A unified and Python-based approach to the physics-dynamics coupling in atmospheric models

One-year Ph.D. interview

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CSCS

Background

Processes occurring in the atmosphere span a wide range of scales.

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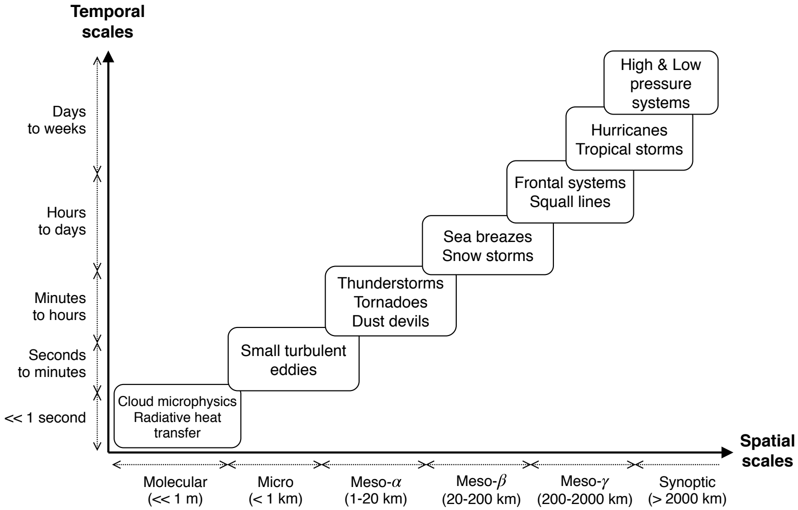

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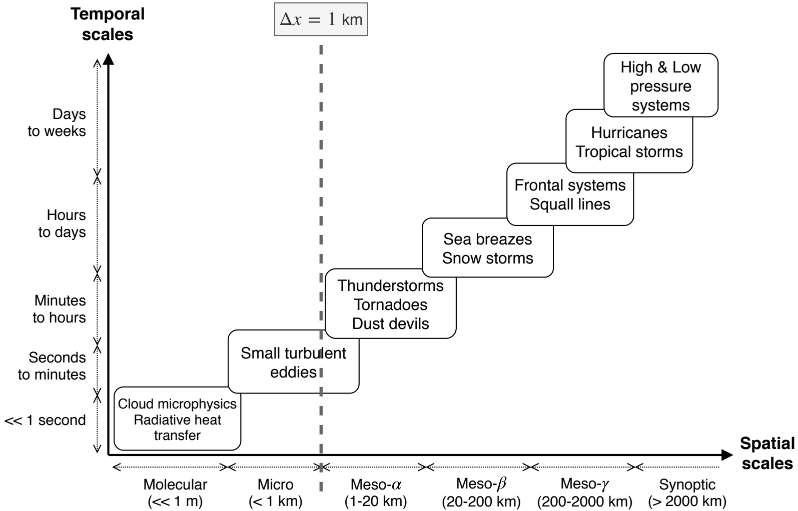

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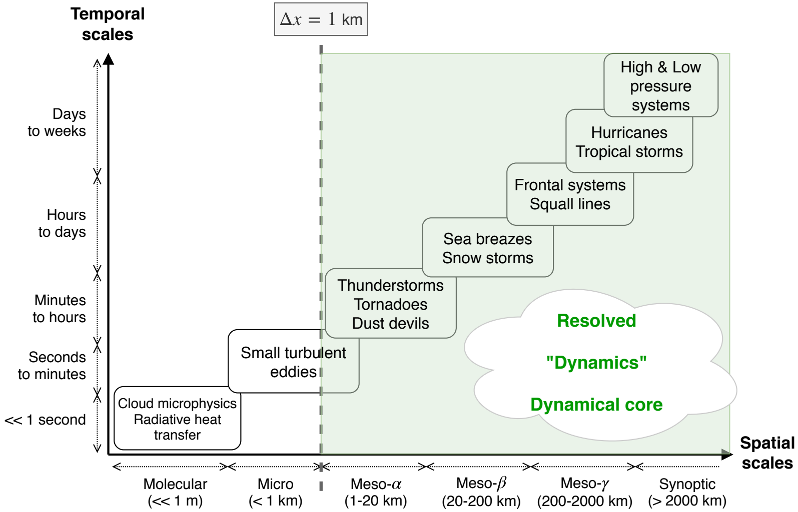

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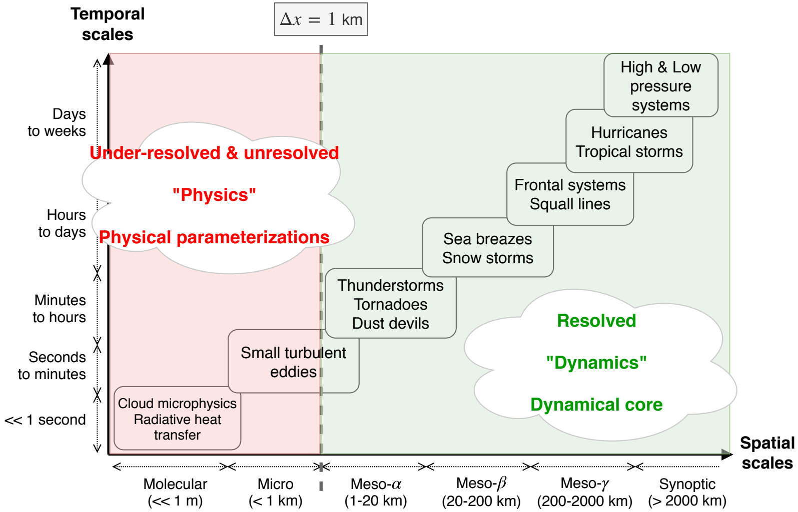

