## CAM-SE: Lecture II

## Peter Hjort Lauritzen

Atmospheric Modeling and Predictability Section<br>Climate and Global Dynamics Laboratory<br>National Center for Atmospheric Research

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## Outline

- Previous talk: derivation of equations of motion ...
- Introduce computational grid and projections
- Introduction to the spectral-element method
- Properties of the spectral-element
- Time-stepping
- Coupling to physics
- Computational performance
- Variable resolution version of CAM-SE

Cubed-sphere geometry (originally introduced by Sadourny (1972))

(a)


- A quadrilateral "box" is referred to as an element $\Omega_{\mathrm{e}}$
- Each 2D element $\Omega_{\mathrm{e}}\left(\mathrm{x}^{1}, \mathrm{x}^{2}\right)$ is defined in terms of central (gnomonic) projection angles ( $\mathbf{x}^{1}, \mathbf{x}^{2}$ )
- The elements are separated by the same central angle -> equi-angular gnomonic grid


## Cubed-sphere geometry (originally introduced by Sadourny (1972))

(a)


```
pure function spherical to_cart(sphere) result (cart)
    implicit none
    type(spherical_polar_t), intent(in) :: sphere
    type(cartesian3D_t) :: cart
    cart%x=sphere%r*COS(sphere%lat)*COS(sphere%lon)
    cart%y=sphere%r*COS(sphere%lat)*SIN(sphere%lon)
    cart%z=sphere%r*SIN(sphere%lat)
```

end function
Spherical_to_cart

Analytical transformation laws for the six cubed sphere faces can be found in Appendix A of Nair et al. (2005):

```
pure function cart2cubedsphere(cart30, face_no) result(cart)
iaplicit none
    type(cartesian3D_t).intent(in) :: cart3d
    integer. intent(in) :: face_no
    type (cartesian2d_t) :: cart
    real(kind=r8) :: x.y
    select case (face_no)
    case (1)
        x = cart3D%y/cart3D%x
        y = cart3D%z/cart3D%x
    case (2)
        x = -cart30%x/cart30%y
        y = cart3D%z/cart30%y
    case (3)
        x = cart30%y/cart30%x
        y = -cart30%z/cart30%x
    case (4)
        x = -cart30%x/cart30%y
        y = -cart3D%z/cart3D%y
    case (5)
        x = -cart3D%y/cart30%z
        y = -cart30%x/cart30%z
    case (6)
        x = cart30zy/cart30%z
        y = -cart30%x/cart30%z
    end select
    cart%x = ATAN(x)
    cart%y = ATAN(y)
end function cart2cubedsphere
```


## Mapping a vector from cube to sphere

The mapping from cube to sphere results in a non-orthogonal curvilinear coordinate system on $\mathcal{S}$, with the metric tensor $G_{i j}$ and analytic Jacobian $\sqrt{G}=\left|G_{i j}\right|^{1 / 2}$, $i, j \in\{1,2\}$. A physical vector quantity such as the wind vector $\mathbf{v}=(u, v)$, defined on $\mathcal{S}$ in orthogonal lat-lon coordinates, can be uniquely expressed in tensor form using conventional notations as the covariant ( $u_{1}, u_{2}$ ) and contravariant ( $u^{1}, u^{2}$ ) vectors using the $2 \times 2$ transformation matrix $\mathbf{D}$ associated with the gnomonic mapping such that $\mathbf{D}^{T} \mathbf{D}=G_{i j}$ (see Nair et al. [2005] for the details):

$$
\left[\begin{array}{l}
u \\
v
\end{array}\right]=\mathbf{D}\left[\begin{array}{l}
u^{1} \\
u^{2}
\end{array}\right]=\mathbf{D}^{-T}\left[\begin{array}{l}
u_{1} \\
u_{2}
\end{array}\right] .
$$

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## The spectral element method: 2D conservation law

