Multi-Implicit Discontinuous Galerkin Method for Low Mach Number Combustion

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Outline

1. Introduction and Motivation
2. Spectral Deferred Correction (SDC) Method
3. Finite Volume Discretization
4. Extensions to DG
5. Preliminary Results
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1. Introduction and Motivation
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Introduction

- Interested in modeling coupled dynamics
- Reacting (low Mach number) fluid flow
- Detailed chemical kinetics
- Vastly different time scales for physical processes:
  - Advection, diffusion, reaction
Low Mach Number Formulation

[Majda, Sethian, (1985)]

- Acoustic propagation typically has negligible impact on the system state
- Sound waves are analytically removed from the system
- The set of conservation laws takes the form of a coupled differential-algebraic system
Governing Equations

Thermodynamic variables: \( \rho \) density, \( Y_j \) mass fractions, \( h \) enthalpy

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (U \rho) \\
\frac{\partial (\rho Y_j)}{\partial t} = -\nabla \cdot (U \rho Y_j) + \nabla \cdot \rho D_j \nabla Y_j + \dot{\omega}_j, \\
\frac{\partial (\rho h)}{\partial t} = -\nabla \cdot (U \rho h) + \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h + \sum_j \nabla \cdot h_j \left( \rho D_j - \frac{\lambda}{c_p} \right) \right) \nabla Y_j,
\]

\( \dot{\omega}_j \) production rate, \( D_j \) diffusion coefficient, \( T \) temperate, \( c_p \) specific heat at constant pressure, \( U \) velocity
Equation of state:

\[ p_0 = \rho R T \sum_j \frac{Y_j}{W_j}, \]

Taking Lagrangian derivative and enforcing constant pressure implies

\[
\nabla \cdot U = \frac{1}{\rho c_p T} \left( \nabla \cdot \lambda \nabla T + \sum_j \Gamma_j \cdot \nabla h_j \right) \\
+ \frac{1}{\rho} \sum_j \frac{W}{W_j} \nabla \cdot \Gamma_j + \frac{1}{\rho} \sum_j \left( \frac{W}{W_j} - \frac{h_j}{c_p T} \right) \dot{\omega}_j =: S
\]
Want to integrate this system in time at advective time scale
For stability, need to treat diffusion and reaction implicitly
Multi-implicit splitting \(\Rightarrow\) weakly couple components of the equation
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Spectral Deferred Correction (SDC) Method

Arbitrary order method for integrating ODEs, e.g.:

\[
\phi_t(t) = F(t, \phi(t)), \quad t \in [t^n, t^n + \Delta t]; \\
\phi(t^n) = \phi^n,
\]

Subdivide time step \([t^n, t^{n+1}]\) into \(m\) time substeps, e.g. according to Gauss-Lobatto rule.
Consider associated integral equation

$$\phi(t) = \phi^n + \int_{t_n}^{t} F(\tau, \phi(\tau)) \ d\tau.$$ 

Update equation:

$$\phi^{(k+1)}(t) = \phi^n + \int_{t_n}^{t} \left[ F(\phi^{(k+1)}) - F(\phi^{(k)}) \right] \ d\tau + \int_{t_n}^{t} F(\phi^{(k)}) \ d\tau,$$
\[
\phi^{(k+1)}(t) = \phi^n + \int_{t^n}^{t} \left[ F(\phi^{(k+1)}) - F(\phi^{(k)}) \right] d\tau + \int_{t^n}^{t} F(\phi^{(k)}) \, d\tau,
\]

Discretize two integrals on RHS with **two** quadrature rules:

- First quadrature rule has order of accuracy \( p \)
- Second quadrature rule has order of accuracy \( q > p \)
- Each iteration increases order of accuracy of solution by \( p \) up to maximum of \( q \)
\[
\phi^{(k+1)}(t) = \phi^n + \int_{t^n}^{t} \left[ F(\phi^{(k+1)}) - F(\phi^{(k)}) \right] d\tau + \int_{t^n}^{t} F(\phi^{(k)}) d\tau,
\]

Discretize two integrals on RHS with \textbf{two} quadrature rules:

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- Each iteration increases order of accuracy of solution by \( p \) up to maximum of \( q \)

For example:

- First term: forward or backward Euler (implicit or explicit method)
- Second term: highly accurate Gauss-Lobatto rule
\[
\phi^{(k+1)}(t) = \phi^n + \int_{t_n}^t \left[ F(\phi^{(k+1)}) - F(\phi^k) \right] d\tau + \int_{t_n}^t F(\phi^k) d\tau,
\]

Discretize two integrals on RHS with \textbf{two} quadrature rules:

- First quadrature rule has order of accuracy \( p \)
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- Each iteration increases order of accuracy of solution by \( p \) up to maximum of \( q \)

For example:

