A high-order partitioned solver for general multiphysics problems and its applications in optimization

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Introduction

- Multiphysics problems

**Figure:** Mars landing  Micro-aerial vehicle  Energy harvesting

Peng and Zhu (2009)
Optimizations for multiphysics problems

Figure: Mars landing  Micro-aerial vehicle  Energy harvesting

- Is there a design to reduce the von-Mises stress?
- What is the energetically-optimal flapping motion?
- How to harvest more wind energy?
Problem formulation

- **Governing multiphysics equations**

\[
\begin{align*}
\partial_t u^i &= \mathcal{L}_i(u^i, c^i, x, t), \quad x \in \Omega^i, \quad t \in (0, T) \\
c^i &= c^i(u^1, \ldots, u^m, x, t),
\end{align*}
\]

for \( i = 1, \ldots, m \)

- **Objective function**

\[
\mathcal{J}(u^1, \ldots, u^m, x, \mu, T) = \int_0^T j(u^1(\tau), \ldots, u^m(\tau), \mu, \tau)\,d\tau
\]
Solution strategies

- Time-dependent multiphysics optimization problem
  - Stability of the multiphysics solver
  - High order accuracy of the objective function and its gradient
  - Efficient multiple queries

- Implicit scheme vs Explicit scheme
- Monolithic procedure vs Partitioned procedure
- Adjoint method vs Direct sensitivity method vs Finite difference
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Governing mutiphysics equations and semi-discretization

- Implicit solver

\[ M \dot{u} = r(u, c(u, t), t), \quad t \in (0, T) \]

- Partitioned Approach: lag one step, solve \( M \dot{u} = r(u, \tilde{c}(u, t), t) \)
  - Facilitates software modularity and mathematical modeling
  - Often low-order accurate\(^1\) (second order accuracy) and suffer from lack of stability\(^2\)

---


Governing multiphysics equations and semi-discretization

- Implicit solver

\[ M \dot{u} = r(u, c(u, t), t), \quad t \in (0, T) \]

- Partitioned Approach: lag one step, solve \( M \dot{u} = r(u, \tilde{c}(u, t), t) \)
  - 😊 facilitates software modularity and mathematical modeling
  - 😞 often low-order accurate\(^1\) (second order accuracy) and suffer from lack of stability\(^2\)

⇒ Can we do better, how stable or how accurate can a partitioned solver be?

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**IMEX scheme I**

- Implicit-explicit Runge Kutta (IMEX) schemes

\[ M \dot{u} = f(u, t) + g(u, t) \]

The non-stiff \( f \) part and stiff \( g \) part are integrated with \( s \)-stage explicit/implicit RK schemes separately.

### Table: Butcher Tableau for \( s \)-stage IMEX scheme

- **Explicit RK coefficients**
  - \( \hat{c}_0 \) 0
  - \( \hat{c}_2 \) \( \hat{a}_{21} \)
  - \( \hat{c}_3 \) \( \hat{a}_{31} \) \( \hat{a}_{32} \)
  - \( \vdots \) \( \vdots \) \( \ddots \)
  - \( \hat{c}_s \) \( \hat{a}_{s1} \) \( \hat{a}_{s2} \) \( \ldots \) \( \hat{a}_{ss-1} \)
  - \( \hat{b}_1 \) \( \hat{b}_2 \) \( \ldots \) \( \hat{b}_{s-1} \) \( \hat{b}_s \)

- **Implicit RK coefficients**
  - \( \hat{c}_1 \) \( a_{11} \) \( a_{12} \)
  - \( \hat{c}_2 \) \( a_{21} \) \( a_{22} \)
  - \( \hat{c}_3 \) \( a_{31} \) \( a_{32} \) \( a_{33} \)
  - \( \vdots \) \( \vdots \) \( \ddots \)
  - \( \hat{c}_s \) \( a_{s1} \) \( a_{s2} \) \( \ldots \) \( a_{ss-1} \) \( a_{ss} \)
  - \( \hat{b}_1 \) \( \hat{b}_2 \) \( \ldots \) \( \hat{b}_{s-1} \) \( \hat{b}_s \)
Algorithm 1 Implicit-Explicit Runge-Kutta scheme

1: for stages $j = 1, \ldots, s$ do

2: Define stage solution: $u_{n,j} = u_{n-1} + \sum_{p=1}^{j-1} \hat{a}_{jp} \hat{k}_{n,p} + \sum_{p=1}^{j} a_{jp} k_{n,p}$

3: Implicit solve for $k_{n,j}$: $M k_{n,j} = \Delta t_n g(u_{n,j}, t_{n-1} + c_j \Delta t_n)$

