

高性能计算对发动机CFD模拟的变革



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阿贡：美国能源部最大的研究机构之一



- 距离芝加哥市中心25英里。建于1946年，是美国第一个国家实验室
- 由芝加哥大学代能源部管理
- 主要研究任务包括基础科学，环境管理，和前沿能源技术
- 3200名员工，其中1000名是科学家和工程师，750人有博士学位
- 年度预算7亿5千万美元（80%来自能源部）
- 自1990年，阿贡已和超过600家公司和许多政府机构合作

<http://www.anl.gov/>

实习机会: <http://www.dep.anl.gov/>



提纲

- 介绍
 - 发动机模拟能有真正的预测性么？
- 预测发动机模拟所必须的开发工作
 - 让CONVERGE能够用于高性能计算
 - 喷嘴内流动
 - 喷嘴内外燃油流动耦合
 - 利用LES的先进湍流模拟
 - 湍流燃烧
 - 不确定性分析
- 模型应用于先进燃烧概念
 - 双燃料燃烧
 - 汽油压燃
- 阿贡的**VERIFI**项目变革研发流程



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发动机模拟能有真正的预测性么？ 发动机流场尺度: 直接求解vs. 模拟

- 缸内流动雷诺数是适中的；喷雾的雷诺数非常高
- 典型流场尺寸的数量级
 - 最大的漩涡 = $O(100 \text{ mm}) ; O(10^{-3} \text{ s})$
 - 滚流和涡流与缸径数量级相当
 - integral length 尺度 = $O(1-10 \text{ mm})$
 - Kolmogorov尺度 = $O(0.01 \text{ mm}) ; O(10^{-5} \text{ s})$
 - 湍流速度 $u' = O(1-10 \text{ m/s})$
- 动能限制Kinetic Energy Budget
 - 典型网格分辨率 ($\sim 0.5 \text{ mm}$) 能求解50-60% 总动能
 - 我们的网格分辨率 ($\sim 0.1 \text{ mm}$) 能求解80-90%总动能
- 但是: 关键的现象在更小的尺度下发生 => 模拟
 - 预混燃烧火焰: 厚度 = $O(0.1 \text{ mm})$
 - 喷雾: 液滴大小 $< 0.025 \text{ mm}$, 蒸发时间 = $O(10^{-7}-10^{-8} \text{ s})$
 - 边界层
- 对于液体喷雾, 混合和燃烧, 亚网格尺度的影响胜过能直接求解的尺度



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梦想: 同时变革发动机和燃料的设计 与不确定性分析结合的超大规模计算所需的软件

依据康明斯发动机研发总监John Deur, 以下的加速层次能显著影响当今的发动机开发过程*

不确定性分析

- [10x] 360度几何
- [10x] 多循环
- [10x] 更准确的湍流模型(LES)
- [10x] 更准确的喷雾动力学

超大规模计算

- [50x] 真实燃料的详细化学反应动力学

按当今的标准需要500,000 倍的提速
(当今工业界的 standards 是用 64 核能在24 小时获得结果)



我们的项目是超大规模的=> 3千万核在24 小时内获得结果!

* DOE Engine Simulation Roadmap Workshop - August 18, 2014

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发动机模拟大致包括:

- 没有被求解的喷嘴内流场
- 简化的燃烧模型
- 粗网格=> 网格收敛
- 简化的湍流模型
- 简易的负荷平衡算法

传统: 大量的模型标定

变革性策略:

- 基于详细化学反应的燃烧模型
- 细网格=>网格收敛
- 高精度湍流模型: LES
- 基于二项流的喷雾模拟
- 喷嘴内流场模拟



- 为高性能计算开发工具

向具有预测性的发动机模拟发展

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我们选择CONVERGE 因为工业界也是如此...

工具	CONVERGE , 大部分源代码
维度和网格类型	3D, 具有自适应网格加密的结构化网格
空间分割策略	2阶精度有限体积
最小和最大的特征网格尺寸	最细网格: 2.5 μm 喷嘴内流体 (3千1百万最大网格量) 32.5 μm 喷雾 (2千2百万最大网格量) 87.5 μm 发动机 (3千5百万最大网格量)
总网格数	5千万最大网格数
并行性	直到 4096 核有良好的拓展性