The governing equations defined in familiar vector form can also be expressed in general tensor form. In order to describe the SE discretization process in simple terms, we consider the the following conservation law on $\mathcal{S}$ for an arbitrary scalar $\phi$ :

$$
\begin{equation*}
\frac{\partial \phi}{\partial t}+\nabla \cdot \mathbf{F}(\phi)=S(\phi) \tag{76}
\end{equation*}
$$

where

$$
\begin{equation*}
\nabla \cdot \mathbf{F}(\phi)=\frac{1}{\sqrt{G}}\left[\frac{\partial \sqrt{G} F^{1}}{\partial x^{1}}+\frac{\partial \sqrt{G} F^{2}}{\partial x^{2}}\right] . \tag{77}
\end{equation*}
$$

In the special case of the flux-form transport equation the contravariant fluxes $\left(F^{1}, F^{2}\right)=$ ( $u^{1} \phi, u^{2} \phi$ ), and $S(\phi)$ is an arbitrary source term.

## The spectral element method: test function

The SE solution process involves casting the partial differential equation in Galerkin form, i.e., by multiplying (76) with a test (weight) function $\psi$ and integrating over the domain $\mathcal{S}$,

$$
\begin{equation*}
\int_{\mathcal{S}} \psi\left[\frac{\partial \phi}{\partial t}+\nabla \cdot \mathbf{F}(\phi)-S(\phi)\right] d \mathcal{S}=0 . \tag{78}
\end{equation*}
$$

A computational form of (78) is obtained by applying Green's theorem, resulting in the weak Galerkin form, as follows:

$$
\begin{equation*}
\int_{\mathcal{S}} \psi \frac{\partial \phi}{\partial t} d \mathcal{S}=\int_{\mathcal{S}} \nabla \psi \cdot \mathbf{F}(\phi) d \mathcal{S}+\int_{\mathcal{S}} \psi S(\phi) d \mathcal{S} \tag{79}
\end{equation*}
$$

where the approximation to the solution $\phi$ and the test function belong to a polynomial space $V^{N}$.

For the efficient evaluation of the integrals, the SE method employs Gauss-Lobatto-Legendre (GLL) quadrature rule for integrals and collocation differentiation for derivative operators.

All the corresponding numerical operations are performed on a square $[-1,1]^{2}$ known as the standard (or reference) element.


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All the corresponding numerical operations are performed on a square $[-1,1]^{2}$ known as the standard (or reference) element.


Then an arbitrary surface integral on $\Omega_{e}$ can be expressed in terms of local coordinates $\xi^{1}, \xi^{2} \in[-1,1]$ and the Jacobian $J_{e}$

$$
\begin{equation*}
\int_{\Omega_{e}} \psi\left(x^{1}, x^{2}\right) d \Omega_{e}=\int_{-1}^{1} \int_{-1}^{1} J_{e}\left(\xi^{1}, \xi^{2}\right) \psi\left(\xi^{1}, \xi^{2}\right) d \xi^{1} d \xi^{2} \approx \sum_{k=0}^{N} \sum_{l=0}^{N} w_{k} w_{l} J_{e}\left(\xi_{k}^{1}, \xi_{l}^{2}\right) \psi\left(\xi_{k}^{1}, \xi_{l}^{2}\right), \tag{80}
\end{equation*}
$$

where $w_{k}, w_{l}$ are the Gauss quadrature weights.

In the case of GLL quadrature rule, the nodal points $\xi_{k}, k=0,1, \ldots, N$, are the roots of the polynomial $\left(1-\xi^{2}\right) P_{N}^{\prime}(\xi)=0, \xi \in[-1,1]$; and the corresponding GLL quadrature weights are given by

$$
w_{k}=\frac{2}{N(N+1)\left[P_{N}\left(\xi_{k}\right)\right]^{2}},
$$

where $P_{N}(\xi)$ is the Legendre polynomial of degree $N$.
Note that there are N+1 GLL point

Then an arbitrary surface integral on
expressed in terms of local coordinates $\xi^{1}, \xi^{2} \in[-1,1]$ and the Jacobian $J_{e}$

$$
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\end{equation*}
$$

where $w_{k}, w_{l}$ are the Gauss quadrature weights.

