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On conservation and dual consistency for summation-by-parts based approximations of parabolic problems

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1. Introduction

We consider the coupling of parabolic problems discretized using difference operators on summation-by-parts (SBP) form with interface conditions imposed weakly. In [1, 2], it was shown that conservation and dual consistency are equivalent concepts for linear conservation laws. Here, we show that these concepts are equivalent also for symmetric or symmetrizable parabolic problems, exemplified by the heat equation. We rewrite the heat equation as a first order system as in the local discontinuous Galerkin method and show the equivalence of dual consistency and conservation for both the first and second order forms [3, 4, 5].

2. The continuous problem

Consider the coupling of two heat equations

$$\begin{aligned} u_t &= (\epsilon u_x)_x, & -1 \leq x \leq 0, & \quad t > 0, \\ v_t &= (\epsilon v_x)_x, & 0 \leq x \leq 1, & \quad t > 0, \\ u(0, t) &= v(0, t), & x = 0, & \quad t > 0, \\ u_x(0, t) &= v_x(0, t), & x = 0, & \quad t > 0, \end{aligned} \tag{1}$$

augmented with initial conditions. In (1), $u(x, t)$ and $v(x, t)$ are the solutions in the left and right domain, respectively. For simplicity, we assume that the thermal diffusivity $\epsilon(x, t) > 0$ is continuous across the interface $x = 0$. For clarity and ease of presentation, the boundary conditions at $x = \pm 1$ are ignored.

The problem (1) is reduced to first order form by introducing the new variables $\tilde{u} = \epsilon u_x, \tilde{v} = \epsilon v_x$

$$\begin{aligned} \tilde{I}U_t + AU + BU_x &= 0, & -1 \leq x \leq 0, \quad t > 0, \\ \tilde{I}V_t + AV + BV_x &= 0, & 0 \leq x \leq 1, \quad t > 0, \\ U(0, t) &= V(0, t), & x = 0, \quad t > 0, \end{aligned} \quad (2)$$

augmented with homogeneous initial conditions. In (2), $U = [u, \tilde{u}]^T, V = [v, \tilde{v}]^T, \tilde{I} = \text{diag}(1, 0), A = \text{diag}(0, 1/\epsilon(x, t))$ and $B = -\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

2.1. Conservation

Let $\varphi(x, t) \in H^2((-1, 1))$ be a function with compact support in $-1 \leq x \leq 1$. Multiplying (1) by $\varphi(x, t)$ and performing integration by parts in space twice, leads to

$$\begin{aligned} \int_{-1}^0 \varphi u_t dx + \int_0^1 \varphi v_t dx &= \int_{-1}^0 (\epsilon \varphi_x)_x u dx + \int_0^1 (\epsilon \varphi_x)_x v dx \\ &+ \epsilon(0, t) \left(\varphi(0, t) (u_x(0, t) - v_x(0, t)) - \varphi_x(0, t) (u(0, t) - v(0, t)) \right). \end{aligned} \quad (3)$$

The interface conditions in (1) remove the interface terms in (3) and conservation follows.

Multiplying (2) with the transpose of the compactly supported vector function $\Phi(x, t) \in [H^1((-1, 1))]^2$, and integrating in space leads to

$$\begin{aligned} \int_{-1}^0 \Phi^T \tilde{I}U_t dx + \int_0^1 \Phi^T \tilde{I}V_t dx + \int_{-1}^0 \Phi^T AU dx + \int_0^1 \Phi^T AV dx \\ = -\Phi^T(0, t)B(U(0, t) - V(0, t)) + \int_{-1}^0 \Phi_x^T BU dx + \int_0^1 \Phi_x^T BV dx. \end{aligned} \quad (4)$$

The interface conditions in (2) remove the interface terms in (4), which (disregarding the zero order terms) implies that (2) is on conservative form.

