#### A general theory of thermocompositional adiabatic and diabatic convection

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#### - Brown dwarfs spectral sequence:



#### - Brown dwarfs spectral sequence:



#### - Brown dwarfs spectral sequence:



- Stratified compressible hydrodynamics

#### Numerical scheme, simulations and HPC implementation -> Thomas Padioleau

with P. Kestener CEA/MdLs: HPC with S. Kokh CEA/DEN: numerical scheme and E. Audit CEA/MdLs

## - Stratified compressible hydrodynamics $\frac{\partial \rho}{\partial t} + \overrightarrow{\nabla} \left( \rho \overrightarrow{u} \right) = 0$

 $\frac{\partial \rho \, \overrightarrow{u}}{\partial t} + \overrightarrow{\nabla} \left( \rho \, \overrightarrow{u} \otimes \overrightarrow{u} + P \right) = \rho \, \overrightarrow{g}$  $\frac{\partial \rho \mathscr{E}}{\partial t} + \overrightarrow{\nabla} \left( \overrightarrow{u} (\rho \mathscr{E} + P) \right) = \rho c_p H(X, T)$  $\frac{\partial \rho X}{\partial t} + \overrightarrow{\nabla} \left( \rho X \overrightarrow{u} \right) = \rho R(X, T)$  $\mathscr{E} = e + \frac{1}{2}u^2 + \phi$  $\overrightarrow{g} = -\overrightarrow{\nabla}\phi$  $P = e(\gamma - 1) = \rho k_b T / \mu(X)$ 

- Stratified compressible hydrodynamics

Compressibility/conservation
finite volume scheme
co-localised variables

#### - Problems

poor accuracy at low Mach
small timestep (dt=dx/c)
poor hydrostatic balance

#### - Stratified compressible hydrodynamics

- Problems e poor accuracy at Low Mach



#### o poor hydrostatic balance



Stratified compressible hydrodynamics
All-regime solver: full scheme



Stratified compressible hydrodynamics
 All-regime solver: full scheme

= 0

= 0

= 0

 $+\rho \frac{\partial u_x}{\partial x}$  $\frac{\partial 
ho}{\partial t}$  $+u_x \frac{\partial \rho}{\partial x}$  $+u_x \frac{\partial \rho u_x}{\partial x}$  $+\rho u_x \frac{\partial u_x}{\partial x} + \frac{\partial P}{\partial x}$  $\partial \rho u_x$  $\partial t$  $+u_x \frac{\partial \rho \mathscr{E}}{\partial x}$  $+\rho \mathscr{E} \frac{\partial u_x}{\partial x} + \frac{\partial P u_x}{\partial x}$  $\partial 
ho \mathcal{E}$  $\partial t$ 

Stratified compressible hydrodynamics
All-regime solver: acoustic step



Stratified compressible hydrodynamics
All-regime solver: acoustic step

$\partial \tau$	$\partial u_x$	- 0	
$\partial t$	дт	-0	$\tau - 1$
$\partial u_x$	$\partial P$	- 0	$\iota = - \rho$
$\partial t$	$\neg \partial m$	-0	$dm = \rho dx$
<u> ISC</u>	$\partial Pu_x$	- 0	
$\partial t$	дт	-0	

Stratified compressible hydrodynamics
 All-regime solver: acoustic step

$\frac{\partial \tau}{\partial t}$	$\frac{\partial u_x}{\partial m}$	= 0	1
$\frac{\partial u_x}{\partial t}$	$+\frac{\partial\Pi}{\partial m}$	= 0	$\tau = - \rho$ $dm = \rho dx$
дЕ дt	$+\frac{\partial \Pi u_x}{\partial m}$	= 0	$a = \rho c_s$
$\frac{\partial \Pi}{\partial t}$	$+a^2 \frac{\partial u_x}{\partial m}$	= 0	

