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Lagrange-Multiplier-Based Partitioned Method for Ocean-Atmosphere Coupling

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Kara Peterson, Pavel Bochev, Paul Kuberry, Nat Trask

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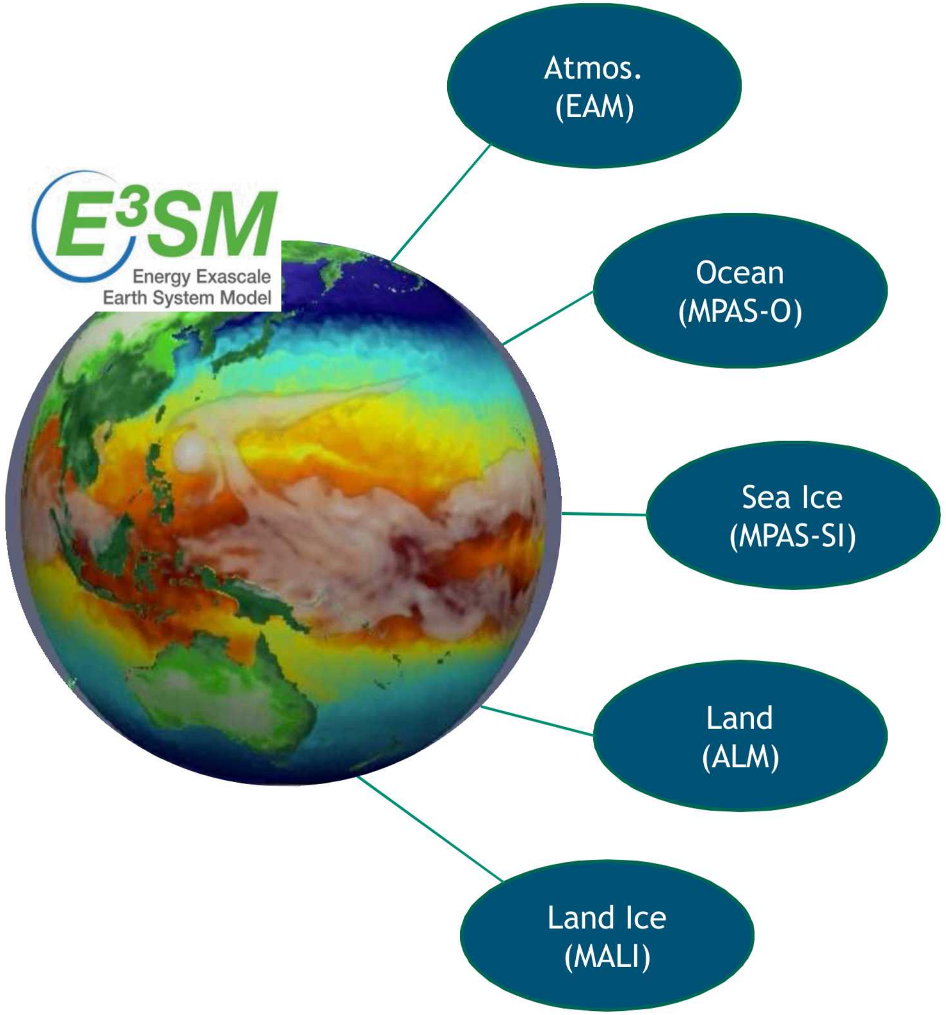
MOTIVATION

CANGA
Coupling Approaches
for Next Generation
Architectures

Earth System Model Coupling

- ESMs include multiple components for the ocean, atmosphere, ice, etc.
- Coupled problem is a complex multi-physics, multiscale problem
- Monolithic solutions of the coupled problem not computationally feasible
- Need stable and accurate methods for partitioned solves

- *Challenges*:
  - Non-conforming grids
  - Independent discretizations
  - Flux conservation and property preservation
  - Stability over long integration times



