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

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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
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

\[
\rho_a \nu_a \frac{\partial u_a}{\partial z} = \rho_o \nu_o \frac{\partial u_o}{\partial z} = \mathbf{\tau} \quad \text{on } \Gamma
\]

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

\[
\mathbf{\tau} = \rho_a C_T \| [\mathbf{u}] \| [\mathbf{u}] \quad Q_{net} = \mathcal{R} + \rho_a C_Q \| [\mathbf{u}] \| [T]
\]

Velocity and temperature jump at interface

\[
[u] = u_a - u_o \quad \text{on } \Gamma
\]

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

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

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

- 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
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

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

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

Atmosphere/ocean tracer

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

Peterson, Bochev, Kuberry, CAMWA 2018
IMPLICIT VALUE RECOVERY

Mixed Formulation
\[ \phi_1 - \nabla \cdot F_1(\phi_1) = f_1 \text{ in } \Omega_1 \]
\[ F_1 \cdot n_1 = -\lambda \text{ on } \gamma \]
\[ \phi_2 - \nabla \cdot F_2(\phi_2) = f_2 \text{ in } \Omega_2 \]
\[ F_2 \cdot n_2 = \lambda \text{ on } \gamma \]
\[ \phi_1 = \phi_2 \text{ on } \gamma \]

Discretize
\[ \varphi_1 \in S^h_1 \subset H^1_\Gamma(\Omega_1) \]
\[ \varphi_2 \in S^h_2 \subset H^1_\Gamma(\Omega_2) \]
\[ \lambda \in G^h_\gamma \subset H^{-1/2}(\gamma) \]

Semi-Discrete System
Index 2 DAE
\[ M_1 \dot{\varphi}_1 + G_1^T \lambda = f_1(\varphi_1) \]
\[ M_2 \dot{\varphi}_2 - G_2^T \lambda = f_2(\varphi_2) \]
\[ G_1 \varphi_1 - G_2 \varphi_2 = 0 \]

Conversion to Index 1 DAE
\[ M_1 \dot{\varphi}_1 + G_1^T \lambda = f_1(\varphi_1) \]
\[ M_2 \dot{\varphi}_2 - G_2^T \lambda = f_2(\varphi_2) \]
\[ G_1 \varphi_1 - G_2 \varphi_2 = 0 \]

Algebraic Form
\[ \begin{bmatrix} M_1 & 0 & G_1^T \\ 0 & M_2 & -G_2^T \\ G_1 & -G_2 & 0 \end{bmatrix} \begin{bmatrix} \dot{\varphi}_1 \\ \dot{\varphi}_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} f_1(\varphi_1) \\ f_2(\varphi_2) \\ 0 \end{bmatrix} \]

- Defines \( \lambda \) as an implicit function of states: can solve for \( \lambda \) 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
**Mixed Formulation**

\[ \dot{\varphi}_1 - \nabla \cdot F_1(\varphi_1) = f_1 \text{ in } \Omega_1 \]
\[ F_1 \cdot n_1 = -\lambda \text{ on } \gamma \]
\[ \dot{\varphi}_2 - \nabla \cdot F_2(\varphi_2) = f_2 \text{ in } \Omega_2 \]
\[ F_2 \cdot n_2 = \lambda \text{ on } \gamma \]
\[ \varphi_1 = \varphi_2 \text{ on } \gamma \]

**Discretize**

\[ \varphi_1 \in S_1^h \subseteq H_1^1(\Omega_1) \]
\[ \varphi_2 \in S_2^h \subseteq H_1^1(\Omega_2) \]
\[ \lambda \in G^h \subseteq H^{-1/2}(\gamma) \]

**Semi-Discrete System**

**Index 2 DAE**

\[ M_1 \dot{\varphi}_1 + G_1^T \lambda = f_1(\varphi_1) \]
\[ M_2 \dot{\varphi}_2 - G_2^T \lambda = f_2(\varphi_2) \]
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**Conversion to index 1 DAE**

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**Algebraic Form**

\[
\begin{bmatrix}
M_1 & 0 & G_1^T \\
0 & M_2 & -G_2^T \\
G_1 & -G_2 & 0
\end{bmatrix}
\begin{bmatrix}
\dot{\varphi}_1 \\
\dot{\varphi}_2 \\
\lambda
\end{bmatrix}
= \begin{bmatrix}
f_1(\varphi_1) \\
f_2(\varphi_2) \\
0
\end{bmatrix}
\]

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

\[ F_1 \cdot n_1 = -F_2 \cdot n_2 = \alpha(\varphi_1 - \varphi_2) \]

Peterson, Bochev, Kuberry, CAMWA 2018
BULK IMPLICIT VALUE RECOVERY

Start with monolithic mixed-like formulation obtained by introducing a new flux variable $\lambda$ and adding the bulk condition as a third equation

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

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

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

Discretize in Space: Seek $\{T^h_a, T^h_o, \lambda^h\} \in S^h_{a,\Gamma}(\Omega_a) \times S^h_{o,\Gamma}(\Omega_o) \times G^h_{\Gamma}$