For the SE discretization it is customary to use Lagrange polynomials $h_{k}(\xi)$, with roots at the GLL quadrature points $\xi_{k}$, as basis functions. This setup provides discrete orthogonality for the basis function $h_{k}(\xi)$, which is formally defined as:


$$
h_{k}(\xi)=\frac{\left(\xi^{2}-1\right) P_{N}^{\prime}(\xi)}{N(N+1) P_{N}\left(\xi_{k}\right)\left(\xi-\xi_{k}\right)} .
$$

$$
\begin{equation*}
\int_{\Omega_{e}} \psi\left(x^{1}, x^{2}\right) d \Omega_{e}=\int_{-1}^{1} \int_{-1}^{1} J_{e}\left(\xi^{1}, \xi^{2}\right) \psi\left(\xi^{1}, \xi^{2}\right) d \xi^{1} d \xi^{2} \approx \sum_{k=0}^{N} \sum_{l=0}^{N} w_{k} w_{l} J_{e}\left(\xi_{k}^{1}, \xi_{l}^{2}\right) \psi\left(\xi_{k}^{1}, \xi_{l}^{2}\right), \tag{80}
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$$

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## The spectral element method: semi-discrete form

$$
\begin{equation*}
\int_{\mathcal{S}} \psi \frac{\partial \phi}{\partial t} d \mathcal{S}=\int_{\mathcal{S}} \nabla \psi \cdot \mathbf{F}(\phi) d \mathcal{S}+\int_{\mathcal{S}} \psi S(\phi) d \mathcal{S}, \tag{79}
\end{equation*}
$$

A semi-discrete form of (79) on an element $\Omega_{e}$ can by obtained by approximating the solution as a tensor product of 1D Lagrange basis $\left\{h_{k}(\xi)\right\}_{k=0}^{N}$ such that

$$
\left.\phi\right|_{\Omega_{e}} \approx \phi^{e}\left(\xi^{1}, \xi^{2}, t\right)=\sum_{k=0}^{N} \sum_{l=0}^{N} \phi_{k l}^{e}(t) h_{k}\left(\xi^{1}\right) h_{l}\left(\xi^{2}\right),
$$

where $\phi_{k l}^{e}(t)=\phi^{e}\left(\xi_{k}^{1}, \xi_{l}^{2}, t\right)$ are the nodal grid-point values of the solution, and defining the test function as $\psi\left(\xi^{1}, \xi^{2}\right)=h_{k}\left(\xi^{1}\right) h_{l}\left(\xi^{2}\right)$.

## The spectral element method: semi-discrete form

$$
\begin{equation*}
\int_{\mathcal{S}} \psi \frac{\partial \phi}{\partial t} d \mathcal{S}=\int_{\mathcal{S}} \nabla \psi \cdot \mathbf{F}(\phi) d \mathcal{S}+\int_{\mathcal{S}} \psi S(\phi) d \mathcal{S}, \tag{79}
\end{equation*}
$$

By using (80) and the discrete orthogonality property of $h_{k}(\xi)$, we get a completely decoupled system of ODEs on $\Omega_{e}$, for each grid-point ( $k, l$ )

$$
\begin{aligned}
\tilde{M}_{k l}^{e} \frac{d}{d t} \phi_{k l}^{e}(t) & =A_{k l}^{e}+S_{k l}^{e} \\
\widetilde{M}_{k l}^{e} & =\int_{-1}^{1} \int_{-1}^{1} J_{e} h_{k}\left(\xi^{1}\right) h_{l}\left(\xi^{2}\right) d \xi^{1} d \xi^{2}=J_{e}(k, l) w_{k} w_{l} \\
A_{k l}^{e} & =\sum_{i=0}^{N} J_{e}^{(1)}(i, l) F_{i l}^{1} D_{i k}^{(1)} w_{i} w_{l}+\sum_{i=0}^{N} J_{e}^{(2)}(k, i) F_{k i}^{2} D_{l i}^{(2)} w_{k} w_{i} \\
S_{k l}^{e} & =J_{e}(k, l) w_{k} w_{l} S\left(U_{k l}\right)
\end{aligned}
$$

where $J_{e}^{(i)}=J_{e} \partial \xi^{i} / \partial x^{i}$ is the metric term and $D_{l k}^{(i)}$ is the derivative matrix $h_{k}^{\prime}\left(\xi_{l}^{i}\right)$, along the $x^{i}$-direction and $i \in\{1,2\}$.

