Improving the Speed and Scalability of the Data Assimilation Research Testbed

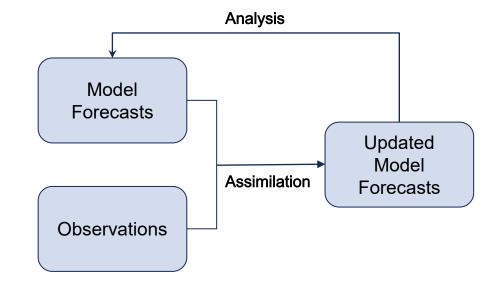
NCAR UCAR Jiachen (Ed) Liu Drexel University Mentors: Helen Kershaw, Jeffrey Anderson



Data assimilation is a process to combine model outputs and observations to improve model forecasts

Example: a temperature forecast

- Model forecast: a three dimensional atmospheric model which computes the temperature
- Observations: observed temperature with a thermometer at a given time
- Assimilation: Generate the statistically optimal value based on the forecast and the observation

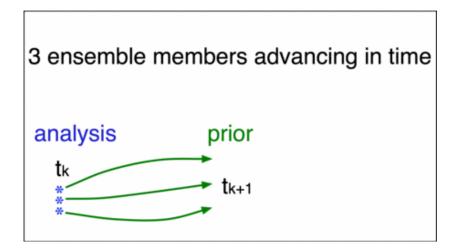




The Data Assimilation Research Testbed (DART) helps researchers perform ensemble data assimilation

Ensemble data assimilation process can capture the uncertainties inherent to model forecasts and observations.

DART provides a platform for flexible and powerful ways to perform ensemble data assimilation with different models.



Ensemble DA with DART



Improving speed and scalability of DART is important for the future

- Although there are modules to utilize parallel computing resources to run DART, it is still computationally expensive.
- The focus of this work is to:
 - 1. Identify the computational barriers in DART with code profiling tools
 - 2. Improve the speed and scalability of DART through algorithmic changes



The speed and scalability of DART with various models are important for the future

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The identification of computational barriers in DART is essential for the future

• Example code profiling result with arm -forge MAP tool of DART

•	•	•	C	
🗉 filter				FORGE
		16 !		
		17		
		18 call initia	lize mpi utilities('Filter')	
		19	,	
98.0%		20 call filter	main()	
50.00		21		
1.9%			<pre>ze mpi utilities()</pre>	
1.90		23	ze_mpi_utilities()	
			611hau	
		24 end program	lliter	
		25		
		26		
			Input/Output Project Files Main Thread Stacks Functions	
×e			Main Thread Stacks Functions	
Total core time	~ MPI	Function(s) on line	Source	
		🔻 🔹 filter [program]		
		▼ / filter	program filter	
		▼ filter_mod::filter_main	call filter_main()	
		▼ assim_tools_mod::filter_assim	call filter_assim(state_ens_handle, obs_fwd_op_ens_handle, seq, keys, &	
65.9%	0.3%	get_close_state_cached [inlined]	call get_close_state_cached(gc_state, base_obs_loc, base_obs_type, &	
17.8%				
3.5%		assim_tools_mod::obs_updates_e	ns call obs_updates_ens(ens_size, num_groups, ens_handle%copies(1:ens_size, state_index), &	
2.5%	0.4%	▶ 56 others		
3.3%	2.9%	▶ forward_operator_mod::get_obs_en		
1.3%	1.3%	▶ filter_mod::obs_space_diagnostics	call obs_space_diagnostics(obs_fwd_op_ens_handle, qc_ens_handle, ens_size, &	
1.0% 2.6%	1.0% 1.5%	state_vector_io_mod::read_state 20 others	call read_state(state_ens_handle, file_info_input, read_time_from_file, time1, &	
1.9%	1.5%	P 20 otners mpi_utilities_mod::finalize_mpi_utilitie	call finalize mpi utilities()	
<0.1%	<0.1%	IT others	s call linalize mpi_utilities()	
<0.178	<0.1%			



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Initial profiling results of DART show that it generally scale well with increased computational resources

• Finite Volume Community Atmosphere Model (CAM-FV) test case

# of nodes	# of processors	Runtime from MAP [s]	filter_mod, compute (%)	filter_mod, mpi (%)	mpi_utilities (%)
2	36	2401.83	70	26.2	3.8
4	36	1071.377	44.5	47.1	8.4
8	36	658.034	24.5	61.8	13.6
10	36	339.992	39.2	34.1	26.6
20	36	285.397	25.8	41.5	32.7
10	4	1184.76	85.2	7.3	7.5
10	16	446.941	60.5	19.4	20



Initial profiling results of DART show that it generally scale well with increased computational resources

- In general, increased number of nodes and/or number of processors per node decrease the total runtime.
- However, as the number of nodes is relatively high, the effect of increasing number of nodes on total runtime reduction decreases.