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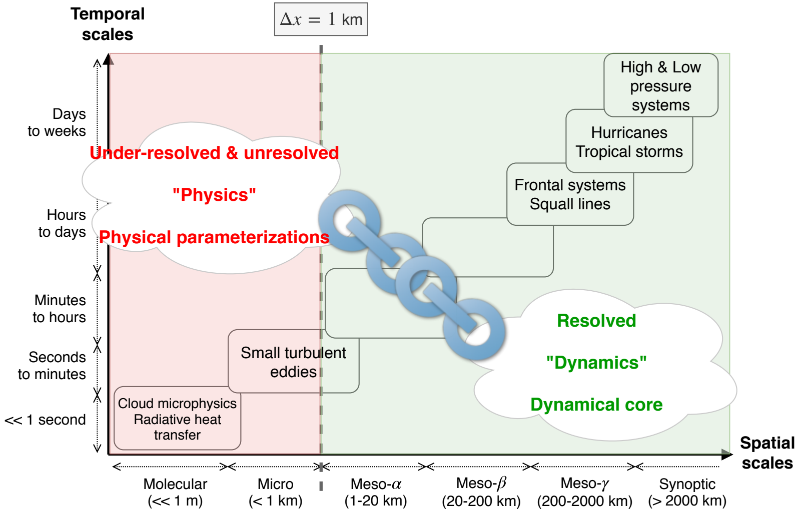

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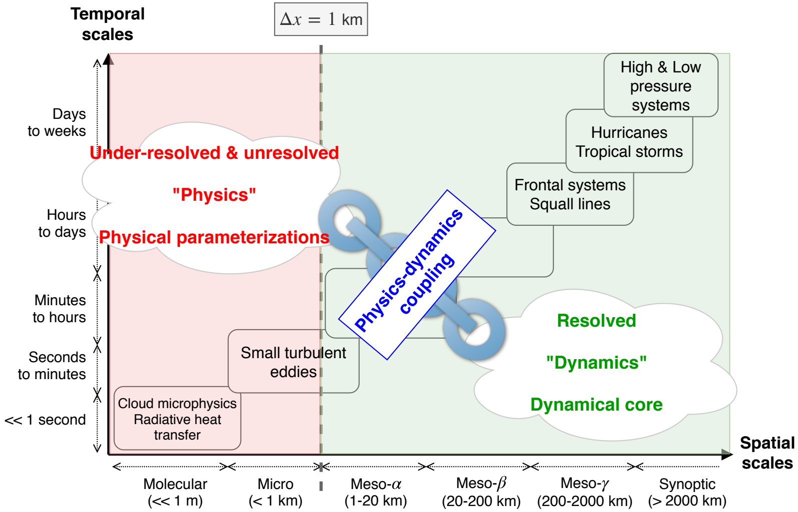


Motivation

- Physical parameterizations express the mutual interaction between subgrid-scale phenomena and large-scale dynamics in terms of the resolved fields.
- Typically devised in a *single-column* fashion.
- For ease of model development, parameterizations studied in isolation.
  - ✓ Consolidated knowledge of single physical and chemical processes.
  - ✓ Error introduced by any parameterization increasingly reduced.
  - ✗ Poor understanding of the impact of physics time-stepping.
  - ✗ Physics-dynamics coupling performed in a crude fashion.
- Arguably, these deficiencies root in the lack of *interoperability*, *usability* and *software reuse* of legacy (Fortran) codes.

Kalnay (2003), Dickinson et al. (2002), Donahue & Caldwell (2018)

Objectives

At the theoretical level:

- Develop a unified framework to analyze different coupling strategies.
- Extend previous studies carried out in more simplified contexts.
- Determine nominal order of convergence.

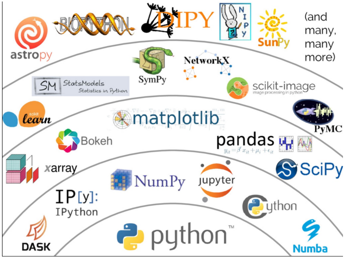
On the software side:

- Build a flexible and modular Python framework (`tasmania`) to ease composition, configuration and simulation of Earth models.

- Each process represented as a Python class.
  - User is given fine-grained control on the execution flow.
  - Wrapping existing Fortran codes is an option. Alternately...
- Inherent execution slowness of the Python interpreter overcome by leveraging `GridTools4Py` (`GT4Py`) - a domain-specific language (DSL) for stencil-based operations.

GridTools4Py: overview

- Developed at CSCS, with `tasmania` serving as major driving application.
- High-level, expressive, declarative definitions of the stencil.
- Internally, `GT4Py` builds an *intermediate representation* (IR) of the stencil as a graph of operations.
  - Allows visual inspection of the operations tree.
- Flexible execution model allowing heterogeneous executors:
  - Pythonic backends for debugging and early testing purposes;
  - Bindings to high-performance `GridTools` backend (in progress).
- Seamless integration with the Python scientific stack enables development of end-to-end applications.
  - Supports standard NumPy arrays.
  - Works in both IPython and Jupyter environments.



