MATH 5344 - PROGRAMMING PROBLEM 2

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1. System Information

System: Nick Moore's Desktop "NickArch"			
Software			
OS	**Python version**	**Numpy version**	**SciPy version**
Arch Linux (Kernel 5.8.14)	3.8.6	1.19.4	1.5.4
Processor Information			
Processor		**Number of Cores**	**Speed**
AMD Ryzen 7 3800X		8 (16 Threads)	3.9GHz Base, Boost to 4.5GHz
Memory Information			
Main RAM		**L2**	**L3**
32 GB @ 3000MHz DDR4		512KB per core	32MB

2. Results from DH GMRES

Matrix: Debye-Huckel #9
Size: 289×289
Solver: GMRES
Preconditioning: ILU right, `fill_factor=15`

Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	68	9.23e-07	2.81e-05	5.91e-4	4.69e-2	4.75e-2	3.62e-16	1.38e-14	8.32e-4
0.1	19	9.61e-07	2.13e-05	6.44e-4	1.29e-2	1.35e-2	3.62e-16	1.38e-14	8.32e-4
0.01	6	1.80e-07	7.59e-06	8.27e-4	3.46e-3	4.28e-3	3.62e-16	1.38e-14	8.32e-4
0.001	2	1.49e-07	2.66e-06	8.17e-4	1.05e-3	1.86e-3	3.62e-16	1.38e-14	8.32e-4
0.0001	1	2.70e-07	1.68e-05	8.08e-4	9.42e-4	1.75e-3	3.62e-16	1.38e-14	8.32e-4

Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	81	6.64e-09	6.60e-08	5.71e-4	0.052	0.0526	3.62e-16	1.38e-14	8.32e-4
0.1	23	1.98e-09	8.21e-08	7.43e-4	4.83e-3	5.57e-3	3.62e-16	1.38e-14	8.32e-4
0.01	8	2.73e-09	1.00e-07	8.12e-4	1.78e-3	2.59e-3	3.62e-16	1.38e-14	8.32e-4
0.001	3	2.42e-10	1.75e-09	8.13e-4	1.15e-3	1.96e-3	3.62e-16	1.38e-14	8.32e-4
0.0001	2	8.05e-11	1.55e-09	8.23e-4	1.04e-3	1.86e-3	3.62e-16	1.38e-14	8.32e-4

Matrix: Debye-Huckel #10									
Size: 545×545									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	87	9.11e-07	1.37e-05	9.96e-4	0.0622	0.0632	3.46e-16	2.95e-14	1.45e-3
0.1	24	7.18e-07	3.12e-05	1.36e-3	0.0377	0.0391	3.46e-16	2.95e-14	1.45e-3
0.01	8	9.22e-07	4.22e-05	1.66e-3	2.59e-3	4.26e-3	3.46e-16	2.95e-14	1.45e-3
0.001	3	8.10e-09	2.13e-07	1.65e-3	1.63e-3	3.28e-3	3.46e-16	2.95e-14	1.45e-3
0.0001	1	3.13e-07	1.41e-05	1.62e-3	0.0013	2.92e-3	3.46e-16	2.95e-14	1.45e-3
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	111	7.78e-09	2.06e-07	1.05e-3	0.0766	0.0776	3.46e-16	2.95e-14	1.45e-3
0.1	29	9.15e-09	7.93e-07	1.34e-3	0.0375	0.0388	3.46e-16	2.95e-14	1.45e-3
0.01	11	1.80e-09	1.44e-07	1.63e-3	3.27e-3	0.0049	3.46e-16	2.95e-14	1.45e-3
0.001	3	8.10e-09	2.13e-07	1.63e-3	1.62e-3	3.25e-3	3.46e-16	2.95e-14	1.45e-3
0.0001	2	4.60e-11	2.59e-09	1.61e-3	1.46e-3	3.07e-3	3.46e-16	2.95e-14	1.45e-3

