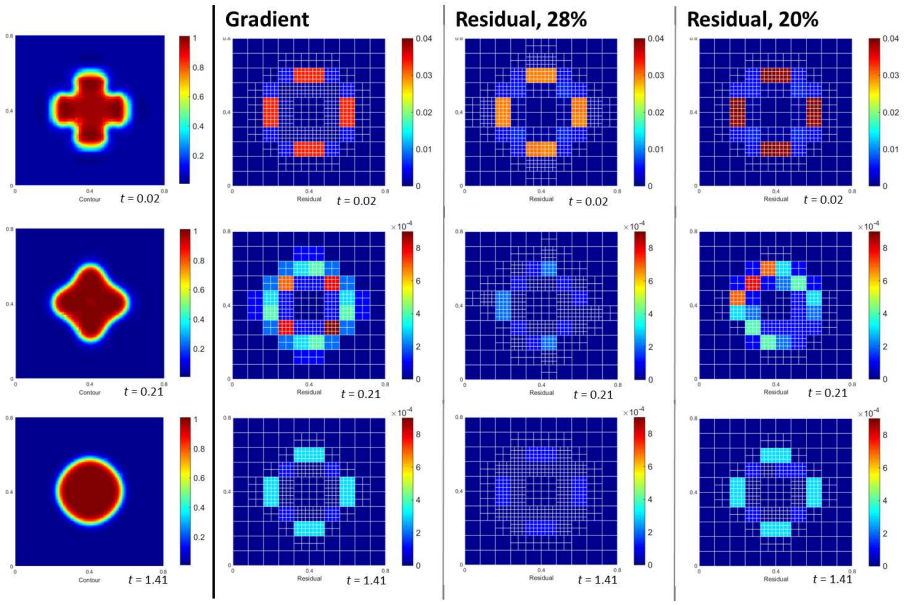

Fig. 4. Evolution of concentration (1st row) and local residuals on refined grid with gradient criterion (2nd row) and with residual criterion of 28% (3rd row) and of 20% (4th row) at $t = 0.02, 0.21$ and 1.41.

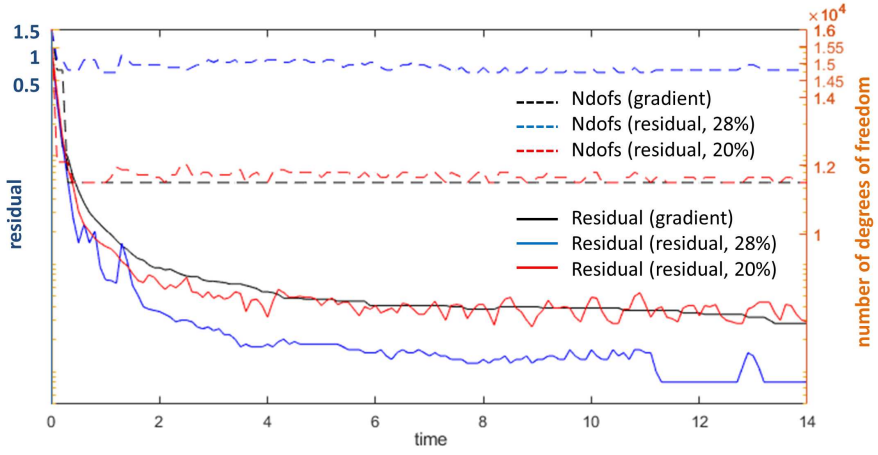

Fig. 5. Total residual (solid line) and Ndofs (dotted line) in time with the gradient criterion (black) and the residual criterion of 28% (blue) and of 20% (red) until $t = 14.0$.

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