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tasmania: Taxonomy of components

```
# Simply retrieve diagnostics
diagnostics = DiagnosticComponent* (state)

# Calculate tendencies, i.e., time-derivatives,
# and retrieve diagnostics
tendencies, diagnostics = TendencyComponent* (state)

# Step the state based on one or more TendencyComponents,
new_state = TendencyStepper* (state, timestep)

# Dynamical core
new_state = DynamicalCore(timestep, state, tendencies)
```

* Abstract base class provided by `sympl` – a package offering functions and objects which could be used by any Earth system model.

Monteiro et al. (2018)

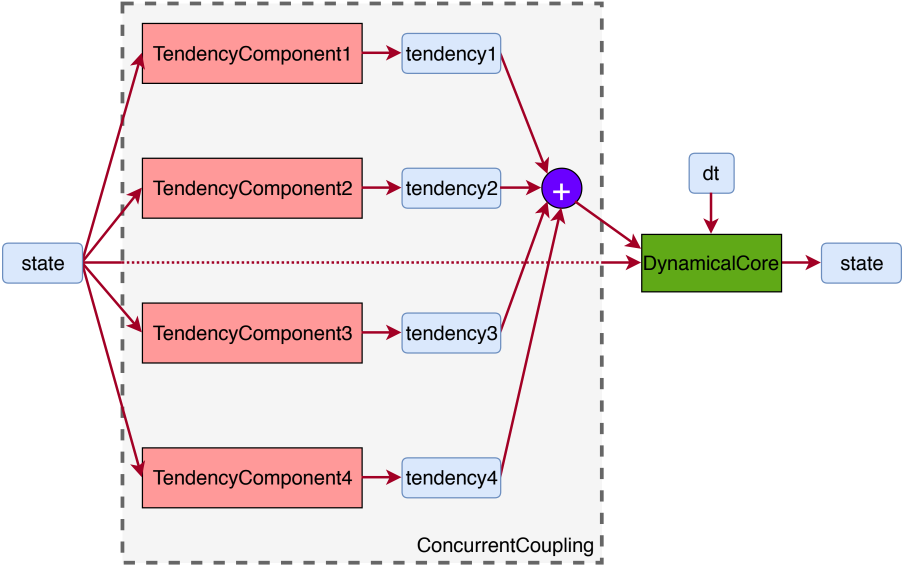
`tasmania`: Couplers

- Couplers automate the execution of a set of physical packages, pursuing a well-defined coupling strategy.
- Three couplers are currently available:
  - `ConcurrentCoupling`,
  - `ParallelSplitting` (not working...),
  - `SequentialUpdateSplitting`,

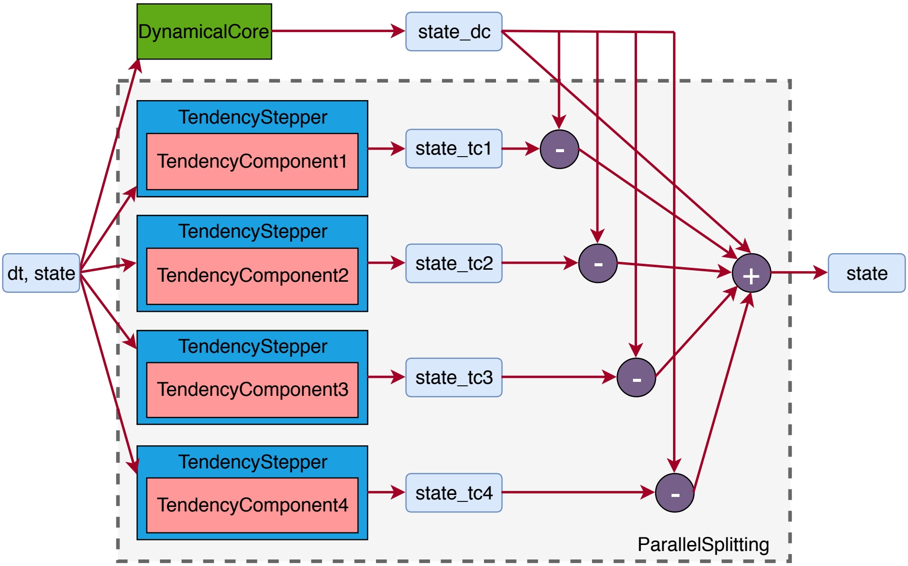
  which support four coupling mechanisms:
  - concurrent coupling (CC) [high order],
  - parallel splitting (PS) [1^{st}-order],
  - sequential-update splitting (SUS) [1^{st}-order],
  - symmetrized sequential-update splitting (SSUS) [2^{nd}-order].
- Couplers assert compatibility between encompassed components.