Matrix: Debye-Huckel #11									
Size: 1089×1089									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	115	8.72e-07	4.40e-05	1.82e-3	0.0849	0.0867	3.64e-16	8.78e-15	3.14e-3
0.1	33	8.38e-07	1.00e-04	2.85e-3	0.0418	0.0446	3.64e-16	8.78e-15	3.14e-3
0.01	11	6.29e-07	2.97e-05	3.53e-3	0.0295	0.0331	3.64e-16	8.78e-15	3.14e-3
0.001	3	4.29e-07	5.04e-05	2.87e-3	1.67e-3	4.54e-3	3.64e-16	8.78e-15	3.14e-3
0.0001	1	2.09e-07	2.73e-06	2.81e-3	1.37e-3	4.18e-3	3.64e-16	8.78e-15	3.14e-3
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	157	9.78e-09	5.68e-07	1.40e-3	0.106	0.107	3.64e-16	8.78e-15	3.14e-3
0.1	44	7.30e-09	2.34e-07	2.42e-3	0.0313	0.0337	3.64e-16	8.78e-15	3.14e-3
0.01	15	3.37e-09	2.94e-07	3.02e-3	0.0272	0.0302	3.64e-16	8.78e-15	3.14e-3
0.001	4	9.81e-09	2.41e-07	3.33e-3	0.0111	0.0145	3.64e-16	8.78e-15	3.14e-3
0.0001	2	9.70e-11	6.81e-09	3.10e-3	1.53e-3	4.62e-3	3.64e-16	8.78e-15	3.14e-3

Matrix: Debye-Huckel #12									
Size: 2113×2113									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	154	9.47e-07	4.56e-05	2.73e-3	0.161	0.164	3.89e-16	2.31e-14	5.61e-3
0.1	42	7.55e-07	1.66e-04	5.41e-3	0.0872	0.0926	3.89e-16	2.31e-14	5.61e-3
0.01	15	2.70e-07	4.30e-05	8.27e-3	0.0205	0.0287	3.89e-16	2.31e-14	5.61e-3
0.001	5	3.12e-08	6.61e-06	6.43e-3	8.55e-3	0.015	3.89e-16	2.31e-14	5.61e-3
0.0001	2	1.81e-08	5.85e-06	6.77e-3	2.82e-3	9.59e-3	3.89e-16	2.31e-14	5.61e-3
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	212	9.64e-09	2.51e-06	2.62e-3	0.267	0.27	3.89e-16	2.31e-14	5.61e-3
0.1	58	6.68e-09	1.39e-06	5.25e-3	0.0673	0.0726	3.89e-16	2.31e-14	5.61e-3
0.01	20	6.63e-09	7.06e-07	8.01e-3	0.0322	0.0402	3.89e-16	2.31e-14	5.61e-3
0.001	6	3.91e-09	7.88e-07	8.99e-3	0.0248	0.0338	3.89e-16	2.31e-14	5.61e-3
0.0001	3	5.77e-11	9.54e-09	9.06e-3	3.19e-3	0.0123	3.89e-16	2.31e-14	5.61e-3

Matrix: Debye-Huckel #13									
Size: 4225×4225									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	208	9.50e-07	1.33e-04	4.79e-3	0.668	0.673	4.24e-16	1.01e-13	0.0118
0.1	58	8.95e-07	1.81e-04	0.0114	0.0883	0.0997	4.24e-16	1.01e-13	0.0118
0.01	20	4.84e-07	1.05e-04	0.0171	0.037	0.0541	4.24e-16	1.01e-13	0.0118
0.001	6	4.16e-07	1.57e-04	0.0203	0.0323	0.0526	4.24e-16	1.01e-13	0.0118
0.0001	2	4.82e-07	5.29e-05	0.0149	7.37e-3	0.0223	4.24e-16	1.01e-13	0.0118
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	251	9.65e-09	2.46e-06	4.89e-3	0.923	0.928	4.24e-16	1.01e-13	0.0118
0.1	82	9.08e-09	3.85e-06	0.0113	0.142	0.153	4.24e-16	1.01e-13	0.0118
0.01	27	6.36e-09	5.71e-07	0.017	0.037	0.054	4.24e-16	1.01e-13	0.0118
0.001	8	3.82e-09	3.92e-07	0.0201	0.0146	0.0347	4.24e-16	1.01e-13	0.0118
0.0001	3	7.68e-09	1.81e-06	0.0218	8.98e-3	0.0307	4.24e-16	1.01e-13	0.0118

