ERROR ESTIMATIONS FOR STOCHASTIC LAGRANGIAN-EULERIAN SIMULATIONS OF SPRAYS

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• Stochastic Lagrangian-Eulerian Methods for Fuel Sprays
• Convergence Rates (Theory)
• Convergence Rates (Demonstrations)
  – 2D, static, analytical
  – 3D, transient, empirical
• De-coupling statistical and spatial errors
DIRECT-INJECTION IS SIGNIFICANT SHARE OF THE MARKET

US DOE Fact of the Week #1018, February 26 2018
FUEL-AIR MIXING KEY TO PERFORMANCE
FULLY RESOLVED SIMULATIONS COMPUTATIONALLY PROHIBITIVE

STOCHASTIC LAGRANGIAN-EULERIAN

PARCELS INSTEAD OF PARTICLES
CONVERGENCE TESTS PRODUCED TROUBLING RESULTS

![Graph showing mean expected error vs mesh resolution.]

The graph illustrates the relationship between mean expected error and mesh resolution, highlighting the troubling results observed in convergence tests.
CURRENT STATUS OF CONVERGENCE OF LE SPRAYS

• Stalsberg-Zarling et al. (2004) – Lagrange Polynomial Interpolation to “smooth” coupling
• Are et al. (2005) – Limits of infinite parcel count
• Senecal et al. (2012), and Van Dam et al. (2016a, 2016b) – Empirically tested the convergence in engine simulations for different QoIs
• Garg et al. (2007, 2009) – Assumed a particular form for the error and tested different coupling schemes empirically, including varying the parcels per cell
  
  Full Error = statistical + bias + discretization errors

\[
\varepsilon_F = \frac{c_F \theta}{\sqrt{N_{\text{parcel}}}} + \frac{b_F (\Delta x)}{N_{\text{parcel}}} + \frac{a_F}{(\Delta x)^p}
\]
Schmidt (2006) and Schmidt and Bedford (2018)

\[ E^2 = \frac{f}{n(\Delta x)^d} + \frac{1}{4} \left[ \sum_{m=1}^{d} \frac{\partial^2 f}{\partial x_m^2} \Delta x^2 \right] \]

\[ n = \frac{b}{\Delta x^a} \]

\[ L_2^2 = \Delta x^d \sum_{\text{cells}} E^2 \]

\[ L_2 \approx \sqrt{\frac{\Delta x^{a-d}}{b} \sum_{\text{cells}} f \Delta x^d + \frac{\Delta x^4}{4} \sum_{\text{cells}} \left[ \sum_{m=1}^{d} \frac{\partial^2 f}{\partial x_m^2} \right]^2 \Delta x^d} \]

\[ \Rightarrow c = \frac{a-d}{2}; \quad a = 2c + d \]
CURRENT STATUS OF CONVERGENCE OF LE SPRAYS

TRANSIENT SIMULATIONS

• If \( N_{PT} = \text{const.}, s \approx \frac{1}{2} N_{PT} N_T^2 \) (for large \( N_T \))
  - \( N_{PT} \cdot N_T = n, N_T = \frac{\tau}{\Delta t} \)
  - Assume \( CFL = \frac{\Delta t U}{\Delta x} = \text{const.} \Rightarrow s = \frac{n\tau U}{2\Delta x} \)

• Plugging into previous equations as the sample size

\[
L_2 \approx \sqrt{\frac{2\Delta x^{a-d+1}}{b\tau U} \sum_{\text{cells}} f \Delta x^d + \frac{\Delta x^4}{4} \sum_{\text{cells}} \left[ \sum_{m=1}^{d} \frac{\partial^2 f}{\partial x_m^2} \right]^2 \Delta x^d}
\]

• \( \Rightarrow c = \frac{a-d+1}{2}; a = 2c + d - 1 \)
$$f_{exact}(x, y) = \frac{\pi^2}{4} \sin(\pi x) \sin(\pi y)$$
PARCEL COUNTS INCREASE VERY QUICKLY