Staniforth (2002a,b), Dubal et al. (2004, 2005, 2006), Strang (1968)

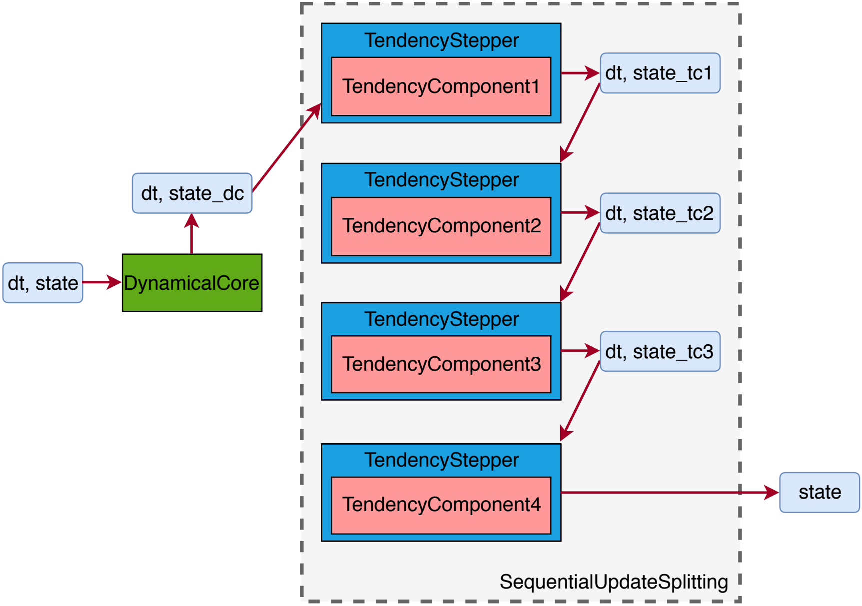
Concurrent coupling (CC)



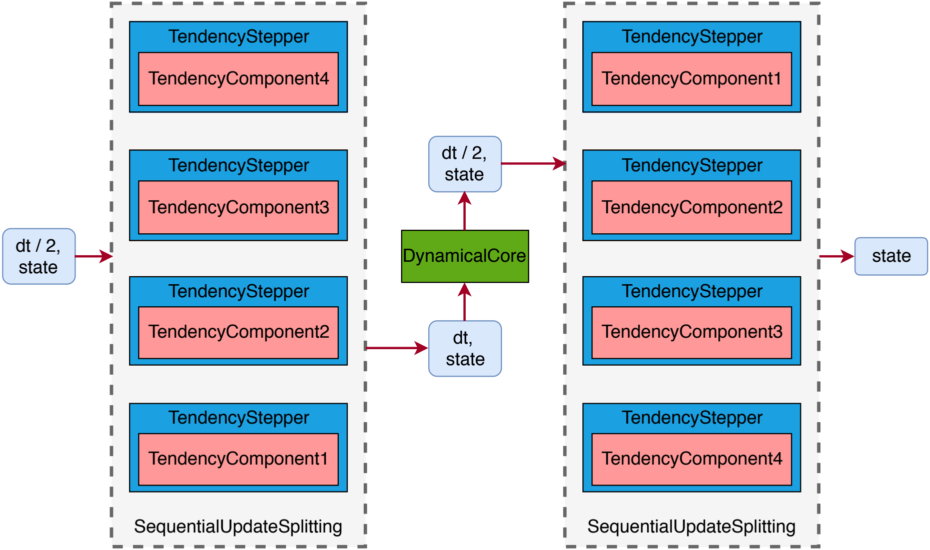
Parallel splitting (PS)



Sequential-update splitting (SUS)



Symmetrized sequential-update splitting (SSUS)



The isentropic system

Isentropic coordinates consist of:

- horizontal, Cartesian coordinates x and y;
- potential temperature θ,

$$\theta := T \left(\frac{p}{p_{\text{ref}}} \right)^{R/c_p} \in [\theta_s, \theta_t] ,$$

with

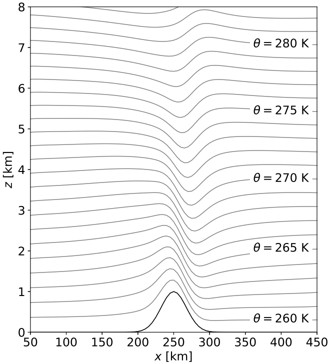
$T =$ temperature,

$p =$ pressure,

$p_{\text{ref}} = 1000$ hPa,

$c_p =$ specific heat for dry at constant pressure,

$R =$ gas constant for dry air.



Isentropic surfaces in a stable atmosphere.

Isentropic model: Hydrostatic dynamics in isentropic coordinates, where the diabatic heat acts as the vertical velocity.

Zeman (2016)

The isentropic model: Prognostic equations

$\sigma := -(1/g)\,\partial p/\partial\theta$ = *isentropic density*, with g = gravitational constant

$\mathbf{v} = [u,\, v]^T$ = horizontal velocity vector

$U := \sigma\, u$ = x-momentum, $V := \sigma\, v$ = y-momentum

$M := c_p\, T + g\, z$ = Montgomery potential, with z = geometric height

f = Coriolis parameter

q = non-precipitating tracer, S_q = physical source-sink rates for q

$$\frac{\partial \sigma}{\partial t} + \frac{\partial u\sigma}{\partial x} + \frac{\partial v\sigma}{\partial y} = -\frac{\partial \dot{\theta}\sigma}{\partial \theta}$$

$$\frac{\partial U}{\partial t} + \frac{\partial uU}{\partial x} + \frac{\partial vU}{\partial y} = -\frac{\partial \dot{\theta}U}{\partial \theta} - \sigma\frac{\partial M}{\partial x} + fV$$

$$\frac{\partial V}{\partial t} + \frac{\partial uV}{\partial x} + \frac{\partial vV}{\partial y} = -\frac{\partial \dot{\theta}V}{\partial \theta} - \sigma\frac{\partial M}{\partial y} - fU$$

$$\frac{\partial \sigma q}{\partial t} + \frac{\partial u\sigma q}{\partial x} + \frac{\partial v\sigma q}{\partial y} = -\frac{\partial \dot{\theta}\sigma q}{\partial \theta} + \sigma S_q$$

