Singletrack Dynamical Core Requirements

The NCAR Singletrack project has the goal of unifying atmospheric simulation models within the organization. This report from the dynamical core subgroup presents the requirements for atmospheric dynamical cores for use in climate, weather and geospace applications. Section 1 is an overview of dynamical core requirements. Section 2 describes metrics and testing needed to determine whether or not, or to what extent, a dynamical core fulfills a given requirement, and section 3 presents the current status of candidate Singletrack dynamical cores relative to these requirements.

1 Dynamical Core Requirements

The following table lists dynamical core requirements, characterizes the need for each requirement within climate, weather, and geospace applications, and characterizes the metrics used to evaluate fulfillment of the requirement by a dynamical core.

Table 1.1: Dynamical Core Requirements

	Requirement	climate	weather	geospace	metrics
(1)	Throughput: cost and scalability	essential	essential	essential	benchmarks
(2)	Efficient tracer transport	essential	essential	essential	benchmarks
(3)	Conservation: mass, scalar mass	essential	essential	essential	by inspection, benchmarks
(4)	Conservation: good energy conservation	essential	desirable	desirable	by inspection, benchmarks
(5)	Conservation: axial angular momentum	highly desirable		essential	by inspection, benchmarks
(6)	Good tracer transport characteristics (tracer correlation, PD and SP options)	essential	essential	essential	by inspection, benchmarks
(7)	Support by developers	essential	essential	essential	agreement to support
(8)	Support simplified setups on the sphere	essential	essential	desirable	agreement to support
(9)	Global mesh refinement	desirable	essential	essential	by inspection

(10)	Cartesian geometry	desirable	essential		by inspection
(11)	Non-Hydrostatics	desirable	essential	highly desirable	by inspection, benchmarks
(12)	Regional capability.		essential		by inspection
(13)	Data assimilation capability. Has to play well with DA.	desirable	essential	essential	by inspection, benchmarks
(14)	Stable over 30 scale heights (~700km)/O(13) in pressure			essential	benchmarks
(15)	Efficient 2 way 3D inline grid coupling	desirable		essential	benchmarks
(16)	Species dependent mean molecular mass and specific heats			essential	by inspection
(17)	Deep atmosphere: variation of gravity, Coriolis force and geometry.			highly desirable	by inspection
(18)	High Top Thermodynamics (prefer solving T rather than theta, which is not well defined above homopause).			essential	by inspection
(19)					
(20)	Strong scaling	essential	desirable	desirable	benchmarks
(21)	platform agnostic	essential	essential	essential	benchmarks
(22)	Single and double-precision integration capability		highly desirable		by inspection, benchmarks
(23)	Dycore characteristics with topography				benchmarks

2 Requirements and Metrics

It is highly desirable that the benchmarks and tests are run in the same (unified) framework rather than in standalone systems (need to coordinate with infrastructure group).

(1) Throughput: Cost and Scalability: Tests need to be devised to measure cost in weather, climate and geospace applications. Ideally these tests would be idealized tests perhaps with scalar (tracer) transport. The test results could be used to infer the cost of

full-physics model applications.

Test (6) with additional tracers as well as high-top configuration (that may have more stringent time-step limitation).

Evaluate throughput and scalability as a function of number of tracers (from O(10) to O(300)) and vertical levels (from O(30) to O(200)).

Assess strong scaling by keeping resolution fixed and scale out to O(10) columns per processor.

(2) Efficient tracer transport: See (1)

(3) Conservation, scalar conservation: Exact conservation (to machine roundoff) of mass and scalar mass is often a property of the dynamical core and can be determined by inspection. In any case, conservation of dry air mass and tracer mass should be evaluated in tests involving moist physics.

See (6).

Conservation in long simulations to assess spurious trends (climate test).

Conservation of dry mass with moist physics.

Assess that water budget is closed.

(4) Conservation - good energy conservation: Energy conservation properties of a dynamical core can be evaluated by inspection (what total energy does the continuous equations of motion conserve), and testing can be done to quantify the magnitude of energy conservation errors for specific applications.

Derive what total energy the continuous equations of motion (on which dycore is based) conserve.

Total energy dissipation of the dynamical core should be assessed with moist physics (for example, aqua-planet).

Discussion with physics group on what discrete energy formula to use in full system.

(5) Conservation - angular momentum: See (4)

Derive what angular momentum the continuous equations of motion (on which dycore is based) conserve in the absence of mountain torques.

Can be tested with Held-Suarez or Aqua-planet forcing.

(6) Good tracer transport characteristics: Many tracer-transport characteristics can be inferred from the design of the schemes (analyses of the scheme), and by idealized transport tests. In any case, these characteristics (shape-preservation, linear and non-linear tracer correlation preservation, filament preservation) should be evaluated in 3D idealized tests.

