Some Applications of HOMs

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Overview:

- Preconditioning: Optimized Schwarz for climate modeling
- Adaptive mesh refinements (on the sphere)
- Efficient time-stepping for AMR and SEM
- Discontinuous Galerkin for non-hydrostatic modeling

Classical Schwarz

Suppose we need to solve:

 $\mathcal{L}u = f$ in Ω , $\mathcal{B}u = g$ on $\partial \Omega$ Partition the original domain into 2 $\begin{array}{rcl} \mathcal{L}u_1^{n+1} &=& f & \text{in } \Omega_1, & \mathcal{L}u_2^{n+1} &=& f & \text{in } \Omega_2, \\ \mathcal{B}(u_1^{n+1}) &=& g & \text{on } \partial\Omega_1, & \mathcal{B}(u_2^{n+1}) &=& g & \text{on } \partial\Omega_2, \\ u_1^{n+1} &=& u_2^n & \text{on } \Gamma_{12}, & u_2^{n+1} &=& u_1^n & \text{on } \Gamma_{21}. \end{array}$

The Robin method

- ✤ Lions (1990)
- Used to accelerate convergence of Schwarz
- Free positive parameter: how to find its correct value?
 Convergence rate not demonstrated theoretically

$$\mathcal{L}u_{j}^{k+1} = u_{j}^{k+1} - \Delta u_{j}^{k+1} = f_{j}$$

$$pu_{j}^{k+1} + \frac{\partial u_{j}^{k+1}}{\partial \mathbf{n}_{jl}} = pu_{l}^{k} + \frac{\partial u_{l}^{k}}{\partial \mathbf{n}_{jl}} \text{ on } \partial\Omega_{j} \cap \partial\Omega_{l} \text{ for } l \in \mathcal{N}(\Omega_{j})$$

$$u_{j}^{k+1} = u_{0} \text{ on } \partial\Omega_{j} \cap \partial\Omega$$

Optimized approach

Inspired by the Robin problem:

 $(\eta - \Delta)u_1^{n+1} = 0 \quad \text{in } \Omega_1, \quad (\eta - \Delta)u_2^{n+1} = 0 \quad \text{in } \Omega_2, \\ (\partial_x + S_1)u_1^{n+1} = (\partial_x + S_1)u_2^n \quad \text{on } \Gamma_{12}, \quad (\partial_x + S_2)u_2^{n+1} = (\partial_x + S_2)u_1^n \quad \text{on } \Gamma_{21}. \end{cases}$ We are looking for the best possible forms of in Fourier space Proceeding as before leads to the solutions: $(\sigma_r(k) = \mathcal{F}(S_r))$ $\hat{u}_1^n(x,k) = \frac{\sigma_1(k) - \sqrt{k^2 + \eta}}{\sigma_1(k) + \sqrt{k^2 + \eta}} e^{-\sqrt{k^2 + \eta}(x-L)} \hat{u}_2^{n-1}(L,k), \quad \hat{u}_2^n(x,k) = \frac{\sigma_2(k) + \sqrt{k^2 + \eta}}{\sigma_2(k) - \sqrt{k^2 + \eta}} e^{-\sqrt{k^2 + \eta}x} \hat{u}_1^{n-1}(0,k)$

New convergence rate:

$$\rho_{opt} = \rho_{opt}(k,\eta,L) = \frac{\sigma_1(k) - \sqrt{k^2 + \eta}}{\sigma_1(k) + \sqrt{k^2 + \eta}} \frac{\sigma_2(k) + \sqrt{k^2 + \eta}}{\sigma_2(k) - \sqrt{k^2 + \eta}} e^{-2\sqrt{k^2 + \eta}L}$$

Optimized Schwarz: algebraic results

- SGT 2006: show how to modify existing Schwarz algorithm to yield optimized versions
- The augmented or "enhanced" system is rediscovered
- Spectral elements are natural candidates:
 - Overlapping grids are cumbersome to construct
 - Block preconditioning costly: FDM when possible
 - Optimal preconditioner is known (SD Kim 2006)
 - Q1-GLL based problem costly to invert does not scale: use MG or other solver to invert