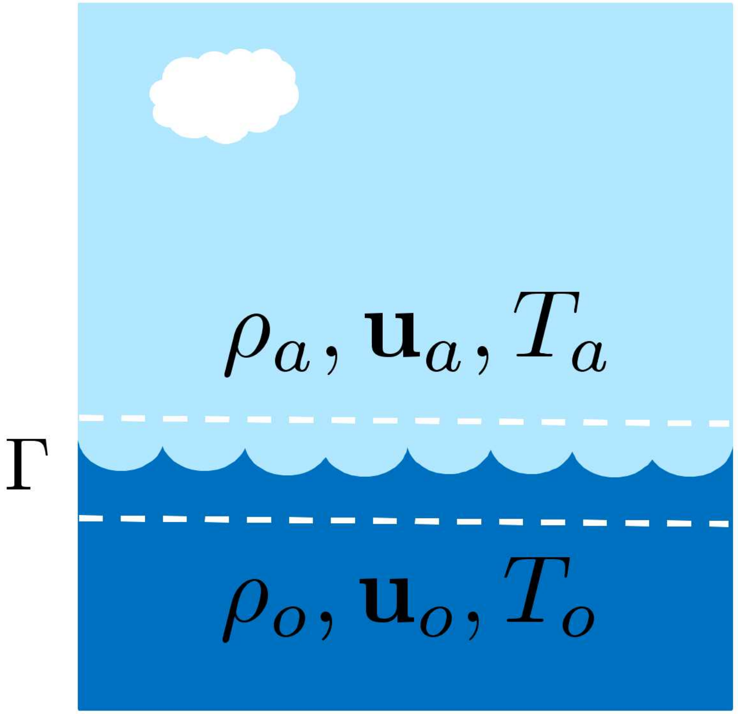
OCEAN-ATMOSPHERE COUPLING

- Consider partial differential equations for atmosphere and ocean circulation with state variables velocity and temperature
- Ocean-atmosphere fluxes are defined by a parameterization of the surface layers: “bulk” formulation
- Coupling conditions

$$\rho_a \nu_a \frac{\partial \mathbf{u}_a}{\partial z} = \rho_o \nu_o \frac{\partial \mathbf{u}_o}{\partial z} = \boldsymbol{\tau} \quad \text{on } \Gamma$$

$$\rho_a K_a \frac{\partial T_a}{\partial z} = \rho_o K_o \frac{\partial T_o}{\partial z} = Q_{net} \quad \text{on } \Gamma$$

$$\boldsymbol{\tau} = \rho_a C_\tau \| [\![\mathbf{u}]\!] \| [\![\mathbf{u}]\!] \quad Q_{net} = \mathcal{R} + \rho_a C_Q \| [\![\mathbf{u}]\!] \| [\![T]\!]$$



Velocity and temperature jump at interface

$$[\![\mathbf{u}]\!] = \mathbf{u}_a - \mathbf{u}_o \quad \text{on } \Gamma$$

$$[\![T]\!] = T_a - T_o \quad \text{on } \Gamma$$

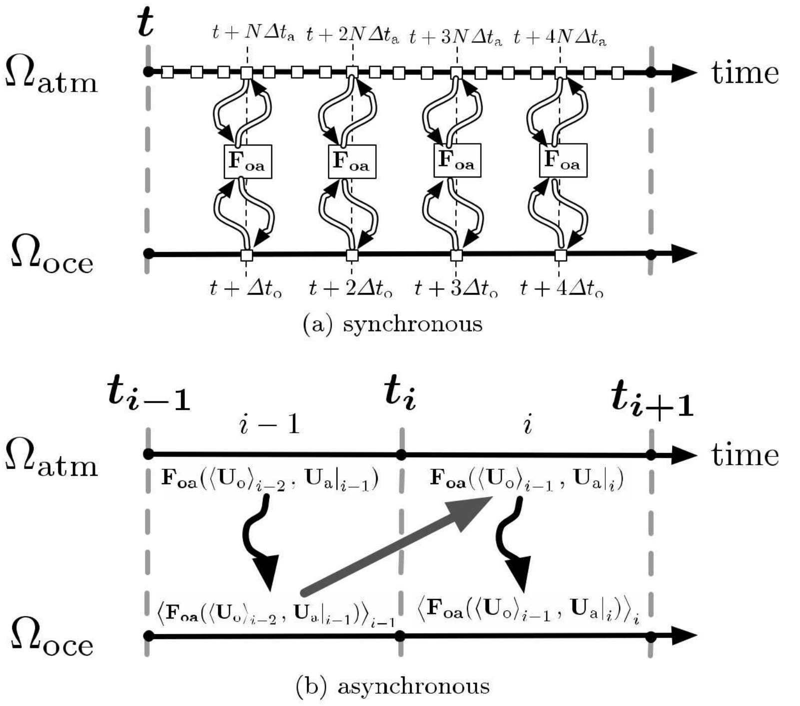
Lemarié, Blayo, Debreu (2015) *Proc. Comp. Sci.*; M. Gross, *et al.* (2018) *MWR*

OCEAN-ATMOSPHERE COUPLING

Typical coupling methods

- Synchronous coupling
  - Exchange instantaneous boundary data at largest time step
  - More frequent communication
  - Can be unstable

- Asynchronous coupling
  - Exchange time-averaged boundary data
  - Long time intervals require fewer communications between models
  - Ensures flux conservation



Schematic of coupling approaches from Gross et al. (2018)

Both methods can be shown to be equivalent to one step of a Schwartz algorithm

Lemarié, Blayo, Debreu (2015) *Proc. Comp. Sci.*; M. Gross, *et al.* (2018) *MWR*

OCEAN-ATMOSPHERE COUPLING

Recent work has investigated relationship between coupling schemes and solution methods for the monolithic ocean-atmosphere system

- Lemarié, Blayo, Debreu (2015): Global-in-time Schwarz method
- Beljaars et al. (2017): Stable parametrized implicit flux coupling for temperature diffusion equation in the context of ice-atmosphere models
- Pelletier, Lemarié, Blayo (2017): Coupling methods for time-dependent Ekman boundary layer model
- Connors, Ganis (2011): Fluid-fluid interaction using a monolithic and a two-way partitioned method.
- Connors, Howell, Layton (2012): Partitioned methods for fluid-fluid interaction