4: Explicit solve for $\hat{k}_{n,j}$: $M \hat{k}_{n,j} = \Delta t_n f(u_{n,j}, t_{n-1} + \hat{c}_j \Delta t_n)$

5: end for

6: Set $u_n = u_{n-1} + \sum_{p=1}^{s} \hat{b}_p \hat{k}_{n,p} + \sum_{p=1}^{s} b_p k_{n,p}$

Computational expense: solve $\frac{\partial g}{\partial u}$

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IMEX scheme based solver

- Semi-discretized equations

\[ M \dot{u} = r(u, c(u, t), t) = f(u, \tilde{c}, t) + g(u, \tilde{c}, t) \]

where \( \tilde{c} \) is an approximation, or predictor, of the coupling term \( c(u, t) \) and the terms are defined as

\[ f(u, \tilde{c}, t) = r(u, c(u, t), t) - r(u, \tilde{c}, t) \]
\[ g(u, \tilde{c}, t) = r(u, \tilde{c}, t) \]

The Jacobian of the implicit part

\[ D_{ug} = \frac{\partial r}{\partial u} + \frac{\partial r}{\partial \tilde{c}} \frac{\partial \tilde{c}}{\partial u} \]
IMEX scheme based partitioned solver

- General partitioned solver
  \[ Ax = b \Rightarrow A \text{ is diagonal or triangular} \]

- IMEX scheme based partitioned solver
  \[ D_u g = \frac{\partial r}{\partial u} + \frac{\partial r}{\partial \tilde{c}} \frac{\partial \tilde{c}}{\partial u} \text{ is diagonal or triangular} \]

\[
\begin{align*}
\frac{\partial r}{\partial u} &= \begin{bmatrix} \frac{\partial r_1}{\partial u_1} & \cdots & \frac{\partial r_m}{\partial u_m} \end{bmatrix} \\
\frac{\partial r}{\partial c} &= \begin{bmatrix} \frac{\partial r_1}{\partial c_1} & \cdots & \frac{\partial r_m}{\partial c_m} \end{bmatrix} \\
\frac{\partial \tilde{c}}{\partial u} &= \begin{bmatrix} \frac{\partial \tilde{c}_1}{\partial u_1} & \cdots & \frac{\partial \tilde{c}_m}{\partial u_m} \end{bmatrix}
\end{align*}
\]

\[ \Rightarrow \frac{\partial \tilde{c}}{\partial u} \text{ is diagonal or triangular} \]
Weakly coupled Gauss-Seidel-type predictor

- Predictor at fully discrete level at stage $j$
  \[
  \tilde{c}^i(u_{n,j}, u_{n-1}, t) = c(u_{n,j}^1, \ldots, u_{n,j}^{i-1}, u_{n-1}^i, \ldots, u_{n-1}^m)
  \]

- The implicit part Jacobian $D_{u}g$ is block lower triangular
  \[
  D_{u}g^i = \begin{cases}
  \frac{\partial r^i}{\partial u^i} & i = j \\
  \frac{\partial r^i}{\partial c^i} \frac{\partial c^i}{\partial u^j} & i > j \\
  0 & i < j.
  \end{cases}
  \]

---

Weakly coupled Gauss-Seidel-type predictor

Algorithm 2 IMEX partitioned multiphysics scheme: weak Gauss-Seidel predictor

1: for stages \( j = 1, \ldots, s \) do
2:     for physical systems \( i = 1, \ldots, m \) do
3:         Define stage solution: \( u_{n,j}^i = u_{n-1}^i + \sum_{p=1}^{j-1} \hat{a}_{jp} \hat{k}_{n,p}^i + \sum_{p=1}^{j} a_{jp} k_{n,p}^i \)
4:         Implicit solve for \( k_{n,j}^i \): \( M_{i} k_{n,j}^i = \Delta t_n g^i (u_{n,j}^i, c^i (u_{1,n,j}^i, \ldots, u_{n-1,n,j}^i, u_{n-1,n,j}^i, \ldots, u_{m,n,j}^i, t_n, j)) \)
5:         Explicit solve for \( \hat{k}_{n,j}^i \): \( M_{i} \hat{k}_{n,j}^i = \Delta t_n f^i (u_{n,j}^i, c^i (u_{1,n,j}^i, \ldots, u_{n-1,n,j}^i, u_{n-1,n,j}^i, \ldots, u_{m,n,j}^i, t_n, j)) \)
6:     end for
7: end for
8: Set \( u_n = u_{n-1} + \sum_{p=1}^{s} \hat{b}_p \hat{k}_{n,p} + \sum_{p=1}^{s} b_p k_{n,p} \)

❌ solved serially

😊 fewer implementation efforts, only the diagonal \( \frac{Dg^i}{Du^i} = \frac{\partial r^i}{\partial u^i} \) of the monolithic implicit Jacobian is required

😊 better stability.
Accuracy analysis

- Order conditions\(^6\)\(^7\) are based on Taylor expansion, local truncation error of \(O(\Delta t^{p+1})\) during one time step.
- Chosen predictors have an interpretation at the semi-discrete level.
- Any of the four proposed predictors for a \(p\)th order IMEX-RK schemes leads to the same \(O(\Delta t^{p+1})\) local truncation error and the same \(O(\Delta t^p)\) global temporal error.

