Diagonal Split-Mass SBP Construction by Constrained Optimization

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We document a diagonal split-mass construction for spherical-symmetry SBP operators in which scalar and vector moments are integrated by separate diagonal matrices. The method enforces hard positivity of both diagonal masses and imposes symmetry, divergence, and quadrature conditions as linear equality constraints in a constrained optimization problem. We describe both full-constraint and divergence-first staged variants, then summarize feasibility and constraint errors for representative runs at $p = 2$ and gradient orders $d = 2, 4, 6$. Feasible configurations satisfy the discrete SBP identity at roundoff level.

I. PROBLEM STATEMENT

On a mirrored uniform grid $x_i \in [-R, R]$ ($i = 1, \dots, N$), let $G \in \mathbb{R}^{N\times N}$ be a first-derivative SBP matrix and

$$B = \mathrm{diag}(B_{11}, \dots, B_{NN}), \qquad B_{11} = -R^p, \quad B_{NN} = R^p, \tag{1}$$

with all other $B_{ii} = 0$.

We seek two diagonal positive-definite mass matrices

$$S = \mathrm{diag}(s_1, \dots, s_N), \qquad V = \mathrm{diag}(v_1, \dots, v_N), \tag{2}$$

with

$$s_i \geq \epsilon, \qquad v_i \geq \epsilon \quad \forall i, \tag{3}$$

where $\epsilon > 0$ is user-selected (default in the implementation is the next-cell volume from $r = 0$, i.e. $\epsilon = 1/3$ for $\Delta r = 1$).

The split SBP relation is

$$SD + G^T V = B, \tag{4}$$

which defines

$$D = S^{-1}(B - G^T V). \tag{5}$$

II. CONSTRAINT FAMILIES

Unknowns are collected as

$$z = [s_1, \dots, s_N, v_1, \dots, v_N]^T \in \mathbb{R}^{2N}. \tag{6}$$

All imposed conditions are linear in z.

A. Reflection symmetry

Let $c = (N + 1)/2$ be the center index. For $k = 1, \dots, c - 1$:

$$s_{c-k} - s_{c+k} = 0, \tag{7}$$
$$v_{c-k} - v_{c+k} = 0. \tag{8}$$

B. Optional anti-stiffness

If enabled:

$$s_c - s_{c+1} = 0, \qquad v_c - v_{c+1} = 0. \tag{9}$$

C. Split quadrature moments

For geometry power p, the target moment is

$$I_q = \int_{-R}^{R} r^q r^p \, dr. \tag{10}$$

For even exponents $q \in \{0, 2, \dots, q_S^{\max}\}$:

$$\sum_{j=1}^{N} s_j x_j^q = I_q. \tag{11}$$

For odd exponents $q \in \{1, 3, \dots, q_V^{\max}\}$:

$$\sum_{j=1}^{N} v_j x_j^q = I_q. \tag{12}$$

Optionally, a $q = -1$ vector moment is also enforced:

$$\sum_{j=1}^{N} v_j \phi_j^{(-1)} = I_{-1}, \tag{13}$$

where $\phi_j^{(-1)} = 1/x_j$ for $x_j \neq 0$ and $\phi_j^{(-1)} = 0$ at $x_j = 0$.

D. Divergence exactness on odd monomials

For odd k, Eq. (4) applied to x^k gives row-wise constraints:

$$(k + p)x_i^{k-1} s_i + \sum_{j=1}^{N} G_{ji} x_j^k v_j = B_{ii} x_i^k. \tag{14}$$

Interior rows use odd degrees up to $k \leq k_{\mathrm{int}}^{\max}$ (via `div_max_odd`). Boundary rows use a possibly reduced cap $k \leq k_{\mathrm{bnd}}^{\max}$ (via `boundary_div_max_odd`).

III. OPTIMIZATION MODEL

With active equality rows $A_{\rm act}z = b_{\rm act}$, we solve

$$\min_{z\in\mathbb{R}^{2N}} \sum_{i=1}^{N}(s_i - |x_i|^p)^2 + \sum_{i=1}^{N}(v_i - |x_i|^p)^2, \tag{15}$$
$$\text{s.t.}\quad A_{\rm act}z = b_{\rm act}, \tag{16}$$
$$s_i \ge \epsilon,\ v_i \ge \epsilon. \tag{17}$$

Ipopt is used with tight feasibility tolerances.

a. Feasibility criterion. A run is marked feasible if termination is successful and

$$\max |A_{\rm act}z - b_{\rm act}| \le \tau, \tag{18}$$

with $\tau = \max(10^{-9}, 10\,\texttt{constr\_viol\_tol})$.

IV. CONSTRAINT APPLICATION STRATEGIES

Two modes are implemented.