PARTITIONED METHOD FOR BULK INTERFACE CONDITIONS

Our approach:

- Consider a simplified scalar equation with representative coupling conditions
- Starting from the monolithic system, develop a non-iterative approach to approximate the Neumann coupling condition
- Use a Lagrange multiplier to ensure flux continuity at the interface
- Motivated by the Implicit Value Recovery (IVR) approach applied to solid mechanics and advection-diffusion problems

Atmosphere/ocean tracer

$$\dot{T}_a + \frac{\partial}{\partial x}(u_a T_a) = \frac{\partial}{\partial z} K_a \frac{\partial T_a}{\partial z}$$

$$K_a \frac{\partial T_a}{\partial z} = K_o \frac{\partial T_o}{\partial z} = \alpha (T_a - T_o)$$

Γ

$$\dot{T}_o + \frac{\partial}{\partial x}(u_o T_o) = \frac{\partial}{\partial z} K_o \frac{\partial T_o}{\partial z}$$

Peterson, Bochev, Kuberry, CAMWA 2018

IMPLICIT VALUE RECOVERY

Mixed Formulation

$$\dot{\varphi}_1 - \nabla \cdot F_1(\varphi_1) = f_1 \text{ in } \Omega_1$$
$$F_1 \cdot \boldsymbol{n}_1 = -\lambda \text{ on } \gamma$$
$$\ddot{\varphi}_2 - \nabla \cdot F_2(\varphi_2) = f_2 \text{ in } \Omega_2$$
$$F_2 \cdot \boldsymbol{n}_2 = \lambda \text{ on } \gamma$$
$$\varphi_1 = \varphi_2 \text{ on } \gamma$$

Discretize

$$\varphi_1 \in S_1^h \subset H^1_{\Gamma_1}(\Omega_1)$$
$$\varphi_2 \in S_2^h \subset H^1_{\Gamma_2}(\Omega_2)$$
$$\lambda \in G_\gamma^h \subset H^{-1/2}(\gamma)$$

Semi-Discrete System Index 2 DAE

$$M_1\dot{\boldsymbol{\varphi}}_1 + G_1^{\mathsf{T}}\lambda = \mathbf{f}_1(\boldsymbol{\varphi}_1)$$
$$M_2\dot{\boldsymbol{\varphi}}_2 - G_2^{\mathsf{T}}\lambda = \mathbf{f}_2(\boldsymbol{\varphi}_2)$$
$$G_1\boldsymbol{\varphi}_1 - G_2\boldsymbol{\varphi}_2 = 0$$

Conversion to index 1 DAE

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Mass matrix $(M_i)_{kl} = (N_{i,k}, N_{i,l})_\Omega$

Coupling matrix $(G_i)_{kl} = (N_{i,k}, \nu_l)_\gamma$

Force vector $\mathbf{f}_{i,k} = -(\nabla N_{i,k}, F_i)_\Omega + (N_{i,k}, f_i)_\Omega$

Algebraic Form

$$\begin{bmatrix} M_1 & 0 & G_1^T \\ 0 & M_2 & -G_2^T \\ G_1 & -G_2 & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{\varphi}}_1 \\ \dot{\boldsymbol{\varphi}}_2 \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1(\boldsymbol{\varphi}_1) \\ \mathbf{f}_2(\boldsymbol{\varphi}_2) \\ 0 \end{bmatrix}$$

- Defines $\boldsymbol{\lambda}$ as an implicit function of states: can solve for $\boldsymbol{\lambda}$ and use as Neumann data
- Explicit time integration effectively decouples the subdomain equations
- Inf-sup condition verified for mortar elements
- No splitting error or stability issues

Peterson, Bochev, Kuberry, CAMWA 2018

IMPLICIT VALUE RECOVERY

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$$F_2\cdot \boldsymbol{n}_2 = \lambda \text{ on } \gamma$$
$$\varphi_1 = \varphi_2 \text{ on } \gamma$$

Discretize

$$\varphi_1 \in S_1^h \subset H^1_{\Gamma_1}(\Omega_1)$$
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$$M_1\dot{\boldsymbol\varphi}_1 + G_1^{\mathsf T}\lambda = \mathbf{f}_1(\boldsymbol\varphi_1)$$
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Algebraic Form