Remark 1. *In this paper, we use a broad definition of conservation where the equations are multiplied by a smooth test function. By performing integration-by-parts we transfer all derivatives to the test function. We say that the problem is conservative if all interface terms vanish. This definition is motivated by the comparison with the problem on first order form. By choosing the test functions to be unity, the usual definition of conservation is obtained.*

2.2. The dual problem

The dual problem [6] associated to (1) is

$$\begin{aligned}
\phi_\tau &= (\epsilon\phi_x)_x, & -1 \leq x \leq 0, \quad \tau > 0, \\
\psi_\tau &= (\epsilon\psi_x)_x, & 0 \leq x \leq 1, \quad \tau > 0, \\
\phi(0, \tau) &= \psi(0, \tau), & x = 0, \quad \tau > 0, \\
\phi_x(0, \tau) &= \psi_x(0, \tau), & x = 0, \quad \tau > 0,
\end{aligned} \tag{5}$$

augmented with homogeneous initial conditions at $\tau = 0$. In (5), the dual time variable is $\tau = T - t$, where T is the final time for the primal problem. We ignore the boundary conditions at $x = \pm 1$ as in the primal problem. In the same way as for the primal problem, (5) can be shown to be conservative. The dual problem associated to (2) is

$$\begin{aligned}
\tilde{I}\Phi_\tau + A\Phi - B\Phi_x &= 0, & -1 \leq x \leq 0, \quad \tau > 0, \\
\tilde{I}\Psi_\tau + A\Psi - B\Psi_x &= 0, & 0 \leq x \leq 1, \quad \tau > 0, \\
\Phi(0, t) &= \Psi(0, t), & x = 0, \quad \tau > 0,
\end{aligned} \tag{6}$$

augmented with homogeneous initial conditions at $\tau = 0$. In (6), $\Phi = [\phi, \tilde{\phi}]^T$ and $\Psi = [\psi, \tilde{\psi}]^T$. Conservation of (6) is shown in the same way as for (2).

3. The semi-discrete approximation

To define a semi-discretization of (1), we discretize the left and right domains by $N + 1$ and $M + 1$ grid points, respectively. Let the vectors $\mathbf{u}, \mathbf{v}, \mathbf{U}$ and $\mathbf{V}$ contain approximations of u, v, U and V , respectively. Then, the first derivative is approximated using SBP operators

$$\begin{aligned}
u_x &\approx D_L \mathbf{u} = P_L^{-1} Q_L \mathbf{u}, & v_x &\approx D_R \mathbf{v} = P_R^{-1} Q_R \mathbf{v}, \\
U_x &\approx (D_L \otimes I_2) \mathbf{U}, & V_x &\approx (D_R \otimes I_2) \mathbf{V},
\end{aligned} \tag{7}$$

where $\otimes$ denotes the Kronecker product and the subscripts L, R refer to the left and right spatial intervals, respectively. For simplicity, we use the first derivative twice as our second derivative operator. In (7), $P_{L,R}$ are symmetric positive definite matrices and $Q_{L,R}$ are almost skew-symmetric matrices satisfying $Q_{L,R} + Q_{L,R}^T = \text{diag}(-1, 0, \dots, 0, 1)$. I_2 is the 2×2 identity matrix.

Now, we discretize (1) in space as in [5] and obtain

$$\begin{aligned} \mathbf{u}_t - D_L(\boldsymbol{\epsilon}_L D_L \mathbf{u}) &= P_L^{-1} [\sigma_L^1(u_N - v_0) + \sigma_L^2((D_L \mathbf{u})_N - (D_R \mathbf{v})_0)] e_N \\ &\quad + P_L^{-1} D_L^T [\sigma_L^3(u_N - v_0) + \sigma_L^4((D_L \mathbf{u})_N - (D_R \mathbf{v})_0)] e_N, \\ \mathbf{v}_t - D_R(\boldsymbol{\epsilon}_R D_R \mathbf{v}) &= P_R^{-1} [\sigma_R^1(v_0 - u_N) + \sigma_R^2((D_R \mathbf{v})_0 - (D_L \mathbf{u})_N)] e_0 \\ &\quad + P_R^{-1} D_R^T [\sigma_R^3(v_0 - u_N) + \sigma_R^4((D_R \mathbf{v})_0 - (D_L \mathbf{u})_N)] e_0, \end{aligned} \quad (8)$$

where the diagonal matrices $\boldsymbol{\epsilon}_L$ and $\boldsymbol{\epsilon}_R$ approximate $\epsilon(x, t)$ point wise on the left and right domains, respectively. In (8), the vectors $e_N = [0, \dots, 0, 1]^T$ and $e_0 = [1, 0, \dots, 0]^T$ have the length of the left and right mesh, respectively. The scalars $u_N, (D_L \mathbf{u})_N, v_0$ and $(D_R \mathbf{v})_0$ are approximations of u, u_x, v and v_x at $x = 0$. Furthermore, the penalty terms on the right-hand side (RHS) impose the interface conditions weakly.