---


Model problem

\begin{align*}
\partial_t u^1 &= \lambda_1 (u^1 + u^2) \\
\partial_t u^2 &= \lambda_2 (u^1 + u^2)
\end{align*}

where $\lambda_1 < 0$ and $\lambda_2 < 0$. The coupling terms are chosen as $c^1 = u^2$, $c^2 = u^1$.

Stability analysis

- More general linear system of ODEs
  \[
  \frac{du}{dt} = A u
  \]
  where \( A = \mathcal{L} + \mathcal{D} + \mathcal{U} \) is an \( n \times n \) matrix, the coupling term is taken as \( c(u) = (\mathcal{L} + \mathcal{U})u \).
  
- If \( A \) is diagonally dominant with negative diagonal entries, the Gauss-Seidel predictor is unconditionally stable for the forward-backward Euler IMEX scheme.
Fully discrete adjoint method

- Solver-consistent discretization of quantities of interest
  \[ J(u_0, \ldots, u_{N_t}, k_{1,1}, \ldots, k_{N_t,s}, \hat{k}_{1,1}, \ldots, \hat{k}_{N_t,s}, \mu) \]

- Auxiliary PDE-constraints
  \[
  \tilde{r}_0 = u^i_0 - \bar{u}^i(\mu) \\
  q^i_{n,j} = u^i_{n,j} - u^i_{n-1} - \sum_{p=1}^{j-1} \hat{a}_{jp} \hat{k}^i_{n,p} - \sum_{p=1}^{j} a_{jp} k^i_{n,p}, \\
  R^i_{n,j} = M k^i_{n,j} - \Delta t_n g(u^i_{n,j}, \tilde{c}^i_{n,j}, \mu) \\
  \hat{R}^i_{n,j} = M \hat{k}^i_{n,j} - \Delta t_n f(u^i_{n,j}, \tilde{c}^i_{n,j}, \mu) \\
  \tilde{r}^i_n = u^i_n - u^i_{n-1} - \sum_{j=1}^{s} b_j k^i_{n,j} - \sum_{j=1}^{s} \hat{b}_j \hat{k}^i_{n,j} \\
  p^i_{n,j} = \tilde{c}^i_{n,j} - c^i(u^1_{n,j}, \ldots, u^{i-1}_{n,j}, u^i_{n,j}, \ldots, u^m_{n-1}, t_{n,j}, \mu) 
  \]
PDE optimization requires repeated queries to primal and dual solvers.

- Primal solver
- Dual solver
- Optimizer
PDE optimization requires repeated queries to primal and dual solvers.
Optimization workflow

- PDE optimization requires repeated queries to primal and dual solvers

\[ \mu, u_1, u_2, \ldots, u_{N_t}, \lambda_{N_t}, \lambda_{N_t-1}, \ldots, \lambda_1 \]

\[ \frac{\partial J}{\partial \mu} \]
PDE optimization requires repeated queries to primal and dual solvers.
PDE optimization requires repeated queries to primal and dual solvers.

![Optimization workflow diagram]

- Optimization workflow
  - PDE optimization requires repeated queries to primal and dual solvers
  - optimizer
  - primal solver
  - dual solver
  - $u_1, u_2, \ldots, u_{N_t}$
  - $\lambda_{N_t}, \lambda_{N_t-1}, \ldots, \lambda_1$
Define Lagrangian

\[ L = J - \sum_{n=0}^{N_t} \sum_{i=1}^{m} \lambda_n^i \tilde{r}_n^i - \sum_{n=1}^{N_t} \sum_{j=1}^{s} \sum_{i=1}^{m} \kappa_{n,j}^i R_{n,j}^i - \sum_{n=1}^{N_t} \sum_{j=1}^{s} \sum_{i=1}^{m} \hat{\kappa}_{n,j}^i \hat{R}_{n,j}^i \]

\[ \quad - \sum_{n=1}^{N_t} \sum_{j=1}^{s} \sum_{i=1}^{m} \tau_{n,j}^i q_{n,j}^i - \sum_{n=1}^{N_t} \sum_{j=1}^{s} \sum_{i=1}^{m} \sigma_{n,j}^i p_{n,j}^i \]