Matrix: Debye-Huckel #14									
Size: 8321×8321									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	284	9.50e-07	5.06e-04	0.0148	2.32	2.33	4.44e-16	1.43e-13	0.0347
0.1	79	7.73e-07	2.21e-04	0.0244	0.26	0.284	4.44e-16	1.43e-13	0.0347
0.01	28	5.29e-07	1.40e-04	0.0379	0.0764	0.114	4.44e-16	1.43e-13	0.0347
0.001	8	7.05e-07	6.44e-05	0.049	0.0235	0.0725	4.44e-16	1.43e-13	0.0347
0.0001	3	1.35e-07	4.36e-05	0.0389	0.0159	0.0549	4.44e-16	1.43e-13	0.0347
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	346	9.62e-09	4.75e-06	9.66e-3	3.39	3.4	4.44e-16	1.43e-13	0.0347
0.1	104	9.20e-09	9.38e-06	0.0243	0.393	0.417	4.44e-16	1.43e-13	0.0347
0.01	35	5.90e-09	1.37e-06	0.0382	0.0914	0.13	4.44e-16	1.43e-13	0.0347
0.001	11	9.15e-09	2.85e-06	0.0493	0.0271	0.0764	4.44e-16	1.43e-13	0.0347
0.0001	4	1.59e-09	7.29e-07	0.0387	0.0266	0.0653	4.44e-16	1.43e-13	0.0347

Matrix: Debye-Huckel #15									
Size: 16641×16641									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	335	9.93e-07	2.57e-03	0.0288	6.19	6.22	4.77e-16	9.31e-14	0.105
0.1	93	9.88e-07	1.67e-03	0.0485	0.586	0.635	4.77e-16	9.31e-14	0.105
0.01	35	9.08e-07	1.10e-03	0.0803	0.153	0.234	4.77e-16	9.31e-14	0.105
0.001	10	9.15e-07	5.14e-04	0.0945	0.0528	0.147	4.77e-16	9.31e-14	0.105
0.0001	4	1.27e-07	2.38e-04	0.0925	0.0622	0.155	4.77e-16	9.31e-14	0.105
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	477	9.64e-09	2.80e-06	0.0188	12.4	12.4	4.77e-16	9.31e-14	0.105
0.1	135	9.76e-09	2.83e-06	0.0472	1.19	1.23	4.77e-16	9.31e-14	0.105
0.01	46	9.01e-09	1.25e-05	0.0751	0.234	0.309	4.77e-16	9.31e-14	0.105
0.001	15	3.39e-09	1.76e-06	0.0921	0.0923	0.184	4.77e-16	9.31e-14	0.105
0.0001	5	8.83e-09	1.03e-05	0.0952	0.0412	0.136	4.77e-16	9.31e-14	0.105

Matrix: Debye-Huckel #16									
Size: 65137×65137									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	468	9.97e-07	2.20e-02	0.102	45.1	45.2	5.40e-16	6.52e-13	0.806
0.1	143	9.92e-07	1.58e-02	0.162	5.02	5.18	5.40e-16	6.52e-13	0.806
0.01	58	9.93e-07	1.07e-02	0.291	1.2	1.49	5.40e-16	6.52e-13	0.806
0.001	20	8.34e-07	1.76e-03	0.395	0.417	0.812	5.40e-16	6.52e-13	0.806
0.0001	7	3.36e-07	3.71e-04	0.523	0.204	0.727	5.40e-16	6.52e-13	0.806
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	760	9.66e-09	1.43e-05	0.0886	118	118	5.40e-16	6.52e-13	0.806
0.1	232	9.81e-09	2.24e-05	0.163	12.2	12.3	5.40e-16	6.52e-13	0.806
0.01	89	9.73e-09	3.51e-05	0.293	2.4	2.69	5.40e-16	6.52e-13	0.806
0.001	26	4.03e-09	1.31e-06	0.399	0.506	0.905	5.40e-16	6.52e-13	0.806
0.0001	9	3.59e-09	2.97e-06	0.526	0.245	0.771	5.40e-16	6.52e-13	0.806

Matrix: Debye-Huckel #17									
Size: 95538×95538									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	521	9.98e-07	5.50e-02	0.173	90.1	90.3	5.23e-16	5.62e-13	1.41
0.1	156	9.90e-07	3.85e-02	0.283	9.45	9.73	5.23e-16	5.62e-13	1.41
0.01	61	9.39e-07	2.23e-02	0.49	2.1	2.59	5.23e-16	5.62e-13	1.41
0.001	21	8.82e-07	3.62e-03	0.639	0.706	1.35	5.23e-16	5.62e-13	1.41
0.0001	7	4.36e-07	3.53e-04	0.845	0.306	1.15	5.23e-16	5.62e-13	1.41
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
1	983	9.94e-09	3.78e-05	0.162	318	318	5.23e-16	5.62e-13	1.41
0.1	295	9.98e-09	3.83e-05	0.275	30.8	31.1	5.23e-16	5.62e-13	1.41
0.01	101	9.97e-09	2.37e-05	0.485	4.61	5.1	5.23e-16	5.62e-13	1.41
0.001	31	4.21e-09	4.78e-06	0.634	1	1.63	5.23e-16	5.62e-13	1.41
0.0001	11	7.12e-09	1.46e-05	0.838	0.413	1.25	5.23e-16	5.62e-13	1.41