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Want to derive a similar scheme for bulk conditions on interface:

$$F_1\cdot\mathbf{n}_1 = -F_2\cdot\mathbf{n}_2 = \alpha(\varphi_1 - \varphi_2)$$

Peterson, Bochev, Kuberry, CAMWA 2018

BULK IMPLICIT VALUE RECOVERY

Start with Monolithic Mixed-like Formulation obtained by introducing a new flux variable λ and adding the bulk condition as a third equation

$$\dot{T}_a + \frac{\partial}{\partial x}(u_a T_a) = \frac{\partial}{\partial z} K_a \frac{\partial T_a}{\partial z} \quad \text{in } \Omega_a \qquad \dot{T}_o + \frac{\partial}{\partial x}(u_o T_o) = \frac{\partial}{\partial z} K_o \frac{\partial T_o}{\partial z} \quad \text{in } \Omega_o$$

$$K_a \frac{\partial T_a}{\partial z} = \lambda \quad \text{on } \Gamma \qquad K_o \frac{\partial T_o}{\partial z} = -\lambda \quad \text{on } \Gamma$$

$$\lambda = \alpha(T_a - T_o) \quad \text{on } \Gamma$$

Discretize in Space: Seek $\{T_a^h, T_o^h, \lambda^h\} \in S_{a,\Gamma}^h(\Omega_a) \times S_{o,\Gamma}^h(\Omega_o) \times G_\Gamma^h$

$$\begin{aligned}
\left(\dot{T}_a, \psi_a\right)_{0,\Omega_a} + \langle \lambda, \psi_a \rangle_\Gamma &= (f_a, \psi_a)_{0,\Omega_a} + \left(K_a \frac{\partial T_a}{\partial z}, \frac{\partial \psi_a}{\partial z}\right)_{0,\Omega_a} - \left(u_a \frac{\partial T_a}{\partial x}, \psi_a\right)_{0,\Omega_a} && \forall \psi_a \in H_\Gamma^1(\Omega_a) \\
\left(\dot{T}_o, \psi_o\right)_{0,\Omega_o} - \langle \lambda, \psi_o \rangle_\Gamma &= (f_o, \psi_o)_{0,\Omega_o} + \left(K_o \frac{\partial T_o}{\partial z}, \frac{\partial \psi_o}{\partial z}\right)_{0,\Omega_o} - \left(u_o \frac{\partial T_o}{\partial x}, \psi_o\right)_{0,\Omega_o} && \forall \psi_o \in H_\Gamma^1(\Omega_o) \\
\langle \alpha(T_a - T_o) - \lambda, \mu \rangle_\Gamma \, dS &= 0 && \forall \mu \in H^{-1/2}(\Gamma)
\end{aligned}$$

Weak form of the additional bulk condition equation

BULK IMPLICIT VALUE RECOVERY

Semi-discrete System

$$
\begin{aligned}
M_a \dot{\mathbf{T}}_a + G_a^T \boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a) \\
M_o \dot{\mathbf{T}}_o - G_o^T \boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o) \\
\alpha G_a \mathbf{T}_a - \alpha G_o \mathbf{T}_o - \widehat{M}_\Gamma \boldsymbol{\lambda} &= 0
\end{aligned}
$$

Mass matrix $(M_i)_{kl} = (N_{i,k}, N_{i,l})_\Omega$

Coupling matrix $(G_i)_{kl} = (N_{i,k}, \nu_l)_\Gamma$

Interface mass matrix $(\widehat{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_\Gamma$

BULK IMPLICIT VALUE RECOVERY

Semi-discrete System

$$\begin{aligned} M_a \dot{\mathbf{T}}_a + G_a^T \boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a) \\ M_o \dot{\mathbf{T}}_o - G_o^T \boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o) \\ \alpha G_a \mathbf{T}_a - \alpha G_o \mathbf{T}_o - \widehat{M}_\Gamma \boldsymbol{\lambda} &= 0 \end{aligned}$$

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Interface mass matrix $(\widehat{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_\Gamma$

Similar in form to IVR system, but cannot simplify by using time derivative of solution on interface.

BULK IMPLICIT VALUE RECOVERY

Semi-discrete System

$$\begin{aligned} M_a\dot{\mathbf{T}}_a + G_a^T\boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a) \\ M_o\dot{\mathbf{T}}_o - G_o^T\boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o) \\ \alpha G_a\mathbf{T}_a - \alpha G_o\mathbf{T}_o - \widehat{M}_\Gamma\boldsymbol{\lambda} &= 0 \end{aligned}$$

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Interface mass matrix $(\widehat{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_\Gamma$

Similar in form to IVR system, but cannot simplify by using time derivative of solution on interface.

Solution: Discretize in time, then solve the fully discrete problem for flux $\boldsymbol{\lambda}$

$$\begin{aligned} M_a\left(\frac{\mathbf{T}_a^{n+1} - \mathbf{T}_a^n}{\Delta t}\right) + G_a^T\boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a^n) \\ M_o\left(\frac{\mathbf{T}_o^{n+1} - \mathbf{T}_o^n}{\Delta t}\right) - G_o^T\boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o^n) \\ \alpha G_a\mathbf{T}_a^{n+1} - \alpha G_o\mathbf{T}_o^{n+1} - \widehat{M}_\Gamma\boldsymbol{\lambda} &= 0 \end{aligned}$$