Next, we discretize (2) as

$$\begin{aligned} (I_N \otimes \tilde{I}) \mathbf{U}_t + [\mathbf{A}_L + D_L \otimes B] \mathbf{U} &= (P_L^{-1} e_N \otimes \Sigma_l)(U_N - V_0), \\ (I_M \otimes \tilde{I}) \mathbf{V}_t + [\mathbf{A}_R + D_R \otimes B] \mathbf{V} &= (P_R^{-1} e_0 \otimes \Sigma_r)(V_0 - U_N), \end{aligned} \quad (9)$$

where I_N and I_M are the identity matrices of size $N + 1$ and $M + 1$ and $\mathbf{A}_L$ and $\mathbf{A}_R$ approximate $A = A(x, t)$ point wise on the left and right domains, respectively.

We can rearrange the terms in (8) such that we get a first order scheme, which is equivalent to (9) if

$$\begin{aligned} \Sigma_l &= \begin{bmatrix} \sigma_L^1 + \alpha_L \sigma_L^3 - \frac{\alpha_L}{\beta} (\sigma_L^2 + \alpha_L \sigma_L^4) (\sigma_L^3 + \sigma_R^3) & -\frac{1}{\beta} (\sigma_L^2 + \alpha_L \sigma_L^4) \\ \frac{-\sigma_L^3}{\epsilon_I} + \frac{\alpha_L}{\beta \epsilon_I} \sigma_L^4 (\sigma_L^3 + \sigma_R^3) & \frac{1}{\beta \epsilon_I} \sigma_L^4 \end{bmatrix}, \\ \Sigma_r &= \begin{bmatrix} \sigma_R^1 - \alpha_R \sigma_R^3 - \frac{\alpha_R}{\beta} (\sigma_R^2 - \alpha_R \sigma_R^4) (\sigma_L^3 + \sigma_R^3) & -\frac{1}{\beta} (\sigma_R^2 - \alpha_R \sigma_R^4) \\ \frac{-\sigma_R^3}{\epsilon_I} + \frac{\alpha_R}{\beta \epsilon_I} \sigma_R^4 (\sigma_L^3 + \sigma_R^3) & \frac{1}{\beta \epsilon_I} \sigma_R^4 \end{bmatrix}, \end{aligned} \quad (10)$$

where $\epsilon_I = \epsilon(0, t)$, $\alpha_L = e_N^T P_L^{-1} e_N$, $\alpha_R = e_0^T P_R^{-1} e_0$ and $\beta = -\epsilon_I + \alpha_L \sigma_L^4 + \alpha_R \sigma_R^4$.

Similarly, we can rewrite the scheme (9) as a second order scheme, which

is equivalent to (8) with $\Sigma_l = \begin{bmatrix} \sigma_l^1 & \sigma_l^2 \\ \sigma_l^3 & \sigma_l^4 \end{bmatrix}$ and $\Sigma_r = \begin{bmatrix} \sigma_r^1 & \sigma_r^2 \\ \sigma_r^3 & \sigma_r^4 \end{bmatrix}$ if