## Story so far: solving equations of motion on each element



Physical Domain

Nodal 1D polynomial basis functions



Computational Domain


GLL Quadrature Grid

## Story so far: solving equations of motion on each element


(a)


Coupling solutions across elements
(b)


Advance solution in each element one Runge Kutta step

## Coupling solutions across elements


(c)


Global C ${ }^{0}$ polynomial
where DSS refers to Direct Stiffness Summation (also referred to as assembly or inverse mass matrix step).

- Choice of GLL quadrature based inner product and nodal basis functions gives a diagonal mass matrix (Maday and Patera, 1987).

Specification of resolution in CAM: number of GLL points is always $4 \times 4$ in each element Number of elements determines resolution


## Specification of resolution in CAM:

 number of GLL points is always $4 \times 4$ in each element Number of elements determines resolution

## Properties of the SE method

A numerical method is mimetic (or compatible) if key integral properties of divergence, gradient and curl-operators are mimicked in discretized space. The CAM-SE discretization satisfies the divergence/gradient adjoint relation

```
In the floating Lagrangian
layer CAM-SE
conserves total energy to
time truncation errors
and conserves mass
\[
\int \phi \nabla \cdot \mathbf{v} d \mathcal{S}+\int \mathbf{v} \cdot \nabla \phi d \mathcal{S}=0
\]
```

in discretized space [Taylor and Fournier, 2010]. This property can be used to show the inherent conservation properties of CAM-SE in terms of mass and energy in the horizontal discretization. This is discussed in detail in Taylor [2011] and hence not repeated here.

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## Time-stepping ( $\mathbf{u}, \mathbf{v}, \mathbf{T}, \mathbf{d M}{ }^{(d)}$ )

## The Kinnmark-Gray 5-stage 3rd-order Runge-Kutta scheme

The thermodynamic equation, momentum equations and dry air-mass continuity equation in CAM-SE are evolved using the 5-stage 3rd-order Runge-Kutta scheme described in Guerra and Ullrich [2016, see their equation (56)]. The stability of this class of time-stepping schemes is discussed in Dubos et al. [2015, see their section 3.4]. For a given initial state vector at timestep $n, \vec{\Lambda}^{(0)}=\vec{\Lambda}^{n}$, the updated state vector $\vec{\Lambda}^{(5)}=\vec{\Lambda}^{n+1}$ is computed as follows:

$$
\begin{aligned}
& \vec{\Lambda}^{(1)}=\vec{\Lambda}^{(0)}+\frac{\Delta t}{5} \vec{\Upsilon}\left(\vec{\Lambda}^{(0)}\right), \\
& \vec{\Lambda}^{(2)}=\vec{\Lambda}^{(0)}+\frac{\Delta t}{5} \vec{\Upsilon}\left(\vec{\Lambda}^{(1)}\right), \\
& \vec{\Lambda}^{(3)}=\vec{\Lambda}^{(0)}+\frac{\Delta t}{3} \vec{\Upsilon}\left(\vec{\Lambda}^{(2)}\right), \\
& \vec{\Lambda}^{(4)}=\vec{\Lambda}^{(0)}+\frac{2 \Delta t}{3} \vec{\Upsilon}\left(\vec{\Lambda}^{(3)}\right), \\
& \vec{\Lambda}^{(5)}=-\frac{1}{4} \vec{\Lambda}^{(0)}+\frac{5}{4} \vec{\Lambda}^{(1)}+\frac{3 \Delta t}{4} \vec{\Upsilon}\left(\vec{\Lambda}^{(4)}\right),
\end{aligned}
$$

where $\vec{\Upsilon}(\vec{\Lambda})$ denotes the discrete right-hand-side terms of the equations of motion. The resulting method is linearly and non-linearly third-order accurate.