BULK IMPLICIT VALUE RECOVERY

Separate system into internal (I) and interface (Γ) degrees of freedom $\quad \mathbf{g}_i(\mathbf{T}_i^n) = \Delta t \mathbf{f}_i(\mathbf{T}_i^n) - M_i \mathbf{T}_i^n$

$$\left[\begin{array}{ccc:cc} M_{a,\Gamma\Gamma} & 0 & \Delta t G_a^T & M_{a,\Gamma I} & 0 \\ 0 & M_{o,\Gamma\Gamma} & -\Delta t G_o^T & 0 & M_{o,\Gamma I} \\ \alpha G_a & -\alpha G_o & -\widehat{M}_\Gamma & 0 & 0 \\ \hdashline M_{a,I\Gamma} & 0 & 0 & M_{a,II} & 0 \\ 0 & M_{o,I\Gamma} & 0 & 0 & M_{o,II} \end{array}\right] \begin{bmatrix} \mathbf{T}_{a,\Gamma}^{n+1} \\ \mathbf{T}_{o,\Gamma}^{n+1} \\ \boldsymbol{\lambda} \\ \mathbf{T}_{a,I}^{n+1} \\ \mathbf{T}_{o,I}^{n+1} \end{bmatrix} = \begin{bmatrix} \mathbf{g}_{a,\Gamma}(\mathbf{T}_a^n) \\ \mathbf{g}_{o,\Gamma}(\mathbf{T}_o^n) \\ 0 \\ \mathbf{g}_{a,I}(\mathbf{T}_a^n) \\ \mathbf{g}_{o,I}(\mathbf{T}_o^n) \end{bmatrix}$$

Solve for flux: with explicit time stepping only involves information from old time step!

$$\boldsymbol{\lambda} = \left(\Delta t G_a^T A_a^{-1} G_a + \Delta t G_o^T A_o^{-1} G_o - \frac{\widehat{M}_\Gamma}{\alpha}\right)^{-1} \left(G_a^T A_a^{-1} \hat{\mathbf{g}}_a(\mathbf{T}_a^n) - G_o^T A_o^{-1} \hat{\mathbf{g}}_o(\mathbf{T}_o^n)\right)$$

where $\quad \hat{\mathbf{g}}_i(\mathbf{T}_i^n) = \mathbf{g}_{i,\Gamma}(\mathbf{T}_i^n) - M_{i,\Gamma I} M_{i,II}^{-1} \mathbf{g}_{i,I}(\mathbf{T}_i^n)$

$$A_i = M_{i,\Gamma} - M_{i,\Gamma I} M_{i,II}^{-1} M_{i,I\Gamma}$$

COUPLING ALGORITHM

1. Compute right-hand side terms

$$\mathbf{g}_i(\mathbf{T}_i^n) = \Delta t \mathbf{f}_i(\mathbf{T}_i^n) - M_i \mathbf{T}_i^n$$

2. Estimate interface boundary condition

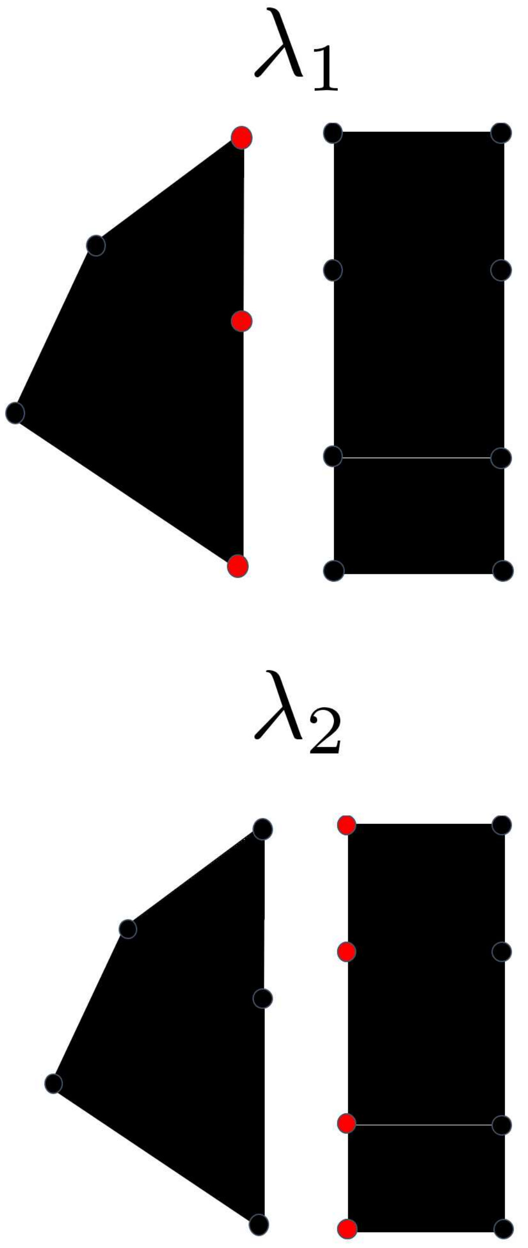
$$\boldsymbol{\lambda} = \left(\Delta t G_a^T A_a^{-1} G_a + \Delta t G_o^T A_o^{-1} G_o - \frac{\widehat{M}_\Gamma}{\alpha} \right)^{-1} \left(G_a^T A_a^{-1} \hat{\mathbf{g}}_a(\mathbf{T}_a^n) - G_o^T A_o^{-1} \hat{\mathbf{g}}_o(\mathbf{T}_o^n) \right)$$