Consider:

$$w_j^{k+1} - \Delta w_j^{k+1} = G_j(x, y)$$

$$pw_j^{k+1} + \frac{\partial w_j^{k+1}}{\partial \mathbf{n}_{jl}} = pw_l^k + \frac{\partial w_l^k}{\partial \mathbf{n}_{jl}} \text{ on } \partial\Omega_j \cap \partial\Omega_l \text{ for } l \in \mathcal{N}(\Omega_j)$$

$$w_j^{k+1} = w_0 \text{ on } \partial\Omega_j \cap \partial\Omega$$

To be solved for all k on any Ω_j : it converges (Lions 1990). Weak form:

$$\int_{\Omega_j} \phi_j w_j^{k+1} + \int_{\Omega_j} \nabla \phi_j \cdot \nabla w_j^{k+1} - \int_{\partial \Omega_j} \phi_j \left(\frac{\partial w_j}{\partial \mathbf{n}}\right)^{k+1} = \int_{\Omega_j} \phi_j G_j.$$

Where test functions are in:

$$H^{1}(\mathcal{Q}_{h}) = \{ v \in L^{2}(\Omega) | v|_{Q} \in H^{1}(Q) \ \forall Q \in \mathcal{Q}_{h} \}$$

ecomposition: $\mathcal{Q}_{h} = \cup_{j} \Omega_{j}$

Define:

$$a_{j}(w_{j}^{k+1},\phi_{j}) \equiv \int_{\Omega_{j}} \phi_{j} w_{j}^{k+1} + \int_{\Omega_{j}} \nabla \phi_{j} \cdot \nabla w_{j}^{k+1}$$
$$f_{j}(\phi_{j}) \equiv \int_{\Omega_{j}} \phi_{j} G_{j}$$
$$T_{j}(w_{j}^{k+1},\phi_{j}) \equiv \sum_{l \in \mathcal{N}(\Omega_{j})} \int_{\Gamma_{jl}} \phi_{j} \left(\frac{\partial w_{j}}{\partial \mathbf{n}_{jl}}\right)^{k+1}$$

Leads to:

 $a_j(w_j^{k+1}, \phi_j) - T_j(w_j^{k+1}, \phi_j) = f_j(\phi_j)$

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Leads to:

 $a_j(w_j^{k+1}, \phi_j) - T_j(w_j^{k+1}, \phi_j) = f_j(\phi_j)$

Remains to introduce the artificial transmission condition...

The normal derivative can be written in terms of the original bilinear operator (Toselli, Widlund 2005)

Avoids the difficult duality pairing for functions on the edges of the subdomains $T_j(w_j^{k+1}, \phi_j) = \int_{\Omega_j} \nabla \phi_j \cdot \nabla w_j^{k+1} + \int_{\Omega_j} \phi_j \Delta w_j^{k+1}$ $= \int_{\Omega_j} \nabla \phi_j \cdot \nabla w_j^{k+1} + \int_{\Omega_j} \phi_j w_j^{k+1} - f_j(\phi_j)$ $= a_j(w_j^{k+1}, \phi_j) - f_j(\phi_j)$

Where we pick $\phi_j \in H^1(\partial \Omega_j)$

Boundary condition is:

T

$$\begin{split} T_{j}(w_{j}^{k+1},\phi_{j}) &= \sum_{l \in \mathcal{N}(\Omega_{j})} T_{j}(w_{j}^{k+1},\phi_{j}|_{\Gamma_{jl}}) \\ &= \sum_{l \in \mathcal{N}(\Omega_{j})} \{ \int_{\Gamma_{jl}} p\phi_{j}(w_{l}^{k}-w_{l}^{k+1}) - T_{l}(w_{l}^{k},\phi_{j}|_{\Gamma_{jl}}) \} \\ &= -\int_{\Omega_{j}} p\phi_{j}w_{j}^{k+1} + \sum_{l \in \mathcal{N}(\Omega_{j})} \{ \int_{\Gamma_{jl}} p\phi_{j}w_{l}^{k} - T_{l}(w_{l}^{k},\phi_{j}|_{\Gamma_{jl}}) \} \end{split}$$

where a sum on neighbors appears.