 $\Pi^{n+1-} = p(\tau^{n+1-}, \mathscr{E}^{n+1-}, u_x^{n+1-})$ 

Stratified compressible hydrodynamics
All-regime solver: acoustic step

$$U_{i+1/2}^{\star} = \frac{u_{x,i} + u_{x,i+1}}{2} - \frac{1}{2a} \left( \Pi_{i+1} - \Pi_i \right)$$
$$\Pi_{i+1/2}^{\star} = \frac{\Pi_i + \Pi_{i+1}}{2} - \frac{a}{2} \left( u_{x,i+1} - u_{x,i} \right)$$

 Stratified compressible hydrodynamics
 All-regime solver: acoustic step  $U_{i+1/2}^{\star} = \frac{u_{x,i} + u_{x,i+1}}{2} - \frac{1}{2a} \left( \Pi_{i+1} - \Pi_i \right)$  $\Pi_{i+1/2}^{\star} = \frac{\Pi_i + \Pi_{i+1}}{2} - \frac{a}{2} \left( u_{x,i+1} - u_{x,i} \right)$  $U_{i+1/2}^{\star} - U_{i-1/2}^{\star}$  $\tau^{n+1-} - \tau^n$ = 0 $\Delta t$  $\Delta m$  $u_x^{n+1-} - u_x^n$  $\prod_{i+1/2}^{\star} - \prod_{i-1/2}^{\star}$ = 0 $\Delta t$  $\Delta m$  $+ \frac{U_{i+1/2}^{\star} \Pi_{i+1/2}^{\star} - U_{i-1/2}^{\star} \Pi_{i-1/2}^{\star}}{+}$  $\mathscr{E}^{n+1-} - \mathscr{E}^n$ = 0 $\Delta m$  $\Delta t$ 

Stratified compressible hydrodynamics
 All-regime solver: transport step



Stratified compressible hydrodynamics
 All-regime solver: transport step

 $+\frac{\partial\rho u_x}{\partial x} - \rho\frac{\partial u_x}{\partial x}$  $\frac{\partial \rho}{\partial t}$ = 0 $+\frac{\partial\rho u_x^2}{\partial x}-\rho u_x\frac{\partial u_x}{\partial x}$  $\partial \rho u_{x}$ = 0 $\partial t$  $+\frac{\partial\rho \mathscr{E}u_x}{\partial x} - \rho \mathscr{E}\frac{\partial u_x}{\partial x}$  $\partial 
ho \mathscr{E}$ = 0 $\partial t$ 

Stratified compressible hydrodynamics
All-regime solver: transport step

$$\frac{\rho^{n+1} - \rho^{n+1-}}{\Delta t} + \frac{[\rho^{n+1-}U^{\star}]}{\Delta x} - \rho^{n+1-}\frac{[U^{\star}]}{\Delta x} = 0$$

$$\frac{(\rho u_x)^{n+1} - (\rho u_x)^{n+1-}}{\Delta t} + \frac{[(\rho u_x)^{n+1-}U^{\star}]}{\Delta x} - (\rho u_x)^{n+1-}\frac{[U^{\star}]}{\Delta x} = 0$$

$$\frac{(\rho \mathscr{E})^{n+1} - (\rho \mathscr{E})^{n+1-}}{\Delta t} + \frac{[(\rho \mathscr{E})^{n+1-}U^{\star}]}{\Delta x} - (\rho \mathscr{E})^{n+1-}\frac{[U^{\star}]}{\Delta x} = 0$$

Stratified compressible hydrodynamics
All-regime solver: full scheme  $\frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{[\rho^{n+1} - U^{\star}]}{\Delta x} = 0$  $\frac{(\rho u_x)^{n+1} - (\rho u_x)^n}{\Delta t} + \frac{[(\rho u_x)^{n+1} - U^* + \Pi^*]}{\Delta x} = 0$  $\frac{(\rho \mathscr{E})^{n+1} - (\rho \mathscr{E})^n}{\Delta t} + \frac{[(\rho \mathscr{E})^{n+1} - U^* + \Pi^* U^*]}{\Delta x} = 0$  $U_{i+1/2}^{\star} = \frac{u_{x,i} + u_{x,i+1}}{2} - \frac{1}{2a} \left( \Pi_{i+1} - \Pi_i \right)$  $\Pi_{i+1/2}^{\star} = \frac{\Pi_i + \Pi_{i+1}}{2} - \frac{a}{2} \left( u_{x,i+1} - u_{x,i} \right)$ 