$$\begin{aligned} \sigma_L^1 &= \sigma_l^1 + \alpha_L \epsilon_I \sigma_l^3 - \frac{\alpha_L \epsilon_I}{\tilde{\beta}} (\sigma_l^2 + \alpha_L \epsilon_I \sigma_l^4) (\sigma_l^3 + \sigma_r^3), & \sigma_L^2 &= -\frac{\epsilon_I}{\tilde{\beta}} (\sigma_l^2 + \alpha_L \epsilon_I \sigma_l^4) \\ \sigma_L^3 &= -\epsilon_I \sigma_l^3 + \frac{\alpha_L \epsilon_I^2}{\tilde{\beta}} \sigma_l^4 (\sigma_l^3 + \sigma_r^3), & \sigma_L^4 &= \frac{\epsilon_I^2}{\tilde{\beta}} \sigma_l^4, \\ \sigma_R^1 &= \sigma_r^1 - \alpha_R \epsilon_I \sigma_r^3 - \frac{\alpha_R \epsilon_I}{\tilde{\beta}} (\sigma_r^2 - \alpha_R \epsilon_I \sigma_r^4) (\sigma_l^3 + \sigma_r^3), & \sigma_R^2 &= -\frac{\epsilon_I}{\tilde{\beta}} (\sigma_r^2 - \alpha_R \epsilon_I \sigma_r^4) \\ \sigma_R^3 &= -\epsilon_I \sigma_r^3 + \frac{\alpha_R \epsilon_I^2}{\tilde{\beta}} \sigma_r^4 (\sigma_l^3 + \sigma_r^3), & \sigma_R^4 &= \frac{\epsilon_I^2}{\tilde{\beta}} \sigma_r^4, \end{aligned} \quad (11)$$

where $\tilde{\beta} = -1 + \alpha_L \epsilon_I \sigma_l^4 + \alpha_R \epsilon_I \sigma_r^4$.

3.1. Conservation

Let $\varphi_L \in V_L$ and $\varphi_R \in V_R$ denote grid functions at the left and right domains where V_L and V_R are discrete subspaces of $H^2((-1, 0))$ and $H^2((0, 1))$, respectively. Multiplying (8) by $\varphi_L^T P_L$ and $\varphi_R^T P_R$ and using $\varphi_L^N = \varphi_R^0 := \varphi_I$ leads to

$$\varphi_L^T P_L \mathbf{u}_t + \varphi_R^T P_R \mathbf{v}_t = [D_L \epsilon_L (D_L \varphi_L)]^T P_L \mathbf{u} + [D_R \epsilon_R (D_R \varphi_R)]^T P_R \mathbf{v} + IT, \quad (12)$$

where

$$\begin{aligned} IT &= \varphi_I (\sigma_L^1 - \sigma_R^1) [u_N - v_0] + \varphi_I (\sigma_L^2 - \sigma_R^2 + \epsilon_I) [(D_L \mathbf{u})_N - (D_R \mathbf{v})_0] \\ &+ (D_R \varphi_R)_0 (\sigma_L^3 - \epsilon_I - \sigma_R^3) [u_N - v_0] + (D_R \varphi_R)_0 (\sigma_L^4 - \sigma_R^4) [(D_L \mathbf{u})_N - (D_R \mathbf{v})_0] \\ &+ [(D_L \varphi_L)_N - (D_R \varphi_R)_0] [\sigma_L^3 (u_N - v_0) - \epsilon_I u_N + \sigma_L^4 ((D_L \mathbf{u})_N - (D_R \mathbf{v})_0)]. \end{aligned}$$

The last term in IT is proportional to the order of the scheme. Following [7], we say that (8) is conservative to the order of the scheme if $IT = 0$, for all $\varphi_L \in V_L$ and $\varphi_R \in V_R$. This holds if $(D_L \varphi_L)_N = (D_R \varphi_R)_0$ and

$$\sigma_L^1 = \sigma_R^1, \quad \sigma_L^2 = \sigma_R^2 - \epsilon_I, \quad \sigma_L^3 = \sigma_R^3 + \epsilon_I, \quad \sigma_L^4 = \sigma_R^4. \quad (13)$$

On the other hand, if (8) is conservative to the order of the scheme, then $IT = 0$ for all possible solutions and test functions which implies that (13) must hold.

We summarize the result in

Proposition 1. *The interface procedure in (8) is conservative if and only if (13) holds.*

Remark 2. *It can be shown that Proposition 1 holds for narrow stencil SBP operators that can accommodate variable coefficients as defined in [8].*