A. Full mode

All selected constraints are active simultaneously.

B. Staged quadrature mode

First, solve with symmetry+divergence rows only. Then attempt quadrature rows one-by-one (ordered by exponent and family), retaining only rows that preserve feasibility under positivity bounds.

This mode prioritizes divergence constraints when full systems are difficult.

V. RUN DESIGN CHOICES

All reported runs use:

- geometry $p = 2$,
- mirrored grid $x = -10 : 1 : 10$ ($N = 21$),
- odd divergence monomials in the interior according to each test,
- hard positivity for both masses ($S, V \succeq \epsilon I$ in diagonal form).

For $d = 2, 4$, we tested representative split quadrature settings and observed feasible solves with small residuals. For $d = 6$, we focused on the case requested by the study: interior $\{Dr, Dr^3\}$ and reduced boundary divergence order.

VI. SUMMARY OF FEASIBLE RUNS

Table I reports feasible representative runs. The quadrature columns show maximum absolute per-moment errors over imposed moments. The divergence columns report maximum residual of imposed divergence constraints, plus origin and boundary subsets.

a. SBP residual on feasible runs. For feasible cases, the matrix residual

$$R_{\rm SBP} = SD + G^T V - B \tag{19}$$

is at roundoff level. For the $d = 6$ feasible runs above, we observed $\max |R_{\rm SBP}| \in [7.1 \times 10^{-15}, 2.8 \times 10^{-14}]$.

VII. WHAT CAUSED INFEASIBILITY IN DIFFICULT $d = 6$ RUNS?

For $d = 6$ with interior $\{Dr, Dr^3\}$ and boundary Dr under the default $\epsilon = 1/3$, the divergence-first base system can be linearly consistent (so not a pure rank mismatch), but still incompatible with strict positivity. Lowering ϵ to 10^{-3} or 10^{-2} restores feasibility for the tested quadrature set.

When boundary divergence is further tightened, genuine linear inconsistency (rank mismatch) can also appear.

VIII. PRACTICAL PROCEDURE

A practical workflow for diagonal split masses is:

1. Choose (d, p) and divergence targets first (interior and boundary separately).
2. Solve divergence+symmetry with hard positivity.
3. If feasible, add quadrature moments (full or staged mode).
4. Report per-family residuals and SBP matrix residual.

IX. REPRODUCIBILITY

All runs are produced with `scripts/diag_mass_qp/diag_mass_qp_core.jl` and `scripts/diag_mass_qp/run_diag_mass_qp.jl`.

Example command (feasible $d = 6$ case):

```
julia --project=. scripts/diag_mass_qp/run_diag_mass_qp.j
  --p 2 --d 6 --epsilon 1e-3 \
  --div-max-odd 3 --boundary-div-max-odd 1 \
  --s-quad-order 2 --v-quad-order 3 --enforce-v-neg1
```

TABLE I. Feasible representative runs for diagonal split masses.

Case	d	ϵ	$k_{\mathrm{bnd}}^{\max}$	Quadrature set	$\max\lvert Az-b\rvert$	$\max E_S$	$\max E_V$	$\max E_{\mathrm{div}}$	$(E_{\mathrm{div}}(0), E_{\mathrm{div}}(\partial))$
A	2	1/3	1	$S:\{0,2\},\ V:\{-1,1,3\}$	1.46×10^{-11}	2.27×10^{-13}	1.46×10^{-11}	1.14×10^{-13}	(n/a, 1.14×10^{-13})
B	4	1/3	1	$S:\{0,2\},\ V:\{-1,1,3\}$	2.91×10^{-11}	1.14×10^{-13}	2.18×10^{-11}	1.22×10^{-13}	(1.22×10^{-13}, 1.14×10^{-13})
C	6	10^{-2}	1	$S:\{0,2\},\ V:\{-1,1,3\}$	1.46×10^{-11}	0	7.28×10^{-12}	4.55×10^{-13}	(2.72×10^{-13}, 2.27×10^{-13})
D	6	10^{-3}	1	$S:\{0,2\},\ V:\{-1,1,3\}$	1.46×10^{-11}	0	1.09×10^{-11}	3.04×10^{-13}	(3.04×10^{-13}, 7.11×10^{-14})
E	6	10^{-2}	0	$S:\{0,2\},\ V:\{-1,1,3\}$	1.42×10^{-13}	0	0	1.42×10^{-13}	(5.55×10^{-17}, n/a)
F	6	10^{-3}	0	$S:\{0,2\},\ V:\{-1,1,3\}$	7.28×10^{-12}	2.27×10^{-13}	2.91×10^{-11}	2.84×10^{-13}	(1.67×10^{-16}, n/a)