Stratified compressible hydrodynamics
All-regime solver: full scheme
Explicit/Explicit scheme
Implicit/Explicit scheme
Low Mach correction

$$U_{i+1/2}^{\star} = \frac{u_{x,i} + u_{x,i+1}}{2} - \frac{1}{2a} \left( \Pi_{i+1} - \Pi_i \right)$$
$$\Pi_{i+1/2}^{\star} = \frac{\Pi_i + \Pi_{i+1}}{2} - \frac{a}{2} \left( u_{x,i+1} - u_{x,i} \right)$$

Stratified compressible hydrodynamics
All-regime solver: full scheme
conservative scheme: Sod test



Stratified compressible hydrodynamics
All-regime solver: full scheme
Low Mach correction: Gresho vortex





- Stratified compressible hydrodynamics - All-regime solver with gravity - hydrostatic balance at cell centre  $\frac{(\rho u_x)^{n+1} - (\rho u_x)^n}{\Delta t} + \frac{\left[(\rho u_x)^{n+1} - U^\star + \Pi^\star\right]}{\Delta x} = -\rho g$ if there is initially no velocity  $\frac{\Pi_{i} + \Pi_{i+1}}{2} - \frac{\Pi_{i} + \Pi_{i-1}}{2} = -\rho_{i}g\Delta x$  $u_x^{n+1} = O(\Delta x), \quad \frac{\partial P}{\partial x} = -\rho g + O(\Delta x)$ 

- Stratified compressible hydrodynamics - All-regime solver with gravity - hydrostatic balance at interface  $\frac{(\rho u_x)^{n+1} - (\rho u_x)^n}{\Delta t} + \frac{[(\rho u_x)^{n+1} - U^* + \Pi^*]}{\Delta x} = -\frac{1}{2} \left( \frac{\rho_i + \rho_{i+1}}{2} + \frac{\rho_i + \rho_{i-1}}{2} \right) g$ if there is initially no velocity  $\frac{\Pi_i + \Pi_{i+1}}{2} - \frac{\Pi_i + \Pi_{i-1}}{2} = -\frac{1}{2} \left( \frac{\rho_i + \rho_{i+1}}{2} + \frac{\rho_i + \rho_{i-1}}{2} \right) g\Delta x$  $\Pi_{i+1} - \Pi_i = \frac{\rho_i + \rho_{i+1}}{2} g \Delta x \qquad \Pi_i - \Pi_{i-1} = \frac{\rho_{i-1} + \rho_i}{2} g \Delta x$  $u_x^{n+1} = 0, \quad \frac{\partial P}{\partial x} = -\rho g$ 

Stratified compressible hydrodynamics
 All-regime solver with gravity
 hydrostatic balance at interface



Stratified compressible hydrodynamics
All-regime solver with gravity
Convective simulation
Low Mach correction



Stratified compressible hydrodynamics
All-regime solver with gravity
Compressible convective simulation



Stratified compressible hydrodynamics
 All-regime solver with gravity
 Parallel HPC Implementation



Problem of portability and performance probability....

Stratified compressible hydrodynamics
All-regime solver with gravity
Parallel HPC Implementation



#### Kokkos Library:

- C++ library for perf. portability
- extracted from Trilinos (Sandia)
- backend: openMP, Pthreads, CUDA
- abstraction of memory space and execution space

Stratified compressible hydrodynamics
All-regime solver with gravity
Memory layout:



Stratified compressible hydrodynamics
All-regime solver with gravity
Kokkos kernel

}

```
void operator ()(const int i) const
{
    a(i, 0) = 1.0*i;
    a(i, 1) = 1.0*i*i;
    a(i, 2) = 1.0*i*i*i;
}
```

```
Kokkos::View<double*[3]> m_a;
```