Matrix: Debye-Huckel #18									
Size: 197830×197830									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	74	9.72e-07	8.85e-02	1.2	7.06	8.26	6.15e-16	2.09e-12	5.26
0.001	29	8.54e-07	1.54e-02	1.66	2.19	3.86	6.15e-16	2.09e-12	5.26
0.0001	83	9.49e-07	2.31e-03	2.21	10.7	12.9	6.15e-16	2.09e-12	5.26
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	154	8.97e-09	8.58e-05	1.2	25.2	26.5	6.15e-16	2.09e-12	5.26
0.001	47	7.07e-09	1.00e-05	1.66	4.01	5.67	6.15e-16	2.09e-12	5.26
0.0001	133	8.91e-09	1.26e-05	2.17	22.4	24.6	6.15e-16	2.09e-12	5.26

Matrix: Debye-Huckel #19									
Size: 436218×436218									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	79	9.80e-07	4.41e-01	2.79	20.9	23.7	5.63e-16	5.46e-12	13.4
0.001	33	9.98e-07	8.42e-02	4.24	6	10.2	5.63e-16	5.46e-12	13.4
0.0001	115	9.35e-07	1.06e-02	5.95	45.9	51.8	5.63e-16	5.46e-12	13.4
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	171	9.80e-09	4.12e-04	2.85	85	87.8	5.63e-16	5.46e-12	13.4
0.001	63	7.72e-09	7.10e-05	4.24	15.7	20	5.63e-16	5.46e-12	13.4
0.0001	172	9.60e-09	4.73e-05	5.9	93.3	99.2	5.63e-16	5.46e-12	13.4

Matrix: Debye-Huckel #20									
Size: 769494×769494									
Solver: GMRES									
Preconditioning: ILU right, `fill_factor=15`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	25	9.84e-07	8.62e-01	6.26	6.33	12.6	6.46e-16	2.11e-11	43.6
0.001	36	9.33e-07	2.30e-01	10.8	12.1	23	6.46e-16	2.11e-11	43.6
0.0001	264	9.73e-07	1.21e-01	13.5	353	367	6.46e-16	2.11e-11	43.6
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	GMRES	total	$\|r\|$	$\|e\|$	time
0.01	199	9.79e-09	2.50e-04	6.11	195	201	6.46e-16	2.11e-11	43.6
0.001	83	9.29e-09	2.19e-04	10.5	43.2	53.7	6.46e-16	2.11e-11	43.6
0.0001	406	9.69e-09	3.77e-05	13.6	801	814	6.46e-16	2.11e-11	43.6

3. Analysis

Question 1: You're running a sparse direct solver in addition to GMRES. For very small systems, the sparse direct solver will be much faster than an iterative solver. At what system size do you see "break even", where the iterative solver is as fast or faster than the sparse direct solver? How does this depend on the preconditioner's drop tolerance? How does the accuracy compare between the iterative and direct solvers?

Answer: The "break even" size appears to be around 65137×65137. It does depend on the drop tolerance. At the sizes between 65317×65137 and 95538×95538, lower drop tolerance improves the speed. At sizes above, 95538×95538, there appears to be a trade-off between the amount of fill and the convergence of GMRES. For these larger sizes, a drop tolerance of 0.001 gives the quickest convergence. It should also be noted that at a stopping tolerance of 10e-8, the Direct Solve is still faster for problems larger than 197830×197830.

In all cases, the direct solve gives a more accurate results, both in term of residuals and errors.

Question 2: What can you say (quantitatively) about conditioning and roundoff in the sparse calculations?

Answer: Even in larger sizes, the direct solver is still able to achieve a residual of around machine epsilon. At high fill drop tolerance, the preconditioner performance is much lower since it still requires a large number of iterations, so there is likely some roundoff error in the calculations. In the cases of lower drop tolerance however, the number of iterations is low and achieves the desired tolerance without any apparent issue.

In larger matrix sizes we see a very high number of iterations required to solve the system for low drop tolerances. This could be due either to eliminating too many values in the preconditioner, or a roundoff issue. This causes GMRES to take many more iterations and causes a high running time.