3. Solve independently in each subdomain

$$\begin{bmatrix} M_{i,\Gamma} & M_{i,\Gamma I} \\ M_{i,I\Gamma} & M_{i,II} \end{bmatrix} \begin{bmatrix} \mathbf{T}_{i,\Gamma} \\ \mathbf{T}_{i,I} \end{bmatrix} = \begin{bmatrix} \mathbf{g}_{i,\Gamma}^n \pm G_i^T \boldsymbol{\lambda} \\ \mathbf{g}_{i,I}^n \end{bmatrix}$$

IMPLEMENTATION

- There is some flexibility in choosing the Lagrange multiplier space
- For the original IVR formulation, we followed the mortar method approach and chose either one of the interface partitions
- Results in a formulation that satisfies the inf-sup condition
- We follow this approach in the bulk IVR method
- Expect to converge optimally, but not pass a patch test



LINEAR SOLUTION

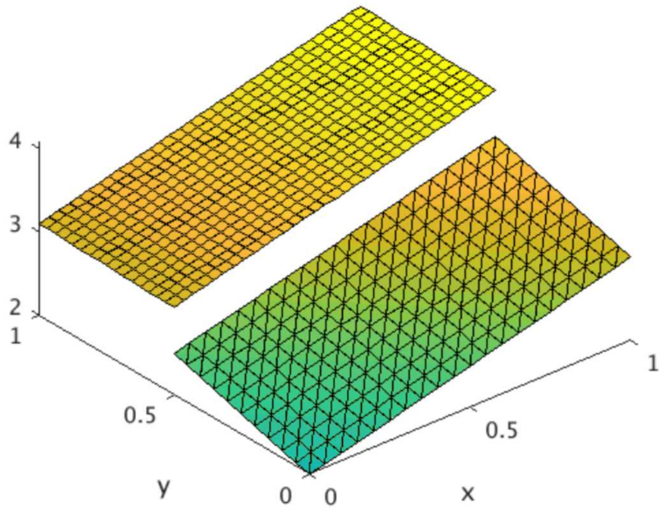
$$T_o = x + y + 2$$

$$T_a = x + \frac{y}{10} + 3$$

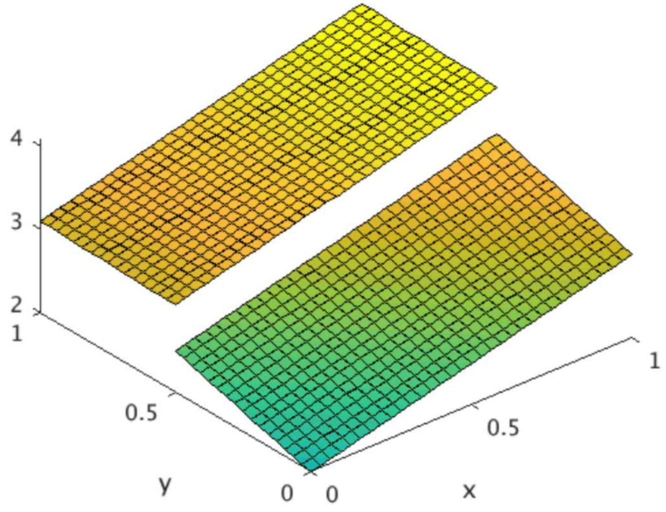
$$K_o = 0.001$$

$$K_a = 0.01$$

Non-matching grids

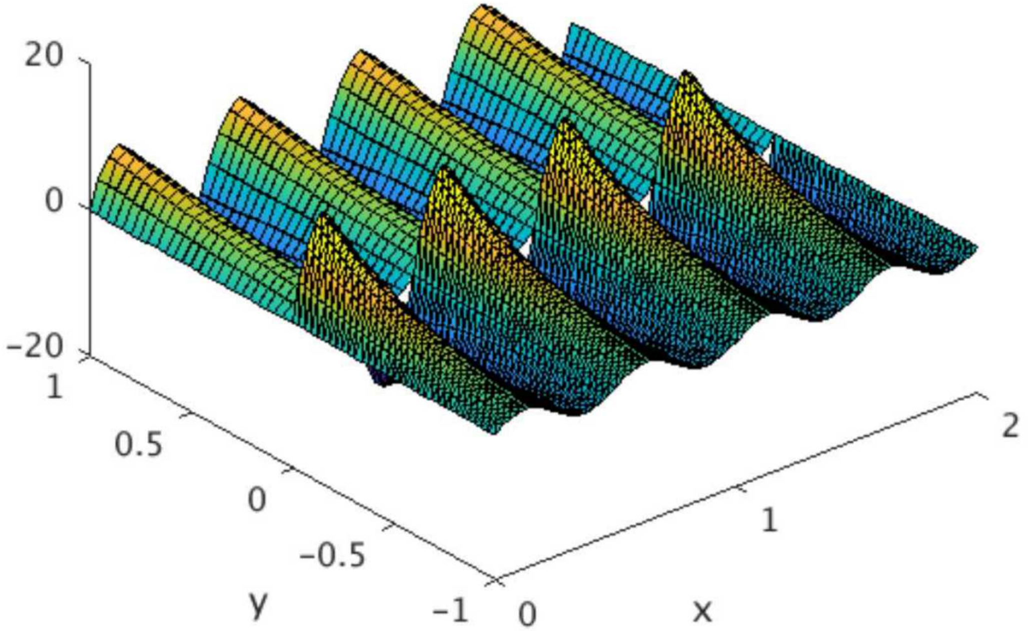


Matching grids



Error Norm	h(Ω_o)	h(Ω_a)	BIVR (λ_o)	BIVR (λ_a)
$L^2(\Omega)$	0.03125	0.03125	1.23e-15	1.23e-15
$H^1(\Omega)$	0.03125	0.03125	1.26e-13	1.26e-13
$L^2(\Omega)$	0.05000	0.03125	7.18e-06	2.14e-07
$H^1(\Omega)$	0.05000	0.03125	7.77e-04	1.64e-05