# of nodes	# of processors	Runtime from MAP [s]	filter_mod, compute (%)	filter_mod, mpi (%)	mpi_utilities (%)
2	36	2401.83	70	26.2	3.8
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Additional profiling results revealed redundant caching in DART consumes significant computational resources

Atmospheric component of the Model for Prediction Across Scales (MPAS - ATM)

25.9%2653 ~	call get_close_state(gc_state,			Scalar floating-point	0.0%
2654	<pre>my_state_loc, my_state_kind, my_state_indx, & num close states, close state ind, close state</pre>				
2655 2656	num_close_st	ates, close_state_ind, clo	ose_state	Vector floating point	0.0%
2657	last base states loc = bas	e obs loc		Scalar integer	1.5%
2658		close states		Vector integer	0.0%
9.1% 2659	last close state ind(:) = clos	e state ind(:)		vector integer	0.0%
29.6% 2660	<pre>last_close_state_dist(:) = clos</pre>	e_state_dist(:)		Memory access*	98.5%
<0.1% 2661	<pre>num_close_states_calls_made = n</pre>	um_close_states_calls_made	e +1	Branch	1.4% I
2662	endif				
2663 2664	endif			Other instructions	0.0%
2664 2665	end subroutine get close state cached			• 07 40/	
2666	end Subroutine get_crose_state_cached			 97.1% memory access instructions, 1.4% implicit memory accesses in other instructions, also counted in their 	
				accesses in other instruction	
	Input/Output Project Fi	les Main Thread Stacks Fu	unctions		
×ð		Main Thread Stacks			
Total core time	Function(s) on line	Source			Position
	🗸 🌠 filter [program]				
	∨ 🖌 filter	program filter			filter.f90:9
	✓ filter_mod::filter_main	call filter_main()			filter.f90:20
	v assim_tools_mod::filter_assim	call filter_assim(state	e_ens_hand	le, obs_fwd_op_ens_h	filter _mod. f90:918
	✓ get_close_state_cached [inlined]	call get_close_state_ca	ached(gc_s	tate, base_obs_loc,	assim_tools_mod.f90:698
29.6%		last_close_state_dist(:) = close		assim_tools_mod.f90:2660
25.9%	> model_mod::get_close_state call get_close_state(gc_state, base_obs_loc, base_obs_loc		 ase obs loc, base ob	assim_tools_mod.f90:2653	
9.1%		last close state ind(:)			assim_tools_mod.f90:2659
<0.1%	> 2 others				
17.8%		call broadcast recy(mar	p pe to ta	sk(ens handle, owner	assim tools mod f90:634
3.5%	<pre>> mpi_utilities_mod::broadcast_recv call broadcast_recv (map_pe_to_task(ens_handle, owner > assim_tools_mod::obs_updates_ens call obs_updates_ens(ens_size, num_groups, ens_handl</pre>				



Additional profiling results revealed redundant caching in DART consumes significant computational resources

9.1%	2659	last_close_state_ind(:) = close_state_ind(:)
29.6%	2660	<pre>last_close_state_dist(:) = close_state_dist(:)</pre>
10 10	0.0.04	

- The purpose of this subroutine is to cache the location and indices of the previous observation so that we can reduce computation time.
- However, these two lines of copying actually consume almost <u>40% of the</u> <u>total runtime of DART</u> for this case!
- It turns out that we don't need these two lines of code to perform the caching. These are redundant copying of very large arrays.



Additional profiling results revealed redundant caching in DART consumes significant computational resources

9.1%	2659	last_close_state_ind(:) = close_state_ind(:)
29.6%	2660	<pre>last_close_state_dist(:) = close_state_dist(:)</pre>
10 10	0000	

- Initial testing with this test case shows that without calling the subroutines, the computation time <u>reduced from 260 seconds to 64 seconds</u>.
- The problem is now resolved with a pull request at https://github.com/NCAR/DART/pull/368



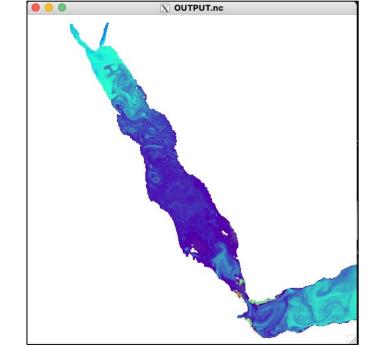
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A high -resolution assimilation run of MIT General Circulation Model for the red sea is a computational problem for DART

- The MIT General Circulation Model for the ocean (MITgcm-ocean) is a numerical model that can compute parameters related to the ocean.
- This specific run is on a 2000x2000x50 (latitude, longitude, depth) grid.
- DART cannot be run on Cheyenne or on the extreme memory nodes (4 TB) at Pittsburgh Supercomputing Center for this specific case.