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$$\frac{\partial \sigma}{\partial t} + \boxed{\frac{\partial u\sigma}{\partial x} + \frac{\partial v\sigma}{\partial y}} = 0$$

$$\frac{\partial U}{\partial t} + \boxed{\frac{\partial uU}{\partial x} + \frac{\partial vU}{\partial y}} = \boxed{-\,\sigma\frac{\partial M}{\partial x}}$$

$$\frac{\partial V}{\partial t} + \boxed{\frac{\partial uV}{\partial x} + \frac{\partial vV}{\partial y}} = \boxed{-\,\sigma\frac{\partial M}{\partial y}}$$

Dry adiabatic configuration:

- $\mathscr{D}$
- $\mathscr{P}_1$

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Dry non-adiabatic configuration:

- $\mathscr{D}$
- $\mathscr{P}_1$
- $\mathscr{P}_2$
- $\mathscr{P}_3$

The isentropic model: Prognostic equations

$\sigma := -(1/g)\,\partial p/\partial\theta$ = *isentropic density*, with g = gravitational constant

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$U := \sigma\, u$ = x-momentum, $V := \sigma\, v$ = y-momentum

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$$\frac{\partial\sigma}{\partial t} + \boxed{\frac{\partial u\sigma}{\partial x} + \frac{\partial v\sigma}{\partial y}} = \boxed{-\frac{\partial\dot{\theta}\sigma}{\partial\theta}}$$

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$$\frac{\partial\sigma q}{\partial t} + \boxed{\frac{\partial u\sigma q}{\partial x} + \frac{\partial v\sigma q}{\partial y}} = \boxed{-\frac{\partial\dot{\theta}\sigma q}{\partial\theta}}\ \boxed{+\,\sigma S_q}$$

Moist non-adiabatic configuration*:

- $\mathscr{D}$
- $\mathscr{P}_1$
- $\mathscr{P}_2$
- $\mathscr{P}_3$
- $\mathscr{P}_4$

*Not tested

The isentropic model: Diagnostic equations

$\Pi := c_p \left(\frac{p}{p_{\text{ref}}} \right)^{R/c_p} = \frac{c_p \, T}{\theta}$ = Exner function

z_s = topography height

$$\begin{cases} \dfrac{\partial p}{\partial \theta} = -g \, \sigma \\ p(\theta = \theta_t) = p_t \end{cases} \quad \text{and} \quad \begin{cases} \dfrac{\partial M}{\partial \theta} = \Pi \\ M(\theta = \theta_s) = \Pi(\theta = \theta_s) \, \theta_s + g \, z_s \end{cases}$$

Adiabatic flow: Convergence analysis (1)

Two-dimensional, dry flow over an isolated *Witch of Agnesi* mountain,

$$z_s(x) = \frac{h\,a^2}{x^2 + a^2}\,,$$

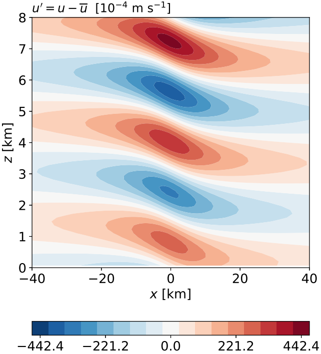
with $h = 1$ m the mountain height and $a = 10$ km its half-width at half-height.

If the flow is isothermal and the mean wind $\overline{u}$ is constant with height, the displacement of a streamline from its height far upstream satisfies

$$\delta(x, z) = \left(\frac{\overline{\rho}}{\rho_0}\right)^{-1/2} h\,a\,\frac{a\cos(l\,z) - x\sin(l\,z)}{x^2 + a^2}\,,$$

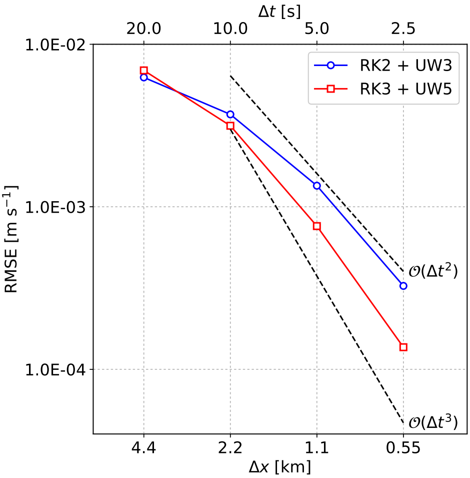
where $\overline{\rho}$ and ρ_0 are the mean and base state density, respectively, and l is the Scorer parameter. Then, the velocity components can be derived as

$$u = \overline{u}\left[1 - \frac{1}{\overline{\rho}}\left(\overline{\rho}\,\delta\right)_z\right] \quad \text{and} \quad w = \overline{u}\,\delta_x\,.$$



Langhans et al. (2012)

Adiabatic flow: Convergence analysis (2)



- Blue: 2-stages Runge-Kutta (RK2) + 3rd-order upwind scheme (UW3) + 2nd-order centered formula for pressure gradient.
- Red: 3-stages Runge-Kutta (RK3) + 5th-order upwind scheme (UW5) + 4th-order centered formula for pressure gradient.
- Root-mean-squared error (RMSE) w.r.t. a high-resolution simulation at $\Delta x = 275$ m.
- Only grid points within 40 km from mountain center and below 8 km considered.
- Similar results with any coupling.