SIMPLE MANUFACTURED SOLUTION



$$T_o = d_o \exp(\beta_o z)\sin(n\pi x)\exp(\omega t)$$

$$T_a = d_a \exp(\beta_a z)\sin(n\pi x)\exp(\omega t)$$

$$\beta_o = 2 \qquad \beta_a = 1$$

$$d_o = 5 \qquad d_a = 1$$

$$K_o = 0.001 \qquad K_a = 0.01$$

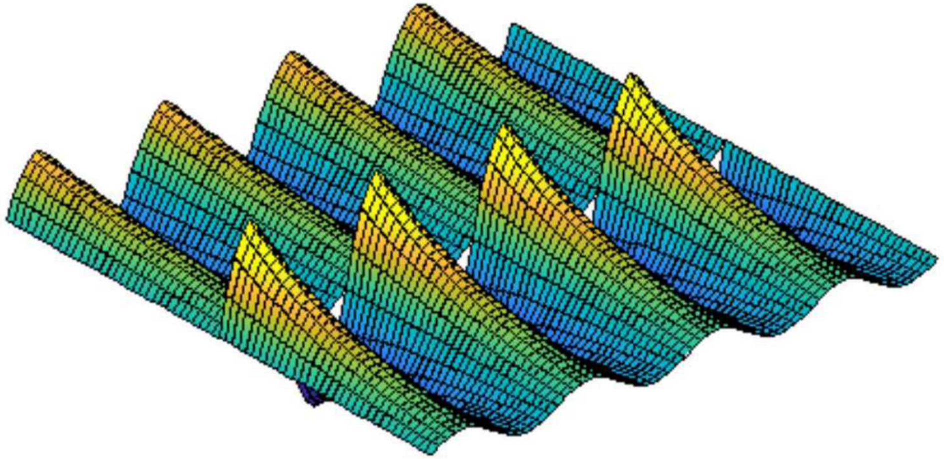
$$\alpha = \frac{K_o \beta_o d_o}{d_a - d_o}$$

$$u_o = u_a = 1$$

Note: developed for testing method convergence and not intended to be physically realistic example.

SIMPLE MANUFACTURED SOLUTION CONVERGENCE

Matching grid solution



$$T_o = d_o \exp(\beta_o z) \sin(n\pi x) \exp(\omega t)$$

$$T_a = d_a \exp(\beta_a z) \sin(n\pi x) \exp(\omega t)$$

Mesh (Ω_o)	Mesh (Ω_a)	Δt	$L^2(\Omega)$	$H^1(\Omega)$
16×8	16×8	1.89e-02	1.44e-00	4.86e01
32×16	32×16	9.43e-03	2.50e-01	2.38e01
64×32	64×32	4.69e-03	4.55e-02	1.19e01
128×64	128×64	1.83e-03	8.76e-03	5.92e00
Rate	-	-	2.38	1.01

SIMPLE MANUFACTURED SOLUTION CONVERGENCE

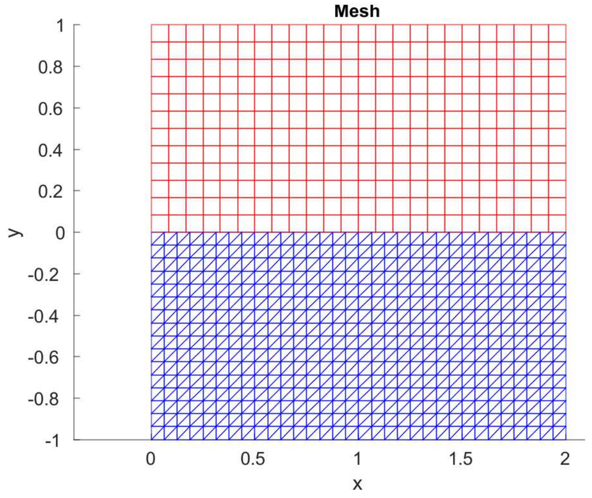
$L^2(\Omega)$ Error norm

Mesh (Ω_o)	Mesh (Ω_a)	Δt	BIVR(λ_o)	BIVR(λ_a)
16×8	12×6	1.33e-02	2.09e-00	2.09e-00
32×16	24×12	6.67e-03	3.40e-01	3.40e-01
64×32	48×24	3.32e-03	6.18e-02	6.18e-02
128×64	96×48	1.66e-03	1.30e-02	1.30e-02
Rate	-	-	2.25	2.25