- First term: forward or backward Euler (implicit or explicit method)
- Second term: highly accurate Gauss-Lobatto rule
- (Formally equivalent to certain RK/DIRK methods)
Multi-implicit SDC

\[
\phi_{m+1,(k+1)}^A = \phi_{m,(k+1)}^A \\
+ \int_{t^m}^{t^{m+1}} \left[ F_A(\phi_{\text{AAD}}^{(k+1)}) - F_A(\phi^{(k)}) \right] dt + \int_{t^m}^{t^{m+1}} F(\phi^{(k)}) dt \\
\phi_{m+1,(k+1)}^{\text{AD}} = \phi_{m,(k+1)}^{\text{AD}} \\
+ \int_{t^m}^{t^{m+1}} \left[ F_A(\phi_{\text{AAD}}^{(k+1)}) - F_A(\phi^{(k)}) + F_D(\phi_{\text{AAD}}^{(k+1)}) - F_D(\phi^{(k)}) \right] dt \\
+ \int_{t^m}^{t^{m+1}} F(\phi^{(k)}) dt, \\
\phi_{m+1,(k+1)} = \phi_{m,(k+1)} \\
+ \int_{t^m}^{t^{m+1}} \left[ F_A(\phi_{\text{AAD}}^{(k+1)}) - F_A(\phi^{(k)}) + F_D(\phi_{\text{AAD}}^{(k+1)}) - F_D(\phi^{(k)}) + F_R(\phi^{(k+1)}) - F_R(\phi^{(k)}) \right] dt + \int_{t^m}^{t^{m+1}} F(\phi^{(k)}) dt.
\]
Multi-implicit SDC

- Explicit advection  $\implies$ discretize update with forward Euler
- Implicit diffusion, reaction  $\implies$ discretize update with backward Euler

\[
\phi_{AD}^{m+1,(k+1)} = \phi_{m,(k+1)} + \Delta t \phi_{AD}^{m,(k)} + \Delta t \left[ F_A(\phi_{m,(k+1)}) - F_A(\phi_{m,(k)}) \right] \\
+ F_D(\phi_{AD}^{m+1,(k+1)}) - F_D(\phi_{m+1,(k)}) + I_m^{m+1} \left[ F(\phi(k)) \right]
\]

\[
\phi^{m+1,(k+1)} = \phi^{m,(k+1)} + \Delta t \phi^{m+1,(k+1)} + \Delta t \left[ F_A(\phi_{m+1,(k+1)}) - F_A(\phi_{m,(k)}) \right] \\
+ F_D(\phi_{AD}^{m+1,(k+1)}) - F_D(\phi_{m+1,(k)}) + F_R(\phi_{m+1,(k+1)}) - F_R(\phi_{m+1,(k)}) + I_m^{m+1} \left[ F(\phi(k)) \right]
\]
Volume Discrepancy Constrained Evolution

Recall velocity constraint: \( \nabla \cdot U = S \),

**Linearization** \( \implies \) pressure no longer constant

Continuity equation \( \implies \)

\[
\nabla \cdot U = \frac{1}{\rho p} \left( -\frac{Dp}{Dt} \right) + S
\]

Define **correction** \( \delta_x = \frac{Dp}{Dt} \), discretize as

\[
\delta_x \approx \frac{1}{p_0} \left( \frac{p_0 - p_{EOS}}{\Delta t} \right)
\]

Solve **corrected** constraint for velocity:

\[
\nabla \cdot U = S + \delta_x
\]

Each MISDC iteration drives the solution to EOS
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Solution represented by cell-averages:

$$\langle \phi \rangle_i \equiv \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \phi(x) \, dx$$

Reconstruct polynomial to 4th order obtain gradients, point values, etc.

$$\hat{\phi}_i = \langle \phi \rangle_i - \frac{1}{24}(\langle \phi \rangle_{i-1} - 2\langle \phi \rangle_i + \langle \phi \rangle_{i+1})$$

$$\tilde{\phi}_{i+\frac{1}{2}} = \frac{-\hat{\phi}_{i-1} + 9\hat{\phi}_i + 9\hat{\phi}_{i+1} - \hat{\phi}_{i+2}}{16}$$

$$\nabla \hat{\phi}_{i+\frac{1}{2}} = \frac{\langle \phi \rangle_{i-1} - 15\langle \phi \rangle_i + 15\langle \phi \rangle_{i+1} - \langle \phi \rangle_{i+2}}{12\Delta x}$$
Numerical Results (Finite Volume)

![Graph showing numerical results for different methods.](image)

- **$L^1$ error for $Y_{\text{HO}_2}$**

- **Axes:**
  - $n$ (horizontal axis)
  - $L^1$ error (vertical axis)

- **Methods shown:**
  - Strang splitting
  - Previous MISDC method
  - New MISDC method

- **Key notes:**
  - Strang splitting is marked by orange dots.
  - Previous MISDC method is marked by blue squares.
  - New MISDC method is marked by orange triangles.