Non-adiabatic flow: Description

- Consider stratified flows past isolated mountains with heated/cooled surface.
- The *modified* thermal forcing is given by

$$\dot{\theta} = \begin{cases} \dfrac{\theta\, R_d\, \alpha}{p\, c_p}\, F_0 \exp\left[-\alpha(z - z_s)\right]\left[\sin(2\pi\omega\, t) + \sin(2\pi\omega_{\mathtt{FW}}\, t)\right] & \text{if } r < L^*, \\ 0 & \text{otherwise}, \end{cases}$$

where

$$F_0 = F_0(t) = \begin{cases} 800 \text{ W m}^{-2} & \text{at day} \\ -75 \text{ W m}^{-2} & \text{at night} \end{cases}, \quad \alpha = \alpha(t) = \begin{cases} 1/600 \text{ m}^{-1} & \text{at day} \\ 1/75 \text{ m}^{-1} & \text{at night} \end{cases},$$

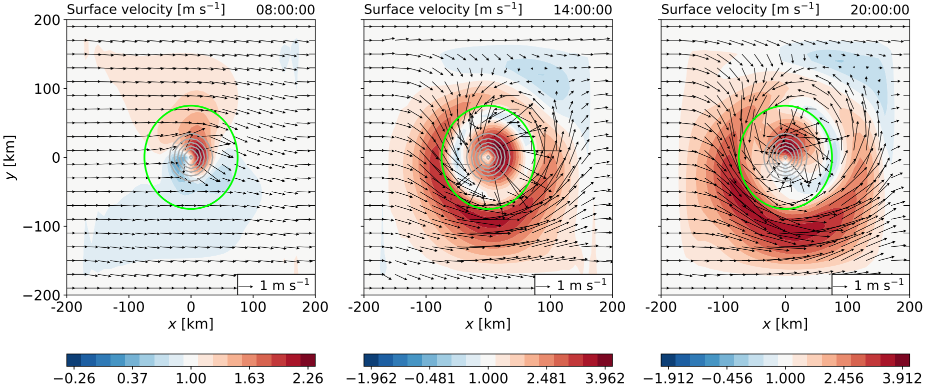
$$z_s = H[1 + (r/L)^2]^{-3/2}, \quad r = \sqrt{x^2 + y^2}, \quad L^* = 3L,$$

$$\omega = 1/24 \text{ h}^{-1} \text{ (diurnal cycle)}, \quad \omega_{\mathtt{FW}} \in \{0, 1/2, 2\} \text{ h}^{-1} \text{ (high-frequency forcing)}.$$

- Configuration: $H = 500$ m, $L = 25$ km, $u(t=0) = 1$ m s^{-1}, $v(t=0) = 0$ m s^{-1}.
- Numerical solver: RK3 + UW5 (horizontal adv.) + UW3 (vertical adv.)
- Resolution: $\Delta x = \Delta y = 10$ km, 50 vertical levels, $\Delta t = 10$ s.

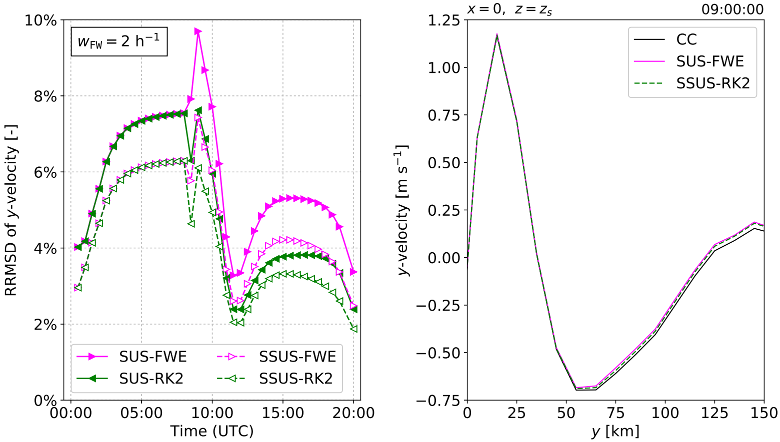
Reisner & Smolarkiewicz (1994)

Non-adiabatic flow: Early results (1)



Near-surface velocity field produced by CC for $\omega_{\mathtt{FW}} = 0$ at 0800 UTC (*left*), 1400 UTC (*center*) and 2000 UTC (*right*). The simulation starts at 0000 UTC and the heating source is switched off until 0800 UTC; the simulation is then conducted for further 12 hours. The green circle encloses the heated/cooled area.

Non-adiabatic flow: Early results (2)



Left: Time series of relative root-mean-squared deviation (RRMSD) of y-velocity yielded by SUS and SSUS, calculated with respect to the CC solution for $\omega_{\mathtt{FW}} = 2$ h^{-1}. Physics time stepping performed via forward Euler (FWE) or two-stages Runge-Kutta (RK2). *Right*: Horizontal profile of y-velocity at 0900 UTC.

