Serial comparison of Proto-based an fortran-based elliptic operators

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1 Context

Chombo solves elliptic equations using the framework in AMRElliptic. The driving classes (`AMRMultigrid, Multigrid, BiCGStabSolver, RelaxSolver` and so on) are templated on data type. The operator base classses `AMRLevelOp`, `MGLevelOp`, and `LinearOp` describe the interface to which an operator much conform to be used by these driver classes. This framework has been shown to be very flexible as operators in many different contexts have been able to use the driver framework.

This operator framework is large, however. The `AMRLevelOp` class hierarchy describes dozens of virtual functions. Over time, optimization efforts have expanded this interface a lot. This means writing one of these classes can be taxing.

The elliptic operators in `Chombo/lib/src/AMRElliptic` are templated on `LevelData<FArrayBox>` and the all computation and memory is on the host. These shall be referred to as the fortran-based operators because they all drop to fortran kernels.

The corresponding elliptic operators in `Chombo/releasedExamples/Proto/common` are templated on proto's `LevelBoxData`. All computation by and memory for the operator is on the device. These shall be referred to as the proto-based elliptic operators.

There are two purposes for this test framework.

- Minimize the operator interface and measure the consequences. The This will have performance penalties but those are measurable. I am very curious as to how big those penalties are and I will expend some effort to find out.
- Use the proto infrastructure to implement a selection of operators on the device and compare their times to the equivalent fortran-based operators on the host. This is a baseline measurement before real optimizations (that can gloriously mess up the code) have been introduced.

Mostly I just want to get everything running in all the configuations Though we will vary a bunch of things, this particular test will be kept simple.

- All computations on the host (specfically, spencer.lbl.gov).
- All computations are in serial.
- All runs have Dirichlet boundary conditions and very simple grids.
- All input files are pretty forgiving in terms of solvability and so on (coefficients set to reasonable constants and so on).
- The varying input files are really just making bigger grids

Later frameworks will address GPU and MPI issues.

2 Test description

There are eight operator classes we are considering.

- `AMRPoissonOp` (constant coefficient Helmholtz on host).
- `VCAMRPoissonOp2` (variable coefficient Helmholtz on host).
- `ViscousTensorOp` (viscous tensor on host).
- `ResistivityOp` (resistivity on host).
- `Proto_Helmholtz_Op` (constant coefficient Helmholtz on device).
- `Proto_Conductivity_Op` (variable coefficient Helmholtz on device).
- `Proto_Viscous Tensor_Op` (viscous tensor on device).
- `Proto_Resistivity_Op` (resistivity on device).

3 Results

Each class is run for both two and three dimensions. Each operator is run with input files for separate cases. For each case, all the operators L were used to solve

$$L\phi = 1$$

with homogeneous Dirichlet boundary conditions. For all the operators, this should be at least solvable. The details for each operator's settings are in the input file for each case (included in the data). Effort was made to match coefficients across the proto- and fortran-based operators. Judging from the wildly variable number of multigrid iterations, it appears these cases are not that closely matched after all. More work will have to be done to bridge that gap.

The cases used for this campaign are as follows.

- `case_0.inputs`: max level = 0, ncells = 32^D.
- `case_1.inputs`: max level = 1, ncells = 32^D.
- `case_2.inputs`: max level = 2, ncells = 32^D.
- `case_3.inputs`: max level = 2, ncells = 64^D.

With eight operators and both two and three dimensions, this should amount to 64 runs.

4 Dataset from February 5, 2024

4.1 Summary of this round of data

This test is mostly to see if I can get everything running. Everything ran. This is very good news. Not everything ran well. Some operators (old and new) did not converge well (or at all). The old resistivity operator seems particularly problematic. Then again, there was no effort to make these test problems reasonable. All the data is included. Keep in mind that all times include very slow things like writing hdf5 files. These are all serial runs meant to provide data for the first round of optimizations.

We plot the final residual and the number of multigrid iterations and amount of time it took to get there. Note that not everything converged. All of these runs had debug false and optimation high.