Boundary condition is:

$$\begin{split} \Gamma_{j}(w_{j}^{k+1},\phi_{j}) &= \sum_{l \in \mathcal{N}(\Omega_{j})} T_{j}(w_{j}^{k+1},\phi_{j}|_{\Gamma_{jl}}) \\ &= \sum_{l \in \mathcal{N}(\Omega_{j})} \{ \int_{\Gamma_{jl}} p\phi_{j}(w_{l}^{k}-w_{l}^{k+1}) - T_{l}(w_{l}^{k},\phi_{j}|_{\Gamma_{jl}}) \} \\ &= -\int_{\Omega_{j}} p\phi_{j}w_{j}^{k+1} + \sum_{l \in \mathcal{N}(\Omega_{j})} \{ \int_{\Gamma_{jl}} p\phi_{j}w_{l}^{k} - T_{l}(w_{l}^{k},\phi_{j}|_{\Gamma_{jl}}) \} \end{split}$$

where a sum on neighbors appears.

Leads to the form required by the algorithm

$$a_j(w_j^{k+1}, \phi_j) + \int_{\Omega_j} p\phi_j w_j^{k+1} = f_j(\phi_j) + \sum_{l \in \mathcal{N}(\Omega_j)} f_l(\phi_l|_{\Gamma_{jl}})$$
$$- \sum_{l \in \mathcal{N}(\Omega_j)} a_l(w_l^k, \phi_l|_{\Gamma_{jl}}) + \sum_{l \in \mathcal{N}(\Omega_j)} \int_{\Gamma_{jl}} p\phi_l w_l^k$$

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$$\tilde{A}_j \boldsymbol{u}_j^{n+1} = \boldsymbol{f}_j + \sum_{k=1}^J \tilde{B}_{jk} \boldsymbol{u}_k^n, \quad j = 1, .., J$$

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After (any)

$$\downarrow
\widetilde{A}_j \boldsymbol{u}_j^{n+1} = \boldsymbol{f}_j + \sum_{k=1}^J \widetilde{B}_{jk} \boldsymbol{u}_k^n, \quad j = 1, .., J$$

$$a_{j}(w_{j}^{k+1},\phi_{j}) + \int_{\Omega_{j}} p\phi_{j}w_{j}^{k+1} = f_{j}(\phi_{j}) + \sum_{l \in \mathcal{N}(\Omega_{j})} f_{l}(\phi_{l}|_{\Gamma_{jl}}) \\ - \sum_{l \in \mathcal{N}(\Omega_{j})} a_{l}(w_{l}^{k},\phi_{l}|_{\Gamma_{jl}}) + \sum_{l \in \mathcal{N}(\Omega_{j})} \int_{\Gamma_{jl}} p\phi_{l}w_{l}^{k} \\ J \\ J \\ \tilde{A}_{j}\boldsymbol{u}_{j}^{n+1} = \boldsymbol{f}_{j} + \sum_{l \in \mathcal{N}(\Omega_{j})} \tilde{B}_{jk}\boldsymbol{u}_{k}^{n}, \quad j = 1, ..., J$$

k=1

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$$a_j(w_j^{k+1}, \phi_j) + \int_{\Omega_j} p\phi_j w_j^{k+1} = f_j(\phi_j) + \sum_{l \in \mathcal{N}(\Omega_j)} f_l(\phi_l|_{\Gamma_{jl}})$$
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Possible to create augmented system!

$$a_j(w_j^{k+1}, \phi_j) + \int_{\Omega_j} p\phi_j w_j^{k+1} = f_j(\phi_j) + \sum_{l \in \mathcal{N}(\Omega_j)} f_l(\phi_l|_{\Gamma_{jl}})$$
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Possible to create augmented system! Not mentioned: difficulties at corners

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Possible to create augmented system! Not mentioned: difficulties at corners Not mentioned: "under" integration for SEM

SEM simple problem

 $\mathcal{L}u = (\eta - \Delta)u = f, \text{ in } \Omega,$

Gander 2006



SEM simple problem



SEM simple problem



Primitive equations

Momentum: $\frac{d\mathbf{v}}{dt} + f\mathbf{k} \times \mathbf{v} + \nabla\Phi + R T \nabla \ln p = 0$

Thermodynamic:

$$\frac{d\,T}{d\,t} - \frac{\kappa\,T\,\omega}{p} = 0$$

Continuity: $\frac{\partial}{\partial t} \left(\frac{\partial p}{\partial \eta} \right) + \nabla \cdot \left(\mathbf{v} \frac{\partial p}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \left(\dot{\eta} \frac{\partial p}{\partial \eta} \right) = 0$

HOMME: high order multiscale modeling environment

Primitive equations: SI

Hydrostatic assumption: $\frac{\partial \Phi}{\partial n} = -\frac{RT}{p} \frac{\partial p}{\partial n}$.