Next, we multiply (9) with $\Phi_L^T(P_L \otimes I_2)$ and $\Phi_R^T(P_R \otimes I_2)$ to get

$$\begin{aligned} & \Phi_L^T(P_L \otimes \tilde{I})\mathbf{U}_t + \Phi_R^T(P_R \otimes \tilde{I})\mathbf{V}_t + \Phi_L^T(P_L \otimes I_2)\mathbf{A}_L\mathbf{U} + \Phi_R^T(P_R \otimes I_2)\mathbf{A}_R\mathbf{V} \\ &= \Phi_I^T(\Sigma_l - \Sigma_r - B)[U_N - V_0] + \Phi_L^T(D_L^T P_L \otimes B)\mathbf{U} + \Phi_R^T(D_R^T P_R \otimes B)\mathbf{V}, \end{aligned} \quad (14)$$

which mimics the continuous formulation in (4). In (14), $\Phi_I := (\Phi_L)_N = (\Phi_R)_0$, and a conservative scheme requires

$$\Sigma_l = \Sigma_r + B. \quad (15)$$

On the other hand, the interface term on the RHS of (14) must vanish for all possible solutions and test functions if (9) is a conservative scheme, which implies that (15) holds.

We summarize the result in

Proposition 2. *The interface procedure in (9) is conservative if and only if (15) holds.*

Remark 3. *If the scheme (8) is conservative, then the first order scheme (9) with penalty matrices given in (10), is conservative. Similarly, if the scheme (9) is conservative, then the second order scheme (8) with penalty coefficients given in (11), is conservative.*

Remark 4. *Since $\sigma_L^4 = \sigma_R^4 \neq 0$ may increase the truncation error of the scheme (8), see [5], an obvious choice is $\sigma_L^4 = \sigma_R^4 = 0$, which is used in the rest of the paper.*

3.2. Dual Consistency

To determine dual consistency, we rewrite (8) in the compact form

$$\mathbf{w}_t + L\mathbf{w} = 0, \quad L = -(D_2 + P^{-1}\Sigma), \quad (16)$$

where $\mathbf{w} = [\mathbf{u}, \mathbf{v}]^T$, $D_2 = \text{diag}(D_L \epsilon_L D_L, D_R \epsilon_R D_R)$, $P^{-1} = \text{diag}(P_L^{-1}, P_R^{-1})$ and

$$\Sigma = F(\Sigma_1 + D\Sigma_2) + D^T F(\Sigma_3 + D\Sigma_4), \quad F = \begin{bmatrix} +E_N & -E_I \\ -E_I^T & +E_0 \end{bmatrix}. \quad (17)$$

In (17), $\Sigma_i = \text{diag}(\sigma_L^i, \sigma_R^i)$, where $\sigma_{L,R}^i$ given in (8), $D = \text{diag}(D_L, D_R)$, while $E_N = e_N e_N^T$ and $E_0 = e_0 e_0^T$. The $(N+1) \times (M+1)$ matrix $E_I = e_N e_0^T$ picks out the parts of the vectors residing at the interface such that $E_I \mathbf{v} = [0, \dots, 0, v_0]^T$ and $E_I^T \mathbf{u} = [u_N, 0, \dots, 0]^T$.

The discrete dual problem corresponding to (16) is (see [6])

$$\boldsymbol{\vartheta}_\tau + P^{-1} L^T P \boldsymbol{\vartheta} = 0, \quad (18)$$

where $\boldsymbol{\vartheta} = [\boldsymbol{\phi}, \boldsymbol{\psi}]^T$. By using the SBP properties of the operators, we expand (18) and write it in component form as

$$\begin{aligned} \boldsymbol{\phi}_t - D_L(\epsilon_L D_L \boldsymbol{\phi}) &= P_L^{-1} [\sigma_L^1 \boldsymbol{\phi}_N - \sigma_R^1 \boldsymbol{\psi}_0 + (\sigma_L^3 - \epsilon_I)(D_L \boldsymbol{\phi})_N - \sigma_R^3 (D_R \boldsymbol{\psi})_0] e_N \\ &\quad + P_L^{-1} D_L^T [(\epsilon_I + \sigma_L^2) \boldsymbol{\phi}_N - \sigma_R^2 \boldsymbol{\psi}_0] e_N, \\ \boldsymbol{\psi}_t - D_R(\epsilon_R D_R \boldsymbol{\psi}) &= P_R^{-1} [\sigma_R^1 \boldsymbol{\psi}_0 - \sigma_L^1 \boldsymbol{\phi}_N + (\epsilon_I + \sigma_R^3)(D_R \boldsymbol{\psi})_0 - \sigma_L^3 (D_L \boldsymbol{\phi})_N] e_0 \\ &\quad + P_R^{-1} D_R^T [(\sigma_R^2 - \epsilon_I) \boldsymbol{\psi}_0 - \sigma_L^2 \boldsymbol{\phi}_N] e_0. \end{aligned} \quad (19)$$