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

Weak form of the additional bulk condition equation
BULK IMPLICIT VALUE RECOVERY

Semi-discrete System

\[
\begin{align*}
M_a \dot{T}_a + G_a^T \lambda &= f_a(T_a) \\
M_o \dot{T}_o - G_o^T \lambda &= f_o(T_o) \\
\alpha G_a T_a - \alpha G_o T_o - \bar{M}_\Gamma \lambda &= 0
\end{align*}
\]

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 \( (\bar{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_\Gamma \)
Semi-discrete System

\[
\begin{align*}
M_a \dot{T}_a + G_a^T \lambda &= f_a(T_a) \\
M_o \dot{T}_o - G_o^T \lambda &= f_o(T_o) \\
\alpha G_a T_a - \alpha G_o T_o - \widehat{M}_\Gamma \lambda &= 0
\end{align*}
\]

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 \((\widehat{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_{\Gamma}\)

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

Semi-discrete System

\[ M_a \dot{T}_a + G_a^T \lambda = f_a(T_a) \]
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Mass matrix \( (M_i)_{kl} = (N_{i,k}, N_{i,l})_\Omega \)
Coupling matrix \( (G_i)_{kl} = (N_{i,k}, \nu_l)_\Gamma \)
Interface mass matrix \( (\hat{M}_\Gamma)_{kl} = (\nu_k, \nu_l)_\Gamma \)

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 \( \lambda \)

\[ M_a \left( \frac{T_a^{n+1} - T_a^n}{\Delta t} \right) + G_a^T \lambda = f_a(T_a^n) \]
\[ M_o \left( \frac{T_o^{n+1} - T_o^n}{\Delta t} \right) - G_o^T \lambda = f_o(T_o^n) \]
\[ \alpha G_a T_a^{n+1} - \alpha G_o T_o^{n+1} - \hat{M}_\Gamma \lambda = 0 \]
Separate system into internal ($I$) and interface ($\Gamma$) degrees of freedom

$$
\begin{bmatrix}
M_{a,\Gamma\Gamma} & 0 & \Delta tG_a^T \\
0 & M_{o,\Gamma\Gamma} & -\Delta tG_o^T \\
\alpha G_a & -\alpha G_o & -\widehat{M}_\Gamma \\
M_{a,\Gamma I} & 0 & M_{a,\Gamma I} \\
0 & M_{o,\Gamma I} & M_{o,\Gamma I} \\
0 & 0 & M_{o,\Gamma I}
\end{bmatrix}
\begin{bmatrix}
T_{a,\Gamma}^{n+1} \\
T_{o,\Gamma}^{n+1} \\
\lambda \\
T_{a,I}^{n+1} \\
T_{o,I}^{n+1}
\end{bmatrix}
= 
\begin{bmatrix}
g_{a,\Gamma}(T_a^n) \\
g_{o,\Gamma}(T_o^n) \\
0 \\
g_{a,I}(T_a^n) \\
g_{o,I}(T_o^n)
\end{bmatrix}
$$

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

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

where

$$
\hat{g}_i(T_i^n) = g_{i,\Gamma}(T_i^n) - M_{i,\Gamma I} M_{i,\Gamma I}^{-1} g_{i,I}(T_i^n)
$$

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

1. Compute right-hand side terms

\[ g_i(T_i^n) = \Delta t f_i(T_i^n) - M_i T_i^n \]

2. Estimate interface boundary condition

\[ \lambda = \left( \frac{\Delta t G^T A^{-1} G_a + \Delta t G^T_o A_o^{-1} G_o - \frac{\hat{M}_T}{\alpha}}{G^T a A_a^{-1} \hat{g}_a(T_a^n) - G^T o A_o^{-1} \hat{g}_o(T_o^n)} \right)^{-1} \]

3. Solve independently in each subdomain

\[
\begin{bmatrix}
M_{i,\Gamma} & M_{i,\Gamma I} \\
M_{i,II} & M_{i,II I}
\end{bmatrix}
\begin{bmatrix}
T_{i,\Gamma} \\
T_{i,I}
\end{bmatrix}
= 
\begin{bmatrix}
g_{i,\Gamma}^{n} \\
g_{i,I}^{n}
\end{bmatrix} \pm G_i^T \lambda
\]
• 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

\[ T_o = x + y + 2 \]
\[ T_a = x + \frac{y}{10} + 3 \]
\[ K_o = 0.001 \]
\[ K_a = 0.01 \]