- **Legend:**
  - Orange dots: Strang splitting
  - Blue squares: Previous MISDC method
  - Orange triangles: New MISDC method

- **Orders of accuracy:**
  - < 1st order
  - 2nd order
  - 4th order
## Premixed Hydrogen Flame

(9 chemical species, 27 reactions)

<table>
<thead>
<tr>
<th>Variable</th>
<th>$L_{128}^1$</th>
<th>$r_{128/256}$</th>
<th>$L_{256}^1$</th>
<th>$r_{256/512}$</th>
<th>$L_{512}^1$</th>
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<tbody>
<tr>
<td>$Y(H_2)$</td>
<td>5.91E-08</td>
<td>4.01</td>
<td>3.67E-09</td>
<td>3.98</td>
<td>2.33E-10</td>
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<tr>
<td>$Y(O_2)$</td>
<td>1.10E-06</td>
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<td>6.83E-08</td>
<td>4.05</td>
<td>4.14E-09</td>
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<tr>
<td>$Y(H_2O)$</td>
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<td>4.01</td>
<td>6.25E-08</td>
<td>4.05</td>
<td>3.76E-09</td>
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<tr>
<td>$Y(H)$</td>
<td>1.17E-09</td>
<td>3.70</td>
<td>9.00E-11</td>
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<td>5.97E-12</td>
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<tr>
<td>$Y(O)$</td>
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<td>3.93</td>
<td>1.77E-09</td>
<td>4.01</td>
<td>1.10E-10</td>
</tr>
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<td>4.01</td>
<td>1.97E-09</td>
<td>4.06</td>
<td>1.18E-10</td>
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<tr>
<td>$Y(HO_2)$</td>
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<td>7.58E-11</td>
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<tr>
<td>$Y(N_2)$</td>
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<td>3.95</td>
<td>1.15E-08</td>
<td>4.07</td>
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<tr>
<td>$\rho$</td>
<td>5.00E-09</td>
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<tr>
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<tr>
<td>$\rho h$</td>
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<td>3.99</td>
<td>4.26E-01</td>
<td>4.07</td>
<td>2.54E-02</td>
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</tbody>
</table>
Premixed Methane Flame

(53 species, 325-step chemical reaction network)

<table>
<thead>
<tr>
<th>Variable</th>
<th>$L_{128}^1$</th>
<th>$r_{128/256}$</th>
<th>$L_{256}^1$</th>
<th>$r_{256/512}^2$</th>
<th>$L_{512}^1$</th>
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<tbody>
<tr>
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<td>3.98</td>
<td>4.42E-09</td>
</tr>
<tr>
<td>$Y(\text{O}_2)$</td>
<td>3.77E-06</td>
<td>3.96</td>
<td>2.42E-07</td>
<td>4.07</td>
<td>1.44E-08</td>
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<tr>
<td>$Y(\text{H}_2\text{O})$</td>
<td>2.30E-06</td>
<td>4.02</td>
<td>1.42E-07</td>
<td>4.05</td>
<td>8.53E-09</td>
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<tr>
<td>$Y(\text{CO}_2)$</td>
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<td>1.15E-07</td>
<td>4.07</td>
<td>6.87E-09</td>
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<tr>
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<td>5.59E-09</td>
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<tr>
<td>$Y(\text{CH}_2(\text{S}))$</td>
<td>8.01E-11</td>
<td>4.14</td>
<td>4.54E-12</td>
<td>3.85</td>
<td>3.15E-13</td>
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<tr>
<td>$Y(\text{O})$</td>
<td>1.05E-07</td>
<td>4.08</td>
<td>6.20E-09</td>
<td>3.90</td>
<td>4.16E-10</td>
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<td>$Y(\text{H})$</td>
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<td>3.83</td>
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<tr>
<td>$\rho$</td>
<td>1.25E-08</td>
<td>4.03</td>
<td>7.64E-10</td>
<td>4.05</td>
<td>4.61E-11</td>
</tr>
<tr>
<td>$T$</td>
<td>3.52E-02</td>
<td>4.01</td>
<td>2.18E-03</td>
<td>4.06</td>
<td>1.31E-04</td>
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<tr>
<td>$\rho h$</td>
<td>4.09E+01</td>
<td>3.97</td>
<td>2.60E+00</td>
<td>4.00</td>
<td>1.62E-01</td>
</tr>
</tbody>
</table>
## Dimethyl Ether Flame

(39 species, 175 reactions)