Tentative schedule

Tasks	**Time**
Start of the Ph.D. project.	November 1, 2017
Familiarize with the weather and climate research fields.	Winter 2018/2019
Develop `tasmania` leveraging `GT4Py-v3`; implement different solvers for the isentropic model, a few parameterizations and various numerical dwarfs within the framework.	January 2018 - November 2018
Shape the theoretical framework and analyze state-of-the-art coupling mechanisms.	Summer 2018
Upgrade `tasmania` to `GT4Py-v4`; report feedbacks to the `GT4Py` development team.	November 2018 - February 2019
Run extensive convergence tests with the isentropic model on CSCS machines.	Spring 2019
Implement a non-hydrostatic model and further parameterizations; perform experiments.	Winter-Summer 2019
Investigate alternative ways to couple physics with dynamics.	Fall 2019 - Winter 2020
Integrate `tasmania` with a domain decomposition library.	Winter-Summer 2020
Writing of the thesis.	Summer-Fall 2020

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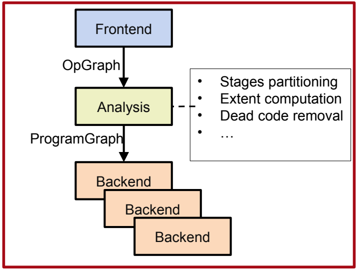
Why Python?

- New generations of domain scientists are more familiar and proficient with high-level programming languages, e.g., Python, than low-level languages, e.g., Fortran, C/C++.
- Python for scientific computing:
  - Python language has clean syntax and great expressiveness;
  - Python integration with other languages is great;
  - Python scientific stack includes an impressive collection of open source software for scientific computing (SciPy ecosystem).
- Main reason behind this success is Python's Buffer Protocol.
  - Low-level API for direct manipulation of memory buffers.
  - Multi-dimensional data structures stored in contiguous memory.
  - It eliminates the need to copy data.

E. Paredes

- The **frontend** builds a intermediate representation of the stencil as a graph of operations.
- During the analysis, the graph is processed and transformed to collect backend-independent information.
  - E.g., stages, temporaries, field accesses.
- The **backend** translates IR in specific code for target hardware.
- Modular design.
  - Ease addition of new components.



E. Paredes, Schulthess et al. (2019)

GridTools4Py: An example

```python
import gridtools as gt

@gt.stencil_function(backend="numpy")
def horizontal_diffusion(data, weight, *, alpha=4.0)):
    laplacian = - alpha * data[0, 0] + \
                (data[-1, 0] + data[1, 0] +
                 data[0, -1] + data[0, 1])
    flux_i = laplacian[1, 0] - laplacian[0, 0]
    flux_j = laplacian[0, 1] - laplacian[0, 0]
    diffusion = weight[0, 0] * (flux_i[-1, 0] - flux_i[0, 0] +
                                 flux_j[0, -1] - flux_j[0, 0])
    return diffusion
```

```python
import numpy as np

in_data  = np.random.rand(64, 64)
weight   = np.random.rand(64, 64)

out_data = horizontal_diffusion(in_data, weight)
```

GridTools4Py: Sketchy roadmap

- First GPL-licensed release of `GT4Py` by Q1 2019.
  - Directly directed towards academics.
  - Life span: $\approx$ 2 years.
  - Thinking about injecting `GT4Py` is some MSc courses to get students involved.
- `GT` backend available by Q2 2019.
  - Still under GPL license.
- Going multinode: integration of `GT4Py` with a domain partition library (cf. L. Strebel's MSc thesis).

`tasmania`: Design principles & requirements

(i) Model conceived as a chain of components, with each component representing a physical or dynamical process.

(ii) User is given fine-grained control on which components to include in the model, and in which order they should be executed.

(iii) Components are highly inter-operable.
   - In principle, any order of execution is supported.

(iv) Components can be instantiated independently, and run stand-alone.
   - E.g., a SCM does not need an underlying dycore to be executed.
   - Particularly useful for early testing of parameterization schemes.

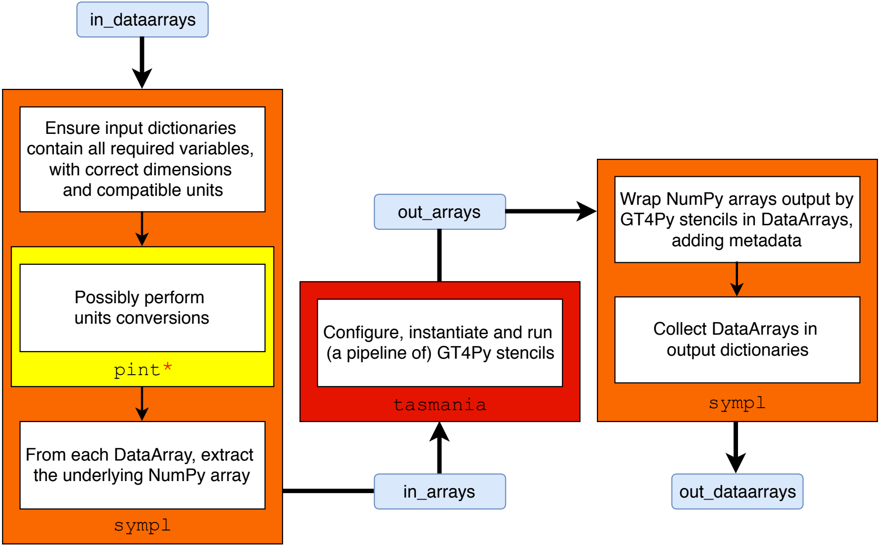
(v) Support for 2D, 3D, and single-column simulations.