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>1st-Order</th>
<th>0th-Order</th>
<th>1st-Order</th>
<th>2nd-Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-1}=0.5$</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
</tr>
<tr>
<td>$2^{-2}=0.25$</td>
<td>32</td>
<td>128</td>
<td>512</td>
<td>2,048</td>
</tr>
<tr>
<td>$2^{-3}=0.125$</td>
<td>32</td>
<td>512</td>
<td>8,192</td>
<td>131,072</td>
</tr>
<tr>
<td>$2^{-4}=0.0625$</td>
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<td>2,048</td>
<td>131,072</td>
<td>8,388,608</td>
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<td>$2^{-5}=0.03125$</td>
<td>32</td>
<td>8,192</td>
<td>2,097,152</td>
<td>536,870,912</td>
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<tr>
<td>$2^{-6}=0.015625$</td>
<td>32</td>
<td>32,768</td>
<td>33,554,432</td>
<td>34,359,738,368</td>
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<tr>
<td>$2^{-7}=0.0078125$</td>
<td>32</td>
<td>131,072</td>
<td>536,870,912</td>
<td>2,199,023,255,552</td>
</tr>
</tbody>
</table>
ERROR TRENDS FOLLOW THE THEORY

L₂ ERROR NORM PLOTTED

\[ N_p = \text{const.} \]

\[ N_{pc} = \text{const.} \]
UNIDIRECTIONAL SPRAY IN A BOX

- 2x2x3 cm box
- D=2 cm injector
- 100 or 10 μm drop size
- $P_{\text{amb}}$ of 1 or 5 bar
- 10 m/s initial velocity
- Sinusoid parcel distribution
- 3 mg/ms injection rate
- 2 ms simulation
- Simulated using OpenFOAM v6
## RAN TESTS FOR 1ST-ORDER CONVERGENCE

<table>
<thead>
<tr>
<th>Run</th>
<th>Δx</th>
<th>Δt</th>
<th>Cell Count</th>
<th>N&lt;sub&gt;PT&lt;/sub&gt;</th>
<th>N at EOI</th>
<th>N/Cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>667 μm</td>
<td>66.7 μs</td>
<td>30x30x45</td>
<td>100</td>
<td>3,000</td>
<td>0.074</td>
</tr>
<tr>
<td>2</td>
<td>333 μm</td>
<td>33.3 μs</td>
<td>60x60x90</td>
<td>800</td>
<td>48,000</td>
<td>0.148</td>
</tr>
<tr>
<td>3</td>
<td>167 μm</td>
<td>16.7 μs</td>
<td>120x120x180</td>
<td>6400</td>
<td>768,000</td>
<td>0.296</td>
</tr>
<tr>
<td>4</td>
<td>83 μm</td>
<td>8.3 μs</td>
<td>240x240x360</td>
<td>51,200</td>
<td>12,300,00</td>
<td>0.593</td>
</tr>
</tbody>
</table>
CONVERGENCE OF THE SPRAY SMOOTHER FOR LOW P_{AMB}, LARGER PARTICLES

STILL INVESTIGATING IF ERROR IS WITH CODE OR THEORY

Pamb 1 bar, 100 μm particles

Pamb 5 bar, 100 μm particles

Pamb 5 bar, 10 μm particles
CONVERGENCE OF THE GAS KE PROBLEMATIC AT SMALLEST MESH RESOLUTIONS

Pamb 1 bar, 100 μm particles

Pamb 5 bar, 100 μm particles

Pamb 5 bar, 10 μm particles
SPLITTING LOCAL ERRORS INTO STOCHASTIC AND SPATIAL COMPONENTS

\[ E^2 = \frac{f}{n(\Delta x)^d} + \frac{1}{4} \sum_{m=1}^{d} \frac{\partial^2 f}{\partial x_m^2} \Delta x^2 \]

- Stochastic Error
- Spatial Error
EXAMPLE MSE PLOT (NX=8, NP=1024)
EMPIRICAL DATA - SINGLE REALIZATION

Exact Solution

Solution Error**2

Estimate Solution

Soln Relative Error
PUTTING THE EMPIRICAL AND THEORETICAL RESULTS SIDE-BY-SIDE WE GET A STRONG CORRELATION (FOR THIS CONDITION)

\[ N_{\text{iter}} = 10^6 \]
At high parcel counts (NP=131072), doesn’t match as well.

\[ N_{\text{iter}} = 25954 \]
NEXT STEPS

- Double-check theoretical MSE against test problem simulations
- MSE with an estimate of f and its second derivative
  - This will introduce local errors and the quality of the error estimate will now itself depend on the number of parcels
- Investigate source of divergence in 3D case
  - Tests with FoamExtend v3 (a fork of OpenFOAM) never converges, so may be issues with the spray-coupling code in OpenFOAM
- Parcel control algorithms
  - Much further down the line
THANK-YOU!