<table>
<thead>
<tr>
<th>Variable</th>
<th>$L_{128}^1$</th>
<th>$r_{128/256}^1$</th>
<th>$L_{256}^1$</th>
<th>$r_{256/512}^1$</th>
<th>$L_{512}^1$</th>
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</thead>
<tbody>
<tr>
<td>$Y(\text{CH}_3\text{OCH}_3)$</td>
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<td>3.83</td>
<td>1.62E-07</td>
<td>3.93</td>
<td>1.06E-08</td>
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<tr>
<td>$Y(\text{O}_2)$</td>
<td>2.99E-06</td>
<td>3.63</td>
<td>2.42E-07</td>
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<td>1.49E-08</td>
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<tr>
<td>$Y(\text{CO}_2)$</td>
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<td>3.83</td>
<td>1.76E-07</td>
<td>4.04</td>
<td>1.07E-08</td>
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<tr>
<td>$Y(\text{H}_2\text{O})$</td>
<td>1.62E-06</td>
<td>3.51</td>
<td>1.42E-07</td>
<td>4.01</td>
<td>8.85E-09</td>
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<tr>
<td>$Y(\text{CH}_3\text{OCH}_2\text{O}_2)$</td>
<td>1.55E-10</td>
<td>4.51</td>
<td>6.76E-12</td>
<td>3.88</td>
<td>4.61E-13</td>
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<tr>
<td>$Y(\text{OH})$</td>
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<tr>
<td>$Y(\text{O})$</td>
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<td>$Y(\text{H})$</td>
<td>8.35E-09</td>
<td>3.68</td>
<td>6.52E-10</td>
<td>3.96</td>
<td>4.20E-11</td>
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<tr>
<td>$Y(\text{N}_2)$</td>
<td>1.09E-06</td>
<td>3.76</td>
<td>8.01E-08</td>
<td>3.93</td>
<td>5.25E-09</td>
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<td>$\rho$</td>
<td>9.44E-09</td>
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<td>7.42E-10</td>
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<td>4.58E-11</td>
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<tr>
<td>$T$</td>
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<td>$\rho h$</td>
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<td>4.15E+00</td>
<td>4.02</td>
<td>2.56E-01</td>
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</tbody>
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Advantages of DG

- Arbitrary order of accuracy
- Unstructured and complex geometries
- Straightforward generalization to multiple dimensions
- Amenable to parallelization
Weak Form

\[ \int_K \frac{\partial \rho}{\partial t} v \, dx = \int_K \rho U \cdot \nabla v \, dx - \int_{\partial K} \hat{\rho U}(n) v \, dA \]

\[ \int_K \frac{\partial (\rho Y_j)}{\partial t} v \, dx = \int_K (\rho Y_j U + \Gamma_j) \cdot \nabla v \, dx + \int_K \dot{\omega}_j v \, dx \]

\[ \quad \quad \quad - \int_{\partial K} \left( \hat{\rho Y_j U}(n) + \hat{\Gamma}_j(n) \right) v \, dA \]

\[ \int_K \frac{\partial (\rho h)}{\partial t} v \, dx = \int_K \rho h U \cdot v \, dx - \int_{\partial K} \hat{\rho h U}(n) v \, dA \]

\[ \quad \quad \quad - \int_K \frac{\lambda}{c_p} \nabla h \cdot \nabla v \, dx + \int_{\partial K} \frac{\lambda}{c_p} \nabla h + \ldots \]
General approach

- Transform second-order equations into system of first-order equations and use LDG method (Cf. Cockburn and Shu)
- Solve weak form of reaction equations $\Rightarrow$ reaction solve couples all nodes within each element (expensive!)

\[
\int_K \frac{u^{(k+1),m+1} - u^{(k+1),m}}{\Delta t_m} \, dx = \int_K r^{(k+1),m+1}_{AD} + \dot{\omega}(u^{(k+1),m+1}) \, dx
\]

- Oscillatory second derivatives $\Rightarrow$ filter $S$ for stability
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Numerical Results (Hydrogen Flame)
### Numerical Results (Hydrogen Flame)

**Error in total concentration of $O_2$ after 1 ms simulation**

<table>
<thead>
<tr>
<th>$n_x$</th>
<th>$p = 1$</th>
<th>Rate</th>
<th>$p = 2$</th>
<th>Rate</th>
<th>$p = 3$</th>
<th>Rate</th>
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<tbody>
<tr>
<td>64</td>
<td>$1.80 \times 10^{-8}$</td>
<td>-</td>
<td>$6.40 \times 10^{-10}$</td>
<td>-</td>
<td>$7.58 \times 10^{-10}$</td>
<td>-</td>
</tr>
<tr>
<td>128</td>
<td>$4.48 \times 10^{-9}$</td>
<td>$2.01$</td>
<td>$3.56 \times 10^{-11}$</td>
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<td>256</td>
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<tr>
<td>512</td>
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<td>$3.22$</td>
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<td>$1.99$</td>
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Thanks!
Volume Discrepancy
Volume Discrepancy (Refinement in Space)