The Lagrangian duality is given by the Karush-Kuhn-Tucker (KKT) system

\[ \frac{\partial L}{u_n^i} = 0, \quad \frac{\partial L}{k_{n,j}^i} = 0, \quad \frac{\partial L}{\hat{k}_{n,j}^i} = 0, \quad \frac{\partial L}{u_{n,j}^i} = 0, \quad \frac{\partial L}{\tilde{c}_{n,j}^i} = 0. \]
Dual PDE solver I

- Primal states/stages required at each state/stage of dual problem
- Linear evolution equations solved backwardly in a partitioned way

\[ \lambda^i_{N_t} = 0 \]

\[ \lambda^i_{n-1} = \lambda^i_n + \sum_{j=1}^{s} \tau_{n,j}^i + \sum_{j=1}^{s} \sum_{p=1}^{i} \frac{\partial c^p_{n,j}}{\partial u_{n-1}^i} T^p \sigma_{n,j}^p \]

\[ M^i T \kappa_{n,j}^i = b_j \lambda^i_n + \sum_{p=j}^{s} a_{p,j} \tau_{n,p}^i \]

\[ M^i T \hat{\kappa}_{n,j}^i = \hat{b}_j \lambda^i_n + \sum_{p=j+1}^{s} \hat{a}_{p,j} \tau_{n,p}^i \]

\[ \tau_{n,j}^i = \frac{\partial J}{\partial u_{n,j}^i} + \Delta t_n \frac{\partial g_{n,j}^i}{\partial u_{n,j}^i} T \kappa_{n,j}^i + \Delta t_n \sum_{k=1}^{m} \frac{\partial f_{n,j}^k}{\partial u_{n,j}^i} T^k \hat{\kappa}_{n,j}^k + \sum_{p=i+1}^{m} \frac{\partial c^p_{n,j}}{\partial u_{n,j}^i} T^p \sigma_{n,j}^p \]

\[ \sigma_{n,j}^i = \Delta t_n \frac{\partial g_{n,j}^i}{\partial \tilde{c}_{n,j}^i} T \kappa_{n,j}^i + \Delta t_n \frac{\partial f_{n,j}^i}{\partial \tilde{c}_{n,j}^i} T \hat{\kappa}_{n,j}^i \]
Gradient reconstruction via dual variables

\[
\frac{dJ}{d\mu} = \frac{\partial J}{\partial \mu} + \sum_{i=1}^{m} \lambda_i \frac{\partial \tilde{u}^i}{\partial \mu} + \sum_{n=1}^{N_t} \sum_{i=1}^{m} \sum_{j=1}^{s} \Delta t_n \frac{\partial g_{n,j}^i}{\partial \mu} T \kappa_{n,j}^i \\
+ \sum_{n=1}^{N_t} \sum_{i=1}^{m} \sum_{j=1}^{s} \Delta t_n \frac{\partial f_{n,j}^i}{\partial \mu} T \hat{\kappa}_{n,j}^i + \sum_{n=1}^{N_t} \sum_{i=1}^{m} \sum_{j=1}^{s} \frac{\partial c_{n,j}^i}{\partial \mu} T \sigma_{n,j}^i
\]
Application: fluid structure interaction problems (FSI)

- Fluid governing equations

\[
\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F}^{\text{inv}}(U) + \nabla \cdot \mathbf{F}^{\text{vis}}(U, \nabla U) = 0 \quad \text{in} \quad \Omega(t)
\]

- Transformation to reference domain\(^7\)

\[
U_X = gU \\
\nabla_X U_X = g \nabla U_X \cdot G + g^{-1} U_X \frac{\partial g}{\partial X}
\]

- Transformed conservation law

\[
\frac{\partial U_X}{\partial t} + \nabla_X \cdot \mathbf{F}^{\text{inv}}_X(U_X) + \nabla_X \cdot \mathbf{F}^{\text{vis}}_X(U_X, \nabla_X U_X) = 0 \quad \text{in} \quad \Omega_0
\]

Application: fluid structure interaction problems (FSI)

- Simple structure model mass-spring-damper systems that can directly be written as a second-order system of ODEs

\[ m_s \ddot{u}_s + c_s \dot{u}_s + k_s u_s = f_{ext}(t) \]

- Deformation of the fluid domain
  - Pseudo-structure
  - Parametrized mapping such as radial basis functions
Application: fluid structure interaction problems (FSI)