};

```
int main (int argc, char* argv[])
{
```

```
Kokkos::initialize(argc, argv);
```

```
Kokkos::View<double*[3]> view("View_name", 15);
```

```
Kokkos::parallel_for(15, InitView(view));
```

```
Kokkos::finalize();
```

## Stratified compressible hydrodynamics All-regime solver with gravity Kokkos kernel



Stratified compressible hydrodynamics
All-regime solver with gravity
2D diabatic convection

$$\frac{\partial \rho}{\partial t} + \overrightarrow{\nabla} \left( \rho \, \overrightarrow{u} \right) = 0$$

 $\frac{\partial \rho \, \overrightarrow{u}}{\partial t} + \overrightarrow{\nabla} \left( \rho \, \overrightarrow{u} \otimes \overrightarrow{u} + P \right) = \rho \, \overrightarrow{g}$  $\frac{\partial \rho \, \mathscr{C}}{\partial t} + \overrightarrow{\nabla} \left( \overrightarrow{u} (\rho \, \mathscr{C} + P) \right) = \rho c_p H(X, T)$  $\frac{\partial \rho X}{\partial t} + \overrightarrow{\nabla} \left( \rho X \, \overrightarrow{u} \right) = \rho R(X, T)$ 

Stratified compressible hydrodynamics
All-regime solver with gravity
2D diabatic convection



#### What is in common between:







#### . What is in common between:

Convective systems but not adiabatic, they are all subject to:
Energy exchange (latent heat, thermal diffusion, radiative transfer)
and/or compositional source terms (chemical reactions, condensation/evaporation, compositional diffusion)





What is adiabatic convection?
 Thermal adiabatic case

 $\theta = T(P_{\rm ref}/P)^{(\gamma-1)/\gamma}$  $\frac{\partial \ln \theta}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} \left( \ln \theta \right) = 0$  $P = \rho k_b T/\mu$ 

What is adiabatic convection?
 Thermal adiabatic case

$$\frac{\partial \ln \theta}{\partial t} + \vec{u} \, \vec{\nabla} \left( \ln \theta \right) = 0 \qquad \qquad \theta = T(P_{\text{ref}}/P)^{(\gamma-1)/\gamma} \\ P = \rho k_b T/\mu \\ - \text{Unstable if:} \quad \frac{\partial \ln \theta_0}{\partial z} < 0 \\ \end{cases}$$



- Schwarzschild criterion (1906)  $\nabla_T - \nabla_{ad} > 0, \quad \nabla_T = \frac{\partial \ln T_0}{\partial \ln P_0}$  $\frac{\partial T_0}{\partial z} < \frac{g}{C_p}$  - What is adiabatic convection? - Thermo-compositional adiabatic case  $\frac{\partial \ln \theta}{\partial t} + \vec{u} \, \vec{\nabla} \left( \ln \theta \right) = 0 \qquad \theta = T(P_{ref}/P)^{(\gamma-1)/\gamma}$   $\frac{\partial X}{\partial t} + \vec{u} \, \vec{\nabla} (X) = 0 \qquad P = \rho k_b T/\mu(X)$  - What is adiabatic convection? - Thermo-compositional adiabatic case  $\frac{\partial \ln \theta}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} \left( \ln \theta \right) = 0$  $\theta = T(P_{\rm ref}/P)^{(\gamma-1)/\gamma}$  $P = \rho k_b T / \mu(X)$  $\frac{\partial X}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} (X) = 0$   $P = \rho k$   $- \text{Unstable if: } \nabla_T - \nabla_{ad} - \nabla_\mu > 0$  $\nabla_T = \frac{\partial \ln T_0}{\partial \ln P_0}, \quad \nabla_\mu = \frac{\partial \ln \mu_0}{\partial \ln P_0}$ - Ledoux criberion (1947)