## Time-stepping ( $\left.\mathbf{u}, \mathbf{v}, \mathbf{T}, \mathbf{d M} \mathbf{M}^{(d)}\right)$

The scheme possesses a stability region which is provably optimal in terms of its extent along the imaginary axis among all 5-stage 3rd-order Runge-Kutta schemes, $[-i \sqrt{15}, i \sqrt{15}]$. Since the largest eigenvalue of the 1D 4th-order spectral element spatial discretization $\left(N_{p}=4\right)$ is $i \sqrt{10 / 3}$, the resulting scheme satisfies a Courant-Friedrichs-Lewy condition given by

$$
\frac{c \Delta t}{\Delta x} \leq \frac{3}{\sqrt{2}}, \quad(1 \mathrm{D} \text { condition })
$$

where $\Delta x$ denotes the average distance between degrees of freedom (equal to $3 \times \Delta x_{e}$, the width of a spectral element), $c$ is the gravity wave speed, and $\Delta t$ is the timestep size. As dimension splitting is not employed in CAM-SE, in 2D and on a uniformly spaced grid this condition is restricted by a further factor of $1 / \sqrt{2}$ to

$$
\frac{c \Delta t}{\Delta x} \leq \frac{3}{2}, \quad \text { (2D condition). }
$$

## Time-stepping (tracers)

- Continuity equation for air is coupled with momentum and thermodynamic equations:
- thermodynamic variables and other prognostic variables feed back on the velocity field
- which, in turn, feeds back on the solution to the continuity equation.
- Hence the continuity equation for air can not be solved in isolation and one must obey the maximum allowable time-step restrictions imposed by the fastest waves in the system.
- The tracer transport equation can be solved in isolation given prescribed winds and air densities, and is therefore not susceptible to the time-step restrictions imposed by the fastest waves in the system.
- For efficiency: Use longer time-step for continuity equation for tracers than for air.


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- The tracer transport equation can be solved in isolation given prescribed winds and air densities, and is therefore not susceptible to the time-step restrictions imposed by the fastest waves in the system.
- For efficiency: Use longer time-step for continuity equation for tracers than for air.

The SE tracer advection algorithm uses a three-stage RK strong-stability-preserving (SSP) time-stepping method, ensuring the time step will preserve any shape-preserving properties preserved by the underlying spatial discretization [Spiteri and Ruuth, 2002]. The shape-preserving filter used is described in Guba et al. [2014b]. The shape-preserving SE tracer advection algorithm is formally second-order accurate.

## Time-steps in CAM-SE



## Time-steps in CAM-SE

$$
\begin{aligned}
\Delta t_{\text {remap }} & =\frac{\Delta t_{\text {phys }}}{\text { se_nsplit }}, \\
\Delta t_{\text {tracer }} & =\frac{\Delta t_{\text {phys }}}{\text { se_nsplit } * \text { se_qsplit }}, \\
\Delta t_{\text {dyn }} & =\frac{\Delta t_{\text {phys }}}{\text { se_nsplit } * \text { se_rsplit } * \text { se_qsplit }}, \\
\Delta t_{\text {hyper }} & =\frac{\Delta t_{\text {phys }}}{\text { se_nsplit } * \text { se_rsplit } * \text { se_hypervis_subcycle } * \text { se_qsplit }}
\end{aligned}
$$

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## Physics dynamics coupling methods in CAM-SE: se_ftype=1



## 10 year average of $\frac{d}{d t}\left|p_{s}\right|$ from AMIP run



## Physics dynamics coupling methods in CAM-SE: se_ftype=0

Advance dynamics core ( 30 minutes): add physics tendency "chunks" during the dynamics time-stepping - every 15 minutes in this example (I refer to it as "dribbling")


Compute physics tendencies based on dynamics updated state

Split physics tendencies into a number of "chunks"