- Three-field and two-field fluid-structure coupling
  - three-field FSI setting
    \[
    M^s \dot{u}^s = r^s(u^s, c^s), \quad M^x \dot{u}^x = r^x(u^x, c^x), \quad M^f \dot{u}^f = r^f(u^f, c^f)
    \]
    coupling terms
    \[
    c^s = c^s(u^s, u^x, u^f), \quad c^x = c^x(u^s), \quad c^f = c^f(u^s, u^x)
    \]
  - two-field FSI setting
    \[
    M^s \dot{u}^s = r^s(u^s, c^s), \quad M^f \dot{u}^f = r^f(u^f, c^f)
    \]
    coupling terms
    \[
    c^s = c^s(u^s, u^f), \quad c^f = c^f(u^s)
    \]
Application: fluid structure interaction problems (FSI)

- 1D three-field coupling piston problem

![One-dimensional piston system](image)

**Figure:** One-dimensional piston system

- Fluid equation: Eulerian equation + FVM
- Deformation of the fluid mesh: linear, isotropic constitutive law and infinitesimal strains assumed

\[
\rho_m \ddot{u}_x = E_m \frac{\partial^2 u_x}{\partial X^2} - c_m \dot{u}_x
\]
Convergence of the IMEX2 (---), IMEX3 (---), and IMEX4 (---) with the **weak** Gauss-Seidel predictor.
Objective function $\mathcal{J} = \int_0^T u_s^2 \, dt$.

Parameter: the stiffness of the piston $\mu_k$, with constraint $0 \leq \mu_k \leq 10$.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$\mathcal{J}$</th>
<th>FD</th>
<th>Direct</th>
<th>Adjoint</th>
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</thead>
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<tr>
<td>IMEX1</td>
<td>5.24027644581e-03</td>
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<td>-6.40416045418e-04</td>
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<td>IMEX4</td>
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<td>-5.75054797593e-04</td>
<td>-5.75054797593e-04</td>
</tr>
</tbody>
</table>

Table: 1D piston problem: the objective function value and its gradients.
Application: fluid structure interaction problems (FSI)

- Objective function $J = \int_0^T u_s^2 dt$.
- Parameter: the stiffness of the piston $\mu_k$, with constraint $0 \leq \mu_k \leq 10$.

![Graphs of $J$ and $\mu_k$ vs. iteration]

Figure: Convergence of the optimizer with IMEX1 (---), IMEX2 (---), IMEX3 (---), and IMEX4 (---).
Application: fluid structure interaction problems (FSI)

- 2D two-field energy harvesting model problem

\[ \theta(t) = \begin{cases} 
\mu_A \cos\left(\frac{2t}{T} (\pi + \mu_\phi)\right), & t < \frac{T}{2} \\
\mu_A \cos\left(2\pi ft + \mu_\phi\right), & t \geq \frac{T}{2}
\end{cases} \]

**Figure:** Foil-damper system

- Fluid equation: isentropic Navier-Stokes equations + DG(p=3)
  \[ s = \frac{p}{\rho^\gamma} \]

- Deformation of the fluid mesh: blending maps
Application: fluid structure interaction problems (FSI)

Convergence of the IMEX2 (---), IMEX3 (--), and IMEX4 (---) with weak Gauss-Seidel type predictors.

Figure: weak Gauss-Seidel predictor
Objective function $J = \frac{1}{T} \int_T^{2T} c_s \dot{u}_s^2 \, dt$.

Parameters: $-55^\circ \leq \mu_{\text{init}}^A \leq 55^\circ$, $-\frac{\pi}{2} \leq \mu_\phi < \frac{\pi}{2}$, and $E_\theta = -\frac{1}{T} \int_T^{2T} M_z \dot{\theta} \, dt \geq -0.15 \times 10^{-2}$

**Figure**: Convergence of the optimizer for the NACA harvesting problem.
Application: fluid structure interaction problems (FSI)

- Objective function \( J = \frac{1}{T} \int_T^{2T} c_s \dot{u}_s^2 dt \).
- Parameters: 
  - \(-55^\circ \leq \mu_A^{\text{init}} \leq 55^\circ\), 
  - \(-\frac{\pi}{2} < \mu_\phi < \frac{\pi}{2}\), and 
  - \( E_\theta = -\frac{1}{T} \int_T^{2T} M_z \dot{\theta} dt \geq -0.15 \).
Summary

- Introduced a framework for constructing high-order, linearly stable, partitioned solvers for general multiphysics problems
- Derived its corresponding adjoint optimization framework
- Demonstrated on an energy harvesting model problem
- Will do more challenging optimization problems in the future
Acknowledgements

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