Linearization (barotropic state): $T^r = 300K$, $p_s^r = 1000hPa$ Semi-Implicit:

$$\frac{dX}{dt} = \mathcal{M}(X)$$

Add zero: $\frac{dX}{dt} = \mathcal{M}(X) + \mathcal{L}X - \mathcal{L}X = \mathcal{N}(X) - \mathcal{L}X$

 $\frac{X^{n+1} - X^{n-1}}{2\Delta t} = \mathcal{N}(X^n) - \frac{1}{2}\mathcal{L}(X^{n+1} + X^{n-1}) = \mathcal{M}(X^n) + \mathcal{L}X^n - \frac{1}{2}\mathcal{L}(X^{n+1} + X^{n-1})$ $\frac{X^{n+1} - X^{n-1}}{2\Delta t} = \mathcal{M}(X^n) - \frac{1}{2}\Delta_{tt}\mathcal{L}X$ "Time diffusion"

PE: vertical structure matrix

Backsub:

 $D = \Delta t^{-1} \mathbf{A}^{-1} (B - G^r)$

 $\ln p_s = \mathcal{P} - \Delta t P \cdot D$

Results of hydrostatic assumption and vertical coordinate choice: $p(\eta, p_s) = A(\eta)p_0 + B(\eta)p_s$

 $\mathbf{A} = R\mathbf{H}^{r}\mathbf{T} + RT^{r}P,$ $G^{r} - \Delta t^{2}\mathbf{A}\nabla^{2}G^{r} = B - \Delta t\mathbf{A}\nabla \cdot \mathcal{V}$

Solve for each k:

$$\left(\nabla^2 - \frac{1}{\Delta t^2 \lambda_k}\right) \Gamma_k^r = C_k$$

 $\begin{array}{rcl} T &=& \mathcal{T} - \Delta t \, \mathbf{T} D \\ \text{Series of 2D Helmholtz} & \mathbf{v} &=& \mathcal{V} - \Delta t \, \nabla G^r \\ \text{Barotropic eigenmodes of atmosphere} \end{array}$

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 $\mathbf{A} = R\mathbf{H}^{r}\mathbf{T} + RT^{r}P, \qquad \qquad \text{Diagonalize}$ $G^{r} - \Delta t^{2}\mathbf{A}\nabla^{2}G^{r} = B - \Delta t\mathbf{A}\nabla \cdot \mathcal{V}$

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Cubed sphere

- ✤ Equiangular projection
- Sadourny (72), Rancic
 (96), Ronchi (96)
- Most models moving towards this approach
- SFC: Dennis 2003

Metric tensor

 $g_{ij} = \frac{1}{r^4 \cos^2 x_1 \cos^2 x_2} \begin{bmatrix} 1 + \tan^2 x_1 & -\tan x_1 \tan x_2 \\ -\tan x_1 \tan x_2 & 1 + \tan^2 x_2 \end{bmatrix}.$ Rewrite div and vorticity $g \nabla \cdot \mathbf{v} = \frac{\partial}{\partial x^j} (g u^j), \quad g \zeta = \epsilon_{ij} \frac{\partial u_j}{\partial x^i}.$



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Held-Suarez numerical experiment: with moisture



Galewski, Sobel and Held 2004

Convergence per mode



- Optimized algorithm: no maxing out
- Communication cost identical
- Twice the cost of CG per iteration
- → Diagonal O(N) while OS is $O(N^3)$
- Best strategy: use OS on first few barotropic modes and diagonal elsewhere
- No coarse solver needed: because of time dependance

Diagonal preconditioning



Optimized Schwarz



New approach

New approach

New approach

Large scale runs

Si vs Exp: Red Storm



Si vs Exp: Blue gene

ne=32, 40km

Si vs Exp: Blue gene



ne=32, 40km

Adaptive Mesh Refinements

Conforming SEM



Linear problem associated with elliptic problem discretized with SEM Au = f $A_L = block\{A_1, A_2, A_3, A_4\}$