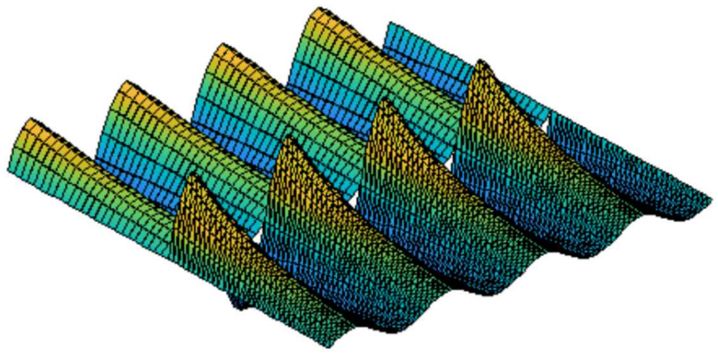
$H^1(\Omega)$ Error norm

Mesh (Ω_o)	Mesh (Ω_a)	Δt	BIVR(λ_o)	BIVR(λ_a)
16×8	12×6	1.33e-02	5.66e01	5.66e01
32×16	24×12	6.67e-03	2.78e01	2.78e01
64×32	48×24	3.32e-03	1.37e01	1.37e01
128×64	96×48	1.66e-03	6.84e00	6.84e00
Rate	-	-	1.01	1.01

Non-matching grids



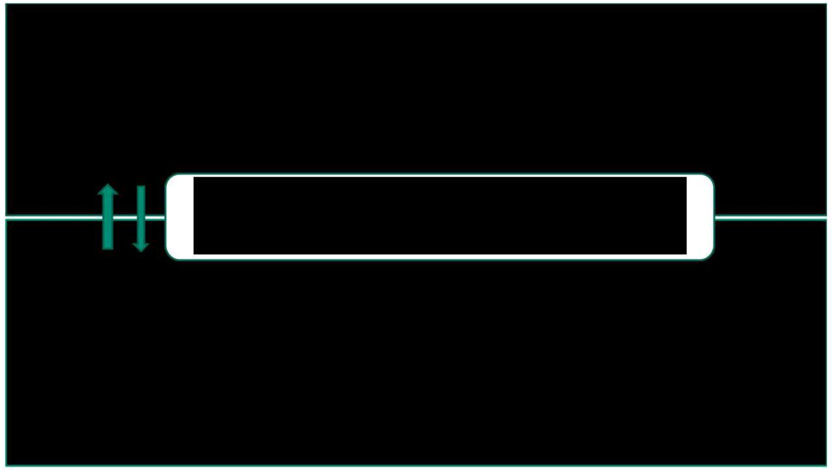
Solution



CONCLUSIONS

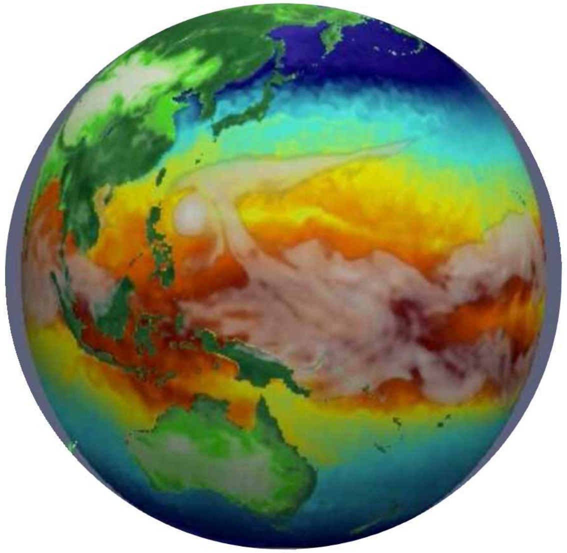
Extended IVR to a Bulk-IVR partitioned scheme for a scalar equation with bulk coupling conditions

- Starts with a well-posed monolithic mixed-like formulation
- Explicit time integration results in an IVR-like structure
- This structure enables solving for the flux on the interface
- Results in a non-iterative partitioned scheme
- Proof-of-concept tested on simple manufactured solutions



Next steps

- Extend Bulk-IVR to simplified coupled fluid equations
- Extend to conjugate heat transfer with imperfect transmission conditions
- Investigate extensions to non-linear coupling conditions
- Evaluate accuracy and stability of method for different spatial and time discretizations



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