4.2 Bug?

Note: I just looked at all the solver tolerances and so on. They seem to match. At the very least, it appears we have a bug in `ResistivityOp`. I just put in a ton of timers and will try again.

5 Dataset from February 7, 2024

After examining time.table files, I found that the fortran-based operators were doing a different form of relaxation than the proto-based ones. To make the comparison more fair, for this round, all operators should be using "slow" Gauss-Seidel relaxation. This is probably not a great long-term solution but it will clarify where we are for this baseline measurement.

5.1 Summary of this round of data

Because of the very different cycle counts, the different operators remain difficult to compare. This should be the focus before more data comparisons of this are made. I also have to resolve the cases that are not converging.

Operator	D	Case	Final Residual	Num. Iteration	Time to solution
Proto_Helmholtz_Op	2	0	7.815970e-14	7	0.07463
Proto_Helmholtz_Op	2	1	6.163958e-13	20	0.22929
Proto_Helmholtz_Op	2	2	5.520029e-13	33	0.39347
Proto_Helmholtz_Op	2	3	7.061018e-13	33	0.51900
Proto_Helmholtz_Op	3	0	3.375078e-13	8	0.87163
Proto_Helmholtz_Op	3	1	6.423750e-13	21	2.56059
Proto_Helmholtz_Op	3	2	6.612488e-13	35	4.43480
Proto_Helmholtz_Op	3	3	6.883383e-13	35	13.27707
AMRPoissonOp	2	0	7.749357e-14	7	0.00847
AMRPoissonOp	2	1	9.574563e-13	7	0.00735
AMRPoissonOp	2	2	7.127632e-14	8	0.01246
AMRPoissonOp	2	3	3.499423e-13	8	0.01599
AMRPoissonOp	3	0	3.325118e-13	8	0.03919
AMRPoissonOp	3	1	6.488143e-13	8	0.04693
AMRPoissonOp	3	2	1.347811e-13	9	0.05338
AMRPoissonOp	3	3	6.195044e-13	9	0.24041

Table 1: Final residual and number of iterations in solution of the constant coefficient Helmholtz equation. The data set is dated February 5, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
Proto_Conductivity_Op	2	0	2.081668e-09	6	0.09689
Proto_Conductivity_Op	2	1	1.405955e-08	19	0.34604
Proto_Conductivity_Op	2	2	1.584777e-07	30	0.51393
Proto_Conductivity_Op	2	3	6.366663e-07	30	0.68123
Proto_Conductivity_Op	3	0	4.222235e-09	7	1.09163
Proto_Conductivity_Op	3	1	4.702191e-08	20	3.40754
Proto_Conductivity_Op	3	2	2.160337e-07	33	5.81398
Proto_Conductivity_Op	3	3	8.665997e-07	33	17.47371
VCAMRPoissonOp2	2	0	3.941292e-11	13	0.01050
VCAMRPoissonOp2	2	1	4.880329e-11	13	0.01244
VCAMRPoissonOp2	2	2	4.877754e-11	13	0.01793
VCAMRPoissonOp2	2	3	6.872614e-11	18	0.02939
VCAMRPoissonOp2	3	0	6.221268e-11	13	0.07810
VCAMRPoissonOp2	3	1	6.221268e-11	13	0.11968
VCAMRPoissonOp2	3	2	6.221268e-11	13	0.12976
VCAMRPoissonOp2	3	3	4.454703e-11	20	1.27999