A. (short time-scale test) Ullrich et al. moist baroclinic wave with a number of passive scalars:

- *terminator chemistry (test linear correlation preservation) - described in DCMIP document*
- *non-linearly correlated inert species (Lauritzen and Thuburn, 2012)*
- *conserving family of species (Lauritzen and Thuburn, 2012)*
- *other inert species initialized with idealized distributions and apply filament diagnostic (Lauritzen et al., 2014)*

B. (longer time-scale test) Age-of-air test with modified Held-Suarez forcing (Gerber, Courant Institute). Add inert tracer to assess long-term trends in mass-conservation

(7) Support by developers: Do the developers of a candidate dynamical core support its porting and use in Singletrack, and do the developers support the Singletrack version to the community following the community release of the Singletrack atmospheric modeling system?

(8) Support simplified setups on the sphere: Are idealized or simplified configurations supported for the dynamical core (e.g. idealized baroclinic waves, gravity wave tests, etc), as part of an evaluation and as part of a community release?

At a minimum the unified framework should support the tests listed in this document.

(9) Global mesh refinement: This can be determined by inspection. Tradeoffs of different approaches may need to be considered and evaluated?

(10) Cartesian geometry: Does the dynamical core support a 3D Cartesian plane configuration? Typically this involves using doubly-periodic lateral boundary conditions. This can be determined by inspection.

(11) Nonhydrostatic: This can be determined by inspection. Testing may be needed to understand the efficacy of the approach.

Reduced radius tests (supercell), gravity wave tests, … (Joe?)

(12) Regional capability: Can the dynamical core be configured to cover only a portion of the sphere, with lateral boundary conditions prescribed from analyses or other (perhaps global) model integrations? This can be determined by inspection.
(13) Data assimilation capability:
(14) Stable over 30 scale heights (~700km)/O(13) in pressure:
(15) Efficient 2 way 3D inline grid coupling:
(16) Species dependent mean molecular mass and specific heats: this can be determined by inspection. Any approximations may need to be evaluated.
(17) Deep atmosphere: variation of gravity, coriolis force and geometry:
(18) High Top Thermodynamics (prefer solving T rather than theta, which is not well defined above homopause): Appropriateness of thermodynamic variables used in the solver.

Modified Held-Suarez test with high top and topography (Hanli)

(19) Scalable on Vector Machines: *To do: determine benchmarks (Rich L)*
(20) Strong scaling: *To do: determine benchmarks (Rich L)*
(21) platform agnostic: *(Rich L)*
(22) The capability of a dynamical core to be integrated in either single- or double-precision. Benchmarks would be used to indicate any issues with solver precision. The advantages of single precision integration is speed, reduced file sizes and better IO performance. The disadvantage may be significantly reduced accuracy in some dynamical core formulations for some applications. See infrastructure team plan.

(23) Topography smoothing and the dynamical core are closely related. It is, in general, desirable to have rougher topography. However, rough topography can trigger grid-scale noise from dynamical core.

Held-Suarez forcing with real-world topography smoothed at different predefined scales.

3 Singletrack candidate dynamical cores

	Requirement	SE	MPAS
(1)	Throughput: cost and scalability		
(2)	Efficient tracer transport		

(3)	Conservation: mass, scalar mass	Yes, by inspection and test results	Yes, by inspection and test results
(4)	Conservation: good energy conservation.	Yes, by inspection and test results	
(5)	Conservation: axial angular momentum	Yes, by inspection and test results	
(6)	Good tracer transport characteristics (tracer correlation, PD, SP options)	Yes (with CSLAM), by inspection and test results	
(7)	Support by developers	Yes, internal	Yes, internal
(8)	Support simplified setups on the sphere	Yes	Yes
(9)	Global mesh refinement	Yes (but not currently supported by CSLAM)	Yes
(10)	Cartesian geometry	Development and testing necessary	Yes
(11)	Non-Hydrostatics	Development and testing necessary	Yes
(12)	Regional capability.	No	In development, prototype being tested
(13)	Data assimilation capability. Has to play well with DA.	Yes, preliminary tests with DART	Yes, with DART and GSI
(14)	Stable over 30 scale heights (~700km)/O(13) in pressure	Development and testing necessary	Development and testing necessary
(15)	Efficient 2 way 3D inline grid coupling	Development and testing necessary	Development and testing necessary
(16)	Species dependent mean molecular mass and specific heats	Infrastructure for 3D variable Cp exists	Development and testing necessary
(17)	Deep atmosphere: variation of gravity, Coriolis force and geometry.	Development and testing necessary	Development and testing necessary
(18)	High Top Thermodynamics (prefer solving T rather than theta, which is not well defined above homopause).	Development and testing necessary	Development and testing necessary
(19)	Scalable on Vector		

	Machines		
(20)	Strong scaling	Yes	
(21)	platform agnostic		
(22)	Single- or double-precision integration capability		Yes