 $v^{T}Au = v^{T}Q^{T}A_{L}Qu = v^{T}Q^{T}M_{L}Qf = v^{T}f$ $A_{k} \qquad v^{T}Q^{T}A_{L}u_{L} = v^{T}Q^{T}M_{L}f_{L}$ $QQ^{T}A_{L}u_{L} = QQ^{T}M_{L}f_{L}$

Conforming SEM



Linear problem associated with elliptic problem discretized with SEM Au = f $A_L = block\{A_1, A_2, A_3, A_4\}$

 $v^T Q^T A_L u_L = v^T Q^T M_L f_L$

 $QQ^T A_L u_L = QQ^T M_L f_L$

 $v^T A u = v^T Q^T A_L Q u = v^T Q^T M_L Q f = v^T f$

Direct stiffness summation: represents boolean operations



SEM vs FVM



Standard test suite is employed

Cosine bell advection Alpha = 0

SEM

Resolution	l_1	l_2	l_∞	$h(m) \max/\min$	Resolution	l_1	l_2	l_∞	$h(m) \max/\min$
2.5	0.0341	0.0301	0.0317	949.1/0	2.5	0.0503	0.0269	0.0195	991.6/-15.1
1.25	0.0097	0.0103	0.0150	984.2/0	1.25	0.0085	0.0056	0.0057	997.5/-4.2
0.625	0.0016	0.0021	0.0044	995.0/0	0.625	0.0019	0.0014	0.0019	999.1/-1.1
0.3125	0.0003	0.0005	0.0014	998.4/0	0.3125	0.0008	0.0006	0.0015	999.7/-0.9

For alpha different than 0 : FV has undershoots

Conservation of mass breaks monotonicity

FV



SWTC1 45 degrees





SWTC5







SWTC5





SWTC6



Time-stepping

OIFS+AMR

- Goal: SEM based AMR for primitive equations
- Oliger and Sundstrom show ill posedness for any kind of boundary conditions
- Scannot use local time stepping: Berger Oliger (84)
- Semi-implicit semi-Lagrangian approach?(Robert 81)

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- Oliger and Sundstrom show ill posedness for any kind of boundary conditions
- <u>Cannot use local time stepping</u>: Berger Oliger (84)
- Semi-implicit semi-Lagrangian approach?(Robert 81)
- SISL is rather inefficient on modern computers
- ✤ Attempts were made by Berhens: shmem only (96)

$$\frac{d\phi(X,t)}{dt} = \frac{\partial\phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = f(\phi(X,t))$$

- Material derivative (hide advective term)
- Spatial position is now a function of time in the Lagrangian frame

Characteristic $\frac{dX}{dt} = u(X, t)$

 $X^{n} = X^{n+1} - \frac{\Delta t}{2} (\mathbf{u}(X^{n}, t^{n}) + \mathbf{u}(X^{n+1}, t^{n+1})), \text{ with } X(t^{n+1}) = x$







- Operator integrating factor splitting
 Maday, Patera, Ronquist (90): OIFS.
- Kelements of order N, KN^d grid points
 Interpolation KN^{2d}
- \sim Scalar advection requires dKN^{d+1}
- \sim OIFS more efficient if sub-step $< N^{d-1}$ "times"
- Purely Eulerian: regular communication patterns
- Nonlinear OIFS: St-Cyr and Thomas (05)
- ∞ Euler (MC2): Girard, Thomas and St-Cyr (07)

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 $t^n + \Delta t$



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 $t^n + \Delta t$



 $t^n + \Delta t$



ODE resulting from SEM discretization (MOL)

$$\frac{du(t)}{dt} = S(u(t)) + F(u(t)), \quad t \in [0, T]$$

with initial condition $u(0) = u_0$

<u>Problem</u>: find integrating factor, $Q_S^{t^*}(t)$ such that $Q_S^{t^*}(t^*) = I$,

$$\frac{d}{dt}Q_S^{t^*}(t) \cdot u = Q_S^{t^*}(t) \cdot F(u).$$

To find the action of $Q_S^{t^*}(t)$ solve:

W

$$\frac{dv^{(t^*,t)}(s)}{ds} = S(v^{(t^*,t)}), \quad 0 \le s \le t-t^*$$

th initial condition $v^{(t^*,t)}(0) = u(t)$

Nonlinear OIFS

St-Cyr and Thomas (2005) sub-step

$$\frac{\partial \tilde{\mathbf{v}}}{\partial s} + \tilde{\zeta} \mathbf{k} \times \tilde{\mathbf{v}} + \frac{1}{2} \nabla \left(\tilde{\mathbf{v}} \cdot \tilde{\mathbf{v}} \right) = 0$$
$$\frac{\partial \tilde{\Phi}}{\partial s} + \nabla \cdot \left(\tilde{\Phi} \tilde{\mathbf{v}} \right) = 0$$

with initial conditions $\tilde{\mathbf{v}}(\mathbf{x}, t^{n-q}) = \mathbf{v}(\mathbf{x}, t^{n-q})$, $\tilde{\Phi}(\mathbf{x}, t^{n-q}) = \Phi(\mathbf{x}, t^{n-q})$.

Nonlinear OIFS

Integration factor applied to the SWE's

$$\frac{d}{dt}Q_{S}^{t^{*}}(t)\begin{bmatrix}\mathbf{v}\\\Phi\end{bmatrix} = -Q_{S}^{t^{*}}(t)\begin{bmatrix}f\,\mathbf{k}\times\mathbf{v}+\nabla\Phi\\\Phi_{0}\,\nabla\cdot\mathbf{v}\end{bmatrix}$$

Backward Differentiation Formula (BDF-2):

Terms responsible for



Non-symmetric due to implicit Coriolis: CGS.

Implicit/Explicit


















Implicit/Explicit



dt=120s





dt=360s





dt=720s





dt=120s





Total number of elements



Comparison with reference solution from NCAR pseudo spectral



Comparison with reference solution from NCAR pseudo spectral



Discontinuous Galerkin

Conservation law:

$$u_t + \nabla \cdot \mathcal{F}(u) = S(u)$$

Weak form:

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_k} \varphi_h u_h \, d\Omega &= \int_{\Omega_k} \varphi_h S(u_h) \, d\Omega + \int_{\Omega_k} \mathcal{F}(u_h) \cdot \nabla \varphi_h \, d\Omega - \int_{\partial \Omega_k} \varphi_h \mathcal{F} \cdot \hat{n} \, ds \\ \text{Numerical flux:} \\ \widehat{\mathcal{F}}(u_h^+, u_h^-) &= \frac{1}{2} \left[\left(\mathcal{F}(u_h^+) + \mathcal{F}(u_h^-) \right) \cdot \hat{n} - \alpha (u_h^+ - u_h^-) \right] \end{aligned}$$

SSP Runge-Kutta with extended linear stability region

$$\frac{d\mathbf{U}_h}{dt} = \mathbf{L}_{\mathbf{h}}(\mathbf{U}_h).$$



Higueras 2004, JSC

Compressible Euler:

 $\underline{\mathbf{U}} \equiv (\rho, \rho u, \rho w, \Theta)^T = (\rho, U, W, \Theta)^T$ $\mathbf{F}(\underline{\mathbf{U}}) \equiv (F,G)$ $F = (U, \frac{UU}{\rho} + p, \frac{WU}{\rho}, \frac{U\Theta}{\rho})^T$ $G = (W, \frac{UW}{\rho}, \frac{WW}{\rho} + p, \frac{W\Theta}{\rho})^T$ $S(\underline{\mathbf{U}}) = (0, 0, -g\rho, 0)^T$ $p = p_0 \left(\frac{R\Theta}{p_0}\right)^{\gamma}$

Warm bubble (Robert 93)



To use or not to use HOMs?

Low order: 2nd or 3rd

- Very dissipative
- ✤ Large dispersion error
- Oscillation control: grid point level
- Limiters not cache efficient
- \sim CFL: dt = O(dx)
- ✤ Costly halos...

- Spectrally accurate
- ✤ No dissipation
- No dispersion error: with filtering
- Oscillation control: questionable
- Matrix-Matrix tensor operations: cache friendly
- ✤ Halos are minimal

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