<table>
<thead>
<tr>
<th>Error Norm</th>
<th>( h(\Omega_o) )</th>
<th>( h(\Omega_a) )</th>
<th>BIVR ( (\lambda_o) )</th>
<th>BIVR ( (\lambda_a) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L^2(\Omega) )</td>
<td>0.03125</td>
<td>0.03125</td>
<td>1.23e-15</td>
<td>1.23e-15</td>
</tr>
<tr>
<td>( H^1(\Omega) )</td>
<td>0.03125</td>
<td>0.03125</td>
<td>1.26e-13</td>
<td>1.26e-13</td>
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<tr>
<td>( L^2(\Omega) )</td>
<td>0.05000</td>
<td>0.03125</td>
<td>7.18e-06</td>
<td>2.14e-07</td>
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<tr>
<td>( H^1(\Omega) )</td>
<td>0.05000</td>
<td>0.03125</td>
<td>7.77e-04</td>
<td>1.64e-05</td>
</tr>
</tbody>
</table>
SIMPLE MANUFACTURED SOLUTION

\[ T_o = d_o \exp(\beta_o z) \sin(n\pi x) \exp(\omega t) \]
\[ T_a = d_a \exp(\beta_a z) \sin(n\pi x) \exp(\omega t) \]

\[ \beta_o = 2 \quad \beta_a = 1 \]
\[ d_o = 5 \quad d_a = 1 \]
\[ K_o = 0.001 \quad K_a = 0.01 \]

\[ \alpha = \frac{K_o \beta_o d_o}{d_a - d_o} \]
\[ u_o = u_a = 1 \]

Note: developed for testing method convergence and not intended to be physically realistic example.
\[ T_o = d_o \exp(\beta_o z) \sin(n\pi x) \exp(\omega t) \]
\[ T_a = d_a \exp(\beta_a z) \sin(n\pi x) \exp(\omega t) \]

<table>
<thead>
<tr>
<th>Mesh ((\Omega_o))</th>
<th>Mesh ((\Omega_a))</th>
<th>(\Delta t)</th>
<th>(L^2(\Omega))</th>
<th>(H^1(\Omega))</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 \times 8</td>
<td>16 \times 8</td>
<td>1.89e-02</td>
<td>1.44e-00</td>
<td>4.86e01</td>
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<tr>
<td>32 \times 16</td>
<td>32 \times 16</td>
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<td>2.50e-01</td>
<td>2.38e01</td>
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<tr>
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<tr>
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<td>128 \times 64</td>
<td>1.83e-03</td>
<td>8.76e-03</td>
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<tr>
<td>Rate</td>
<td>-</td>
<td>-</td>
<td>2.38</td>
<td>1.01</td>
</tr>
</tbody>
</table>
SIMPLE MANUFACTURED SOLUTION CONVERGENCE

$L^2(\Omega)$ Error norm

<table>
<thead>
<tr>
<th>Mesh ($\Omega_o$)</th>
<th>Mesh ($\Omega_a$)</th>
<th>$\Delta t$</th>
<th>BIVR($\lambda_o$)</th>
<th>BIVR($\lambda_a$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 $\times$ 8</td>
<td>12 $\times$ 6</td>
<td>1.33e-02</td>
<td>2.09e-00</td>
<td>2.09e-00</td>
</tr>
<tr>
<td>32 $\times$ 16</td>
<td>24 $\times$ 12</td>
<td>6.67e-03</td>
<td>3.40e-01</td>
<td>3.40e-01</td>
</tr>
<tr>
<td>64 $\times$ 32</td>
<td>48 $\times$ 24</td>
<td>3.32e-03</td>
<td>6.18e-02</td>
<td>6.18e-02</td>
</tr>
<tr>
<td>128 $\times$ 64</td>
<td>96 $\times$ 48</td>
<td>1.66e-03</td>
<td>1.30e-02</td>
<td>1.30e-02</td>
</tr>
<tr>
<td>Rate</td>
<td>-</td>
<td>-</td>
<td>2.25</td>
<td>2.25</td>
</tr>
</tbody>
</table>

$H^1(\Omega)$ Error norm

<table>
<thead>
<tr>
<th>Mesh ($\Omega_o$)</th>
<th>Mesh ($\Omega_a$)</th>
<th>$\Delta t$</th>
<th>BIVR($\lambda_o$)</th>
<th>BIVR($\lambda_a$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 $\times$ 8</td>
<td>12 $\times$ 6</td>
<td>1.33e-02</td>
<td>5.66e01</td>
<td>5.66e01</td>
</tr>
<tr>
<td>32 $\times$ 16</td>
<td>24 $\times$ 12</td>
<td>6.67e-03</td>
<td>2.78e01</td>
<td>2.78e01</td>
</tr>
<tr>
<td>64 $\times$ 32</td>
<td>48 $\times$ 24</td>
<td>3.32e-03</td>
<td>1.37e01</td>
<td>1.37e01</td>
</tr>
<tr>
<td>128 $\times$ 64</td>
<td>96 $\times$ 48</td>
<td>1.66e-03</td>
<td>6.84e00</td>
<td>6.84e00</td>
</tr>
<tr>
<td>Rate</td>
<td>-</td>
<td>-</td>
<td>1.01</td>
<td>1.01</td>
</tr>
</tbody>
</table>
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
REFERENCES