Table 2: Final residual and number of iterations in solution of the variable coefficient Helmholtz equation. The data set is dated February 5, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
`Proto_Viscous_Tensor_Op`	2	0	1.039169e-13	12	0.61612
`Proto_Viscous_Tensor_Op`	2	1	5.695444e-13	23	1.22842
`Proto_Viscous_Tensor_Op`	2	2	5.443423e-13	32	1.78032
`Proto_Viscous_Tensor_Op`	2	3	8.972822e-13	32	2.28227
`Proto_Viscous_Tensor_Op`	3	0	3.987921e-13	13	10.45855
`Proto_Viscous_Tensor_Op`	3	1	4.504175e-13	25	21.21297
`Proto_Viscous_Tensor_Op`	3	2	4.360956e-13	33	28.45970
`Proto_Viscous_Tensor_Op`	3	3	5.653440e-03	10	27.78179
`ViscousTensorOp`	2	0	1.759459e-11	11	0.11242
`ViscousTensorOp`	2	1	9.671908e-11	22	0.11848
`ViscousTensorOp`	2	2	9.324896e-11	20	0.12169
`ViscousTensorOp`	2	3	4.322143e-11	21	0.22275
`ViscousTensorOp`	3	0	6.480527e-11	63	8.08230
`ViscousTensorOp`	3	1	7.077317e-11	70	8.75837
`ViscousTensorOp`	3	2	9.199486e-11	62	7.71172
`ViscousTensorOp`	3	3	9.661738e-11	68	67.7667

Table 3: Final residual and number of iterations in solution of the viscous tensor equation. The data set is dated February 5, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
`Proto_Resistivity_Op`	2	0	1.514344e-13	7	0.44804
`Proto_Resistivity_Op`	2	1	4.618528e-13	24	1.64127
`Proto_Resistivity_Op`	2	2	4.672929e-13	35	2.51303
`Proto_Resistivity_Op`	2	3	6.417089e-13	35	3.28381
`Proto_Resistivity_Op`	3	0	3.852474e-14	9	7.14071
`Proto_Resistivity_Op`	3	1	6.714629e-13	27	22.9827
`Proto_Resistivity_Op`	3	2	5.753176e-13	45	39.2442
`Proto_Resistivity_Op`	3	3	6.127321e-13	45	126.269
`ResistivityOp`	2	0	1.075184e-11	12	0.07357
`ResistivityOp`	2	1	5.151905e-01	100	0.86896
`ResistivityOp`	2	2	7.756453e-01	100	0.89232
`ResistivityOp`	2	3	1.046114e+00	100	1.19475
`ResistivityOp`	3	0	7.031487e-12	10	1.15735
`ResistivityOp`	3	1	5.094567e-01	100	13.5964
`ResistivityOp`	3	2	6.155470e-01	100	13.3735
`ResistivityOp`	3	3	6.747065e-01	100	94.4081

Table 4: Final residual and number of iterations in solution of the magnetic resistivity equation. The data set is dated February 5, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Time to solution
Proto_Helmholtz_Op	2	0	7.815970e-14	7	0.07802
Proto_Helmholtz_Op	2	1	6.163958e-13	20	0.22959
Proto_Helmholtz_Op	2	2	5.520029e-13	33	0.39283
Proto_Helmholtz_Op	2	3	7.061018e-13	33	0.51628
Proto_Helmholtz_Op	3	0	3.375078e-13	8	0.87581
Proto_Helmholtz_Op	3	1	6.423750e-13	21	2.56837
Proto_Helmholtz_Op	3	2	6.612488e-13	35	4.43307
Proto_Helmholtz_Op	3	3	6.883383e-13	35	13.2446
AMRPoissonOp	2	0	7.749357e-14	7	0.00866
AMRPoissonOp	2	1	8.455459e-13	12	0.01329
AMRPoissonOp	2	2	1.201261e-13	13	0.01791
AMRPoissonOp	2	3	3.961276e-13	13	0.02261
AMRPoissonOp	3	0	3.325118e-13	8	0.05562
AMRPoissonOp	3	1	7.107648e-13	13	0.09404
AMRPoissonOp	3	2	1.330047e-13	14	0.11897
AMRPoissonOp	3	3	6.328271e-13	14	0.64701