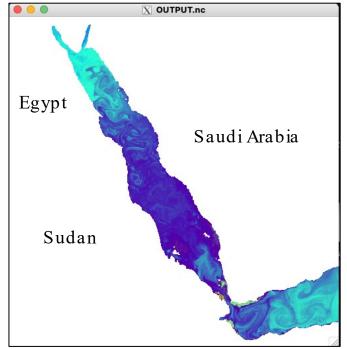


Sample output from MITgcm -ocean for the red sea



A high -resolution assimilation run of MIT General Circulation Model for the red sea is a computational problem for DART

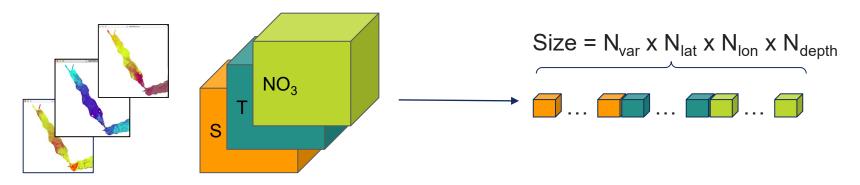
- Memory overflow is likely the problem.
- The grid has land which is not used in the data assimilation process.
- In the state file, these values are usually *fill values*.
- Analysis shows **92%** of the grid are fill values.



Sample output from MITgcm-ocean for the red sea



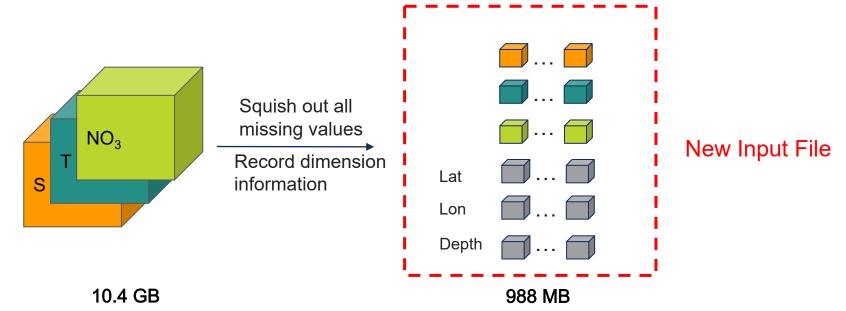
DART handles the state information by generating a 1 -D DART vector



- The state might have several variables (salinity, temperature, nitrate concentration, etc.)
- DART reduces everything into a 1-D DART vector and performs data assimilation.
- The missing values (land cells in an ocean model) stay in the vector.



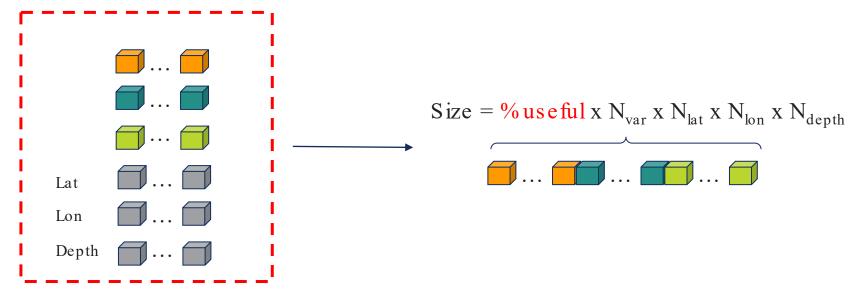
The squished state approach can significantly reduce the size of the state vector



- The new input file does not have missing values at all.
- Additional dimension information is required because we squished the grid.



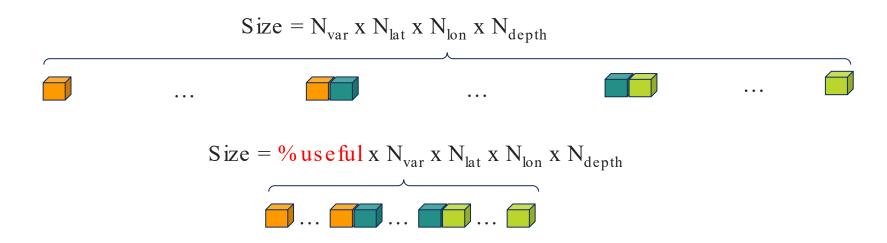
The squished state approach can significantly reduce the size of the state vector



• If %useful is small, the size of the state vector can be reduced significantly, so the assimilation might be able to run



The squished state approach can significantly reduce the size of the state vector



 The DART model size (number of variables)<u>decreased from ~2.63e9 to</u> ~2.0e8.



The squished state approach improves the speed and scalability of DART*

	Medium Case (500x500x50)	Large Case (2000x2000x50)	
Original	361s	N/A	
Squished State	150s	1500s	

- The computation time for the medium case decreased from 361 seconds to 150 seconds.
- The large case now runs properly.
- The squishing process can be done fairly easily without significant additional computational resources.



Future Work

- Make the squishing process "online" with DART
 - The users only need to specify if they want to use the squished state method.
- Write subroutines which reformulate the squished DART array back into its original form.



Acknowledgements

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