Dual consistency requires that (19) is a consistent approximation of (5), which leads to

Proposition 3. *The scheme (19) is dual consistent if only if (13) holds.*

Proof. The left-hand side (LHS) of (19) approximate the equations in (5). If (13) is satisfied, then the RHS of (19) imposes the dual interface conditions in (5). On the other hand, the interface terms on the RHS of (19) should vanish if $\boldsymbol{\varphi}$ and $\boldsymbol{\psi}$ satisfies the numerical interface conditions exactly. In other words, if (13) is not satisfied, the numerical scheme (19) would impose interface conditions at $x = 0$ that do not exist in the adjoint problem. $\square$

To determine dual consistency, we rewrite (9) in compact form

$$\tilde{\mathbf{I}} \mathbf{W}_t + \mathcal{L} \mathbf{W} = 0, \quad \mathcal{L} = \mathcal{D}_2 - \mathcal{P}^{-1} S, \quad \tilde{\mathbf{I}} = \text{diag}(I_N \otimes \tilde{I}, I_M \otimes \tilde{I}), \quad (20)$$

and $\mathbf{W} = [\mathbf{U}, \mathbf{V}]$. In (20), $\mathcal{D}_2 = \text{diag}(\mathbf{A}_L + D_L \otimes B, \mathbf{A}_R + D_R \otimes B)$, and

$$S = \begin{bmatrix} +E_N \otimes \Sigma_l & -E_I \otimes \Sigma_l \\ -E_I^T \otimes \Sigma_r & +E_0 \otimes \Sigma_r \end{bmatrix}, \quad \mathcal{P}^{-1} = \text{diag}(P_L^{-1} \otimes I_2, P_R^{-1} \otimes I_2).$$

The discrete dual problem corresponding to (20) is

$$\tilde{\mathbf{I}} \boldsymbol{\theta}_\tau + \mathcal{P}^{-1} \mathcal{L}^T \mathcal{P} \boldsymbol{\theta} = 0, \quad (21)$$

where $\boldsymbol{\theta} = [\boldsymbol{\Phi}, \boldsymbol{\Psi}]^T$. By expanding (21) in component form, we find

$$\begin{aligned} (I_N \otimes \tilde{I})\boldsymbol{\Phi}_t + [\mathbf{A}_L - D_L \otimes B]\boldsymbol{\Phi} &= (P_L^{-1}e_N \otimes (\Sigma_l^T - B^T))\boldsymbol{\Phi}_N - (P_L^{-1}e_N \otimes \Sigma_r^T)\boldsymbol{\Psi}_0, \\ (I_M \otimes \tilde{I})\boldsymbol{\Psi}_t + [\mathbf{A}_R - D_R \otimes B]\boldsymbol{\Psi} &= (P_R^{-1}e_0 \otimes (\Sigma_r^T + B^T))\boldsymbol{\Psi}_0 - (P_R^{-1}e_0 \otimes \Sigma_l^T)\boldsymbol{\Phi}_N. \end{aligned} \quad (22)$$

Proposition 4. *The scheme (22) is dual consistent if only if (15) holds.*

Proof. The terms on the LHS in (22) approximate the two systems of equations in (6). If (15) is satisfied, the RHS of (22) imposes the dual interface conditions in (6). On the other hand, the interface terms on the RHS of (22) should vanish if $\boldsymbol{\Phi}$ and $\boldsymbol{\Psi}$ satisfies the numerical interface conditions exactly. In other words, if (15) is not satisfied, the numerical scheme (22) would impose interface conditions at $x = 0$ that do not exist in the adjoint problem. $\square$

4. Equivalence of conservation and dual consistency

We are now ready to state the main results.

Proposition 5. *The approximation (16) is conservative if and only if it is dual consistent.*

Proof. It follows immediately from Propositions (1) and (3). $\square$

Proposition 6. *The approximation (20) is conservative if and only if it is dual consistent.*

Proof. It follows immediately from Propositions (2) and (4). $\square$

Remark 5. *Proposition 5 and 6 imply that the conservation relations in Remark 3 also lead to dual consistency.*

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