What is adiabatic convection? - Thermo-compositional diabatic case  $\frac{\partial \ln \theta}{\partial t} + \vec{u} \, \vec{\nabla} \left( \ln \theta \right) = \frac{H(X,T)}{T} \quad \theta = T(P_{\text{ref}}/P)^{(\gamma-1)/\gamma}$   $\frac{\partial X}{\partial t} + \vec{u} \, \vec{\nabla} (X) = R(X,T)$   $P = \rho k_b T/\mu(X)$  - What is adiabatic convection?  $-\frac{Thermo-compositional}{\partial \ln \theta} + \overrightarrow{u} \overrightarrow{\nabla} (\ln \theta) = \frac{H(X,T)}{T} \quad \theta = T(P_{\text{ref}}/P)^{(\gamma-1)/\gamma}$  $P = \rho k_b T / \mu(X)$  $\frac{\partial X}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla}(X) = R(X, T)$ - Unstable if:  $\nabla_T - \nabla_{ad} - \nabla_\mu > 0$ or  $(\nabla_T - \nabla_{ad})\omega'_X - \nabla_\mu \omega'_T < 0$  $\omega'_X = R_X + R_T (T_0 \partial \ln \mu_0 / \partial X)$ with  $\omega_T' = H_T + H_X (T_0 \partial \ln \mu_0 / \partial X)^{-1}$ and

#### - Thermohaline or fingering convection





 $(\nabla_T - \nabla_{ad})\omega'_X - \nabla_\mu \omega'_T < 0$ with  $R = \kappa_\mu \Delta X \quad \omega'_X = -k^2 \kappa_\mu \quad (R_T = 0)$ 

and  $H = \kappa_T \Delta T$   $\omega'_T = -k^2 \kappa_T$   $(H_X = 0)$ 



Stern 1960



Ulrich 1972

 $(\nabla_T - \nabla_{ad})\kappa_{\mu} - \nabla_{\mu}\kappa_T > 0$ 

and simulations from Traxler et al. 2011, Brown et al. 2013 Garaud et al. 2015, Sengupta & Garaud 2018

#### - Steam/liquid or moist convection





 $\nabla_T - \nabla_{\rm ad} > 0$ 





von Bezold 1893

Dry adiabat

Moist « pseudo-adiabat »

#### - Steam/Liquid or moist convection



### $(\nabla_{T} - \nabla_{ad})\omega'_{X} - \nabla_{\mu}\omega'_{T} < 0$ with $R = R_{cond}(X, T)$ and $X = X_{eq}(P, T)$ and $H = -R_{cond}L/c_{p}$ $\nabla_{T} - \nabla_{ad}\frac{1 - \rho_{0}\frac{\partial X_{eq}}{\partial P}L}{1 + \frac{\partial X_{eq}}{\partial T}\frac{L}{c_{p}}} > 0$

Moist « pseudo-adiabat »



#### - steam/liquid or moist convection





 $(\nabla_{T} - \nabla_{ad})\omega'_{X} - \nabla_{\mu}\omega'_{T} < 0$ with  $R = R_{cond}(X, T)$  and  $X = X_{eq}(P, T)$ and  $H = -R_{cond}L/c_{p}$  $\nabla_{T} - \nabla_{ad}\frac{1 - \rho_{0}\frac{\partial X_{eq}}{\partial P}L}{1 + \frac{\partial X_{eq}}{\partial T}\frac{L}{c_{p}}} > 0$ 

Moist « pseudo-adiabat »

von Bezold 1893

### Thermo-compositional diabatic convection



 $(\nabla_T - \nabla_{ad})\omega'_X - \nabla_\mu \omega'_T < 0$ with  $\omega'_X = R_X + R_T (T_0 \partial \ln \mu_0 / \partial X)$ and  $\omega'_T = H_T + H_X (T_0 \partial \ln \mu_0 / \partial X)^{-1}$ and probably many more...