Table 5: Final residual and number of iterations in solution of the constant coefficient Helmholtz equation. The data set is dated February 7, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
Proto_Conductivity_Op	2	0	2.081668e-09	6	0.09638
Proto_Conductivity_Op	2	1	1.405955e-08	19	0.31747
Proto_Conductivity_Op	2	2	1.584777e-07	30	0.52062
Proto_Conductivity_Op	2	3	6.366663e-07	30	0.67664
Proto_Conductivity_Op	3	0	4.222235e-09	7	1.08044
Proto_Conductivity_Op	3	1	4.702191e-08	20	3.40413
Proto_Conductivity_Op	3	2	2.160337e-07	33	5.83492
Proto_Conductivity_Op	3	3	8.665997e-07	33	17.5112
VCAMRPoissonOp2	2	0	3.941292e-11	13	0.00963
VCAMRPoissonOp2	2	1	4.880329e-11	13	0.01524
VCAMRPoissonOp2	2	2	4.877754e-11	13	0.01581
VCAMRPoissonOp2	2	3	6.872614e-11	18	0.03154
VCAMRPoissonOp2	3	0	6.221268e-11	13	0.07995
VCAMRPoissonOp2	3	1	6.221268e-11	13	0.11737
VCAMRPoissonOp2	3	2	6.221268e-11	13	0.12495
VCAMRPoissonOp2	3	3	4.454703e-11	20	1.29137

Table 6: Final residual and number of iterations in solution of the variable coefficient Helmholtz equation. The data set is dated February 7, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
Proto_Viscous_Tensor_Op	2	0	1.039169e-13	12	0.61725
Proto_Viscous_Tensor_Op	2	1	5.695444e-13	23	1.23255
Proto_Viscous_Tensor_Op	2	2	5.443423e-13	32	1.77953
Proto_Viscous_Tensor_Op	2	3	8.972822e-13	32	2.29478
Proto_Viscous_Tensor_Op	3	0	3.987921e-13	13	10.51760
Proto_Viscous_Tensor_Op	3	1	4.504175e-13	25	21.16876
Proto_Viscous_Tensor_Op	3	2	4.360956e-13	33	28.51970
Proto_Viscous_Tensor_Op	3	3	5.653440e-03	10	27.69634
ViscousTensorOp	2	0	1.759459e-11	11	0.11060
ViscousTensorOp	2	1	9.671908e-11	22	0.11815
ViscousTensorOp	2	2	9.324896e-11	20	0.12216
ViscousTensorOp	2	3	4.322143e-11	21	0.21566
ViscousTensorOp	3	0	6.480527e-11	63	8.13374
ViscousTensorOp	3	1	7.077317e-11	70	8.70458
ViscousTensorOp	3	2	9.199486e-11	62	7.89806
ViscousTensorOp	3	3	9.661738e-11	68	66.9880

Table 7: Final residual and number of iterations in solution of the viscous tensor equation. The data set is dated February 7, 2024.

Operator	D	Case	Final Residual	Num. Iteration	Solution Time
Proto_Resistivity_Op	2	0	1.514344e-13	7	0.45358
Proto_Resistivity_Op	2	1	4.618528e-13	24	1.65240
Proto_Resistivity_Op	2	2	4.672929e-13	35	2.52877
Proto_Resistivity_Op	2	3	6.417089e-13	35	3.30563
Proto_Resistivity_Op	3	0	3.852474e-14	9	7.08352
Proto_Resistivity_Op	3	1	6.714629e-13	27	22.9359
Proto_Resistivity_Op	3	2	5.753176e-13	45	39.1402
Proto_Resistivity_Op	3	3	6.127321e-13	45	125.603
ResistivityOp	2	0	1.075184e-11	12	0.07385
ResistivityOp	2	1	5.151905e-01	100	0.86797
ResistivityOp	2	2	7.756453e-01	100	0.89139
ResistivityOp	2	3	1.046114e+00	100	1.18931
ResistivityOp	3	0	7.031487e-12	10	1.12118
ResistivityOp	3	1	5.094567e-01	100	13.0433
ResistivityOp	3	2	6.155470e-01	100	12.6258
ResistivityOp	3	3	6.747065e-01	100	90.5228

Table 8: Final residual and number of iterations in solution of the magnetic resistivity equation. The data set is dated February 7, 2024.