## Physics dynamics coupling methods in CAM-SE: se_ftype=1

$\mathbf{1 0}$ year average of $\frac{d}{d t}\left|p_{s}\right|$ from AMIP run


## Physics dynamics coupling methods in CAM-SE: se_ftype=1

## 10 year average of $\frac{d}{d t}\left|p_{s}\right|$ from AMIP run



## Physics-dynamics coupling: "dribbling" tendencies



Physics-dynamics coupling: "dribbling" tendencies


Physics-dynamics coupling: "dribbling" tendencies


Physics-dynamics coupling: "dribbling" tendencies


## Physics-dynamics coupling: "dribbling" tendencies



## Physics-dynamics coupling: "dribbling" tendencies

Example from fully coupled climate model: water conservation errors



## Physics dynamics coupling methods in CAM-SE: se_ftype=2

Advance dynamics core ( 30 minutes): for ( $\mathbf{u}, \mathbf{v}, \mathbf{T}$ ) add physics tendency "chunks" during the dynamics timestepping - every 15 minutes in this example (I refer to it as "dribbling")


Compute physics tendencies based on dynamics updated state

Split physics tendencies into a number of "chunks" for $\mathbf{u}, \mathbf{v}, \mathbf{T}$
Update tracer state with physics tendencies

Instantaneous PSL for CAM-SE at approximately $\mathbf{1} \mathbf{4}$ degree horizontal resolution
ftype $=2$
ftype $=1$


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## Computation throughput (ne30 ~ 1 degree)




## Computation throughput (ne30 ~ 1 degree)




Data produced by John Dennis (CISL)

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## Variable horizontal resolution

- One of the advantages of the spectral-element method is that it can relatively easily be adapted to variable resolution meshes (as long as elements are quadrilateral)

A direct way to address this problem is establishing a transformation $\mathcal{J}_{e}: \Omega_{e} \rightarrow[-1,1]^{2}$, where $\mathcal{J}_{e}$ may be considered as a composite mapping combining the gnomonic and the quadrilateral to standard-element mapping. Let the Jacobian associated with the composite mapping be $J_{e}=J_{e}(\sqrt{G})$. Then an arbitrary surface integral on $\Omega_{e}$ can be expressed in terms of local coordinates $\xi^{1}, \xi^{2} \in[-1,1]$ and the Jacobian $J_{e}$

$$
\begin{equation*}
\int_{\Omega_{e}} \psi\left(x^{1}, x^{2}\right) d \Omega_{e}=\int_{-1}^{1} \int_{-1}^{1} J_{e}\left(\xi^{1}, \xi^{2}\right) \psi\left(\xi^{1}, \xi^{2}\right) d \xi^{1} d \xi^{2} \approx \sum_{k=0}^{N} \sum_{l=0}^{N} w_{k} w_{l} J_{e}\left(\xi_{k}^{1}, \xi_{l}^{2}\right) \psi\left(\xi_{k}^{1}, \xi_{l}^{2}\right), \tag{80}
\end{equation*}
$$

where $w_{k}, w_{l}$ are the Gauss quadrature weights.



## Challenges: diffusion

CAM-SE, Zarzycki et al., 2014, JClim


Let's say 100 km cell is our "reference" and $\mathrm{y}=$ 3.321
$\left(\frac{50}{100}\right)^{3.321}=\frac{1}{10}$
Our diffusion coefficient $\left(\mathrm{K}_{4}\right)$ in the 50 km box is $1 / 10^{\text {th }}$ that of 100 km box!

## V-R applications: tropical cyclones



V-Rap andications: tropical

## cyclones

- Community $\underline{A} t m o s p h e r e ~ M o d e l ~ S p e c t r a l ~ E l e m e n t ~(C A M-~$ SE)
- Atmospheric Model Intercomparison Project (AMIP) protocols
- 1980-2002 (23 years)
- Prescribed SSTs, ozone, aerosols, solar insolation
- Simulate historic, observed climate



## Uniform global simulation



## Variable-resolution global circulation



Precipitable water, Sept 1-16

## Tropical cyclones



## Numerical weather prediction

- 8 day forecast $=\sim 1.5$ hours of wall clock time on 800 cores (NCAR Yellowstone)
- $6-7 x$ cheaper than a globally-uniform 13 km forecast



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