(vi) User-interface abstracts away details of the computing architecture.
   - Separation of concerns between domain and computer scientists.

tasmania: Some (technical) details

- state, tendencies and diagnostics are plain dictionary where:
  - *keys* are strings denoting quantity names, which should be compliant with the CF Conventions;
  - *values* are xarray's DataArrays storing values and metadata (dimensions, coordinates, units) for those quantities.
- DataArray's API similar to that for pandas' Series.
- Each component specifies fundamental properties (name, dimensions, units) of both the variables which it requires in input, and the quantities which it calculates and outputs.
- This allows for effective runtime checks on input arguments.

tasmania: Intra-component workflow



* Package to define, operate and manipulate physical quantities.

Unified theoretical framework (1)

Canonical problem

$\psi = \psi(\boldsymbol{x}, t)$ = prognostic variable

$\mathscr{D}$ = spatial operator modeling the dynamics

$\mathscr{P}_m$ = $m-$th physical process, with $\mathscr{P} = \sum_{m=1}^{M} \mathscr{P}_m$

$R = R(\boldsymbol{x}, t)$ = forcing term independent of ψ (e.g., orographic forcing)

$$\frac{\partial \psi}{\partial t} - \mathscr{D}\psi = \sum_{m=1}^{M} \mathscr{P}_m \psi + R(\boldsymbol{x}, t) = \mathscr{P}\psi + R(\boldsymbol{x}, t)$$

Exact solution

If $\mathscr{D}$ and $\mathscr{P}$ do not depend on time, and $R \equiv 0$:

$$\begin{aligned} \psi(t) &= \psi(0) \exp\left[t\big(\mathscr{D} + \mathscr{P}\big)\right] \\ &= \psi(0) \left[I + t\,(\mathscr{D} + \mathscr{P}) + (1/2)\, t^2\, (\mathscr{D} + \mathscr{P})^2 + (1/6)\, t^3\, (\mathscr{D} + \mathscr{P})^3 + \ldots \right] \end{aligned}$$

$$\Rightarrow \psi(t+\Delta t) = \underbrace{\left[I + \Delta t\,(\mathscr{D} + \mathscr{P}) + (1/2)\Delta t^2\, (\mathscr{D} + \mathscr{P})^2 + (1/6)\Delta t^3\, (\mathscr{D} + \mathscr{P})^3 + \ldots \right]}_{\textbf{Exact update operator}} \psi(t)$$

Unified theoretical framework (2)

Semi-discretized form

$\psi_j = \psi_j(t) \approx \psi(\boldsymbol{x}_j, t)$

$\mathbb{D}$, $\mathbb{P}_m$ = numerical approximations of $\mathscr{D}$ and $\mathscr{P}_m$, respectively

$R_j(t) = R(\boldsymbol{x}_j, t)$

$$\frac{d\psi_j}{dt} - \mathbb{D}\psi_j = \mathbb{P}\psi_j + R_j(t) \qquad \text{(Set of ODEs)}$$

Note. In what follows, subscripts denoting the spatial location are omitted.

Fully-discretized version

- For the sake of tractability, we limit ourselves to two-time-level multi-step time integration schemes.
- The discretization of an ODE $\dot{\psi} = f(t,\ \psi)$ can be cast into the form

  $$\psi^{n+1} = \mathbf{L}\psi^n,$$

  with $\mathbf{L} = \mathbf{L}(t,\ \Delta t,\ f)$ the (nonlinear) numerical update operator.

Unified theoretical framework: Coupling

SUS

(i) $\psi^{n+1,0} = \mathbf{L}_D(\Delta t,\ \mathbb{D})\,\psi^n$

(ii) $\psi^{n+1,m} = \mathbf{L}_m(\Delta t,\ \mathbb{P}_m)\,\psi^{n+1,m-1}$,
for $m = 1,\ldots,M$

(iii) $\psi^{n+1} = \mathbf{L}_R(\Delta t,\ R)\,\psi^{n+1,M}$

PS

(i) $\psi^{n+1,D} = \mathbf{L}_D(\Delta t,\ \mathbb{D})\psi^n$

(ii) $\psi^{n+1,m} = \mathbf{L}_m(\Delta t,\ \mathbb{P}_m)\psi^n$,
for $m = 1,\ldots,M$

(iii) $\psi^{n+1,R} = \mathbf{L}_R(\Delta t,\ R)\psi^n$

(iv) $$\frac{\psi^{n+1}-\psi^n}{\Delta t} = \frac{\psi^{n+1,D}-\psi^n}{\Delta t} + \sum_{m=1}^{M}\frac{\psi^{n+1,m}-\psi^n}{\Delta t} + \frac{\psi^{n+1,R}-\psi^n}{\Delta t}$$

CC

$\psi^{n+1} = \mathbf{L}(\Delta t,\ \mathbb{D}+\mathbb{P}+R)\ \psi^n$

SSUS

$0 < \eta < 1$

(i) $\widetilde{\psi}^0 = \mathbf{L}_R(\eta\Delta t,\ R)\,\psi^n$

(ii) $\widetilde{\psi}^m = \mathbf{L}_m(\eta\Delta t,\ \mathbb{P}_m)\,\widetilde{\psi}^{m-1}$,
for $m = 1,\ldots,M$

(iii) $\psi^{n+1,M+1} = \mathbf{L}_D(\Delta t,\ \mathbb{D})\,\widetilde{\psi}^M$

(iv) $\psi^{n+1,m} = \mathbf{L}_m((1-\eta)\Delta t,\ \mathbb{P}_m)\,\psi^{n+1,m+1}$,
for $m = M,\ldots,1$

(iv) $\psi^{n+1} = \mathbf{L}_R((1-\eta)\Delta t,\ R)\,\psi^{n+1,1}$