#### - CO/CH4 radiative convection



 $(\nabla_T - \nabla_{ad})\omega'_X - \nabla_\mu \omega'_T < 0$ with  $R = -(X - X_{eq})/\tau_{chem}$ and  $H = 4\pi\kappa/c_p \left(J - \sigma T^4\right)$ 

Brown dwarfs and giant exoplanets



Moist convection



CO/CH4 radiative convection

$$\frac{\partial \ln \theta}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} \left( \ln \theta \right) = \omega_T' \frac{\delta T}{T_0}$$

 $\frac{\partial X}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} (X) = \omega'_X \delta X$  $\delta X \partial \ln \mu_0 / \partial X = \delta T / T_0$ 

 $\frac{\partial \ln \theta}{\partial t} + \overrightarrow{u} \,\overrightarrow{\nabla} \left( \ln \theta \right) = \omega_T' \frac{\delta T}{T_0}$  $\frac{\partial X}{\partial t} + \overrightarrow{u} \,\overrightarrow{\nabla} (X) = \omega_X' \delta X$ 

 $\delta X \partial \ln \mu_0 / \partial X = \delta T / T_0$ 

 $\frac{\partial \ln \theta'}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} (\ln \theta') = 0$ 

with  $\ln \theta' = \ln \theta - X \frac{\partial \ln \mu_0}{\partial X} \frac{\omega'_T}{\omega'_X}$ 

 $\frac{\partial \ln \theta}{\partial t} + \overrightarrow{u} \,\overrightarrow{\nabla} \left( \ln \theta \right) = \omega_T' \frac{\delta T}{T_0}$  $\frac{\partial X}{\partial t} + \overrightarrow{u} \,\overrightarrow{\nabla} (X) = \omega_X' \delta X$  $\delta X \partial \ln \mu_0 / \partial X = \delta T / T_0$ 

 $\frac{\partial \ln \theta'}{\partial t} + \overrightarrow{u} \overrightarrow{\nabla} (\ln \theta') = 0$ 

with  $\ln \theta' = \ln \theta - X \frac{\partial \ln \mu_0}{\partial X} \frac{\omega'_T}{\omega'_X}$ 

 $\ln \theta' = \ln \theta - XL/c_p T_0$  for moist convection

Can define an adiabatic convective flux:

$$F_{\rm ad} = \rho c_p w_{\rm ad} T_0 (\nabla_T - \nabla_{\rm ad})$$

## Can define a diabatic convective flux: $F_{\rm d} = \rho c_p w_{\rm d} T_0 (\nabla_T - \nabla_{\rm ad} - \nabla_\mu \omega_T' / \omega_X')$



similar to mass/flux convection parametrizations used for moist convection (review: Arakawa & Jung 2011)

# Bifurcation between adiabatic and diabatic convection Boiling crisis in steam/liquid convection





Nukiyama 1934

#### Bifurcation between adiabatic and diabatic convection - Boiling crisis in steam/liquid convection







Nukiyama 1934

- Could provide a natural explanation of the boiling crisis?

#### - Bifurcation between adiabatic and diabatic convection

- L/T transition in brown-dwarf spectra?





### - Bifurcation between adiabatic and diabatic convection

- L/T transition in brown-dwarf / ctra?

(Den) Hu

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O,

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or willingd)



#### A giant cooling crisis?

#### - Bifurcation between adiabatic and diabatic convection

- L/T transition in brown-dwarf spectra?





- Bifurcation between adiabatic and diabatic convection

- Spatial bifurcation: thermohaline staircase



$$F_{d} = \rho c_{p} w_{d} T_{0} (\nabla_{T} - \nabla_{ad} - \nabla_{\mu} \kappa_{T} / \kappa_{\mu})$$

$$X_{d} = \rho w_{d} \left(\frac{\partial \log \mu_{0}}{\partial X}\right)^{-1} (\nabla_{\mu} - (\nabla_{T} - \nabla_{ad}) \kappa_{\mu} / \kappa_{T})$$

$$F_{ad} = \rho c_{p} w_{ad} T_{0} (\nabla_{T} - \nabla_{ad})$$

$$X_{ad} = \rho w_{ad} \left(\frac{\partial \log \mu_{0}}{\partial X}\right)^{-1} (\nabla_{\mu})$$

#### - Conclusions:

- Stratified all-regime compressible hydrodynamic solvers can be developed with efficient HPC support (MPI+Kokkos) to study these convective instabilities
- Thermohaline, fingering, moist, steam/liquid,
   CO/CH4 radiative convection all derive from
   this diabatic branch of convection
- Extension at high order, implicit acoustic waves and radiative transfer (Trilinos)