湍流模型	RANS: RNG k-ε; LES: Smagorinsky, Dynamic Structure
喷雾模型	Eulerian-Eulerian Near Nozzle Model Lagrangian Models:
喷嘴内流动	Homogeneous Relaxation Model (HRM)
时间步长	依据喷雾, 蒸发, 燃烧的变量
湍流-燃烧相互作用模型	详细化学反应机理直接积分 well-mixed model Multi-Flamelet Representative Interactive Flamelet (RIF)

所用的工作都在期刊和会议论文中发表 (<http://verifi.anl.gov/publications/>)

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让CONVERGE能够用于高性能计算

1. S. Som, D.E. Longman, S.M. Aithal, R. Bair, M. Garcia, S. Quan, K.J. Richards, P.K. Senecal, T. Shethaji, M. Weber, SAE Paper No. 2013-01-1095, April 2013
2. J. Kodavasal, K. Harms, P. Srivastava, S. Som, S. Quan, K.J. Richards, M. Garcia, *Proceedings of the ASME 2015 Internal Combustion Engine Division Fall Technical Conference*, ICEF2015-1035, November 2015
3. J. Kodavasal, K. Harms, P. Srivastava, S. Som, S. Quan, K.J. Richards, M.G. Martinez, "Performance Enhancement of an Internal Combustion Engine CFD Simulation on IBM BG/Q," *ISC High Performance Computing Conference*, Frankfurt, Germany, July 2015. Winner of ISC Best poster award

阿贡的计算资源

集群

Fusion Cluster

- 320 节点
 - 2560 核
 - 12.5 兆字节存储
 - 500兆字节磁盘
 - 最高25.9兆次浮点运算
- ### Blues Cluster
- 310 节点
 - 4960 核
 - 最高107.8兆次浮点运算

超级计算机



PETAFLOPS POWER

48 racks
1,024 nodes per rack
1.6 GHz 16-way core processor
16 GB RAM per node
384 I/O nodes
240 GB/s, 35 PB storage

That's a total of **768K cores**,
768 terabytes of RAM,
and a peak performance of
10 petaflops.
The system is capable of carrying out
10 quadrillion floating-point
operations per second.

2017年以后的下一代计算机



50 架

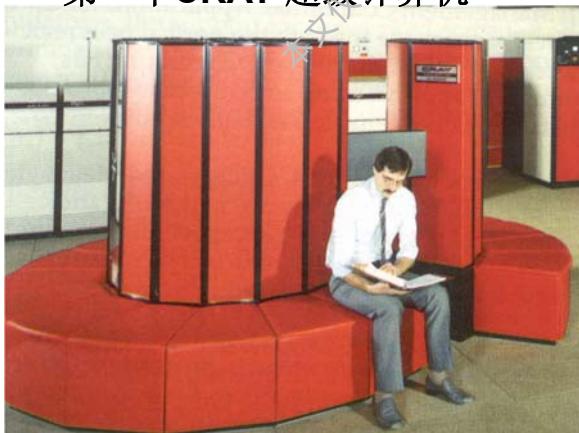
180千兆次浮点运算

0.18 百万兆次: 还不是超大规模计算

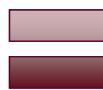
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高性能计算：过去，现在，未来!!

第一个CRAY 超级计算机



IPAD2



6千万 IPAD2

阿贡10兆次浮点超级计算机

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高性能计算使过去不可能的模拟成为可能..

- 将单个发动机模拟拓展到**1000核** (性能计算)

- 3千-5千万网格
- 先进的负荷均衡算法, 解决I/O 问题
- 500-1000 核上2-3 周

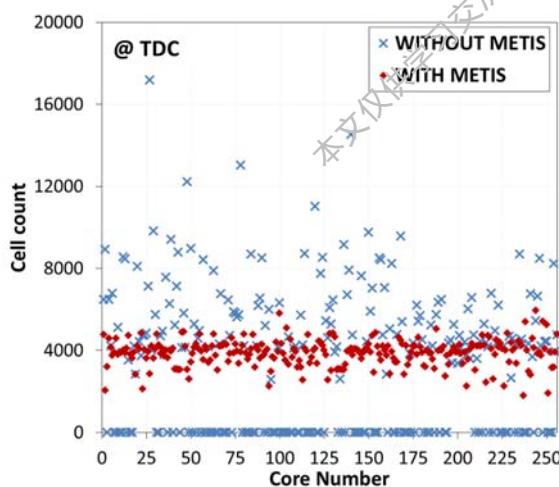


- 使用**1000多核完成多数 (100s)** 较小的模拟 (性能计算)

- 1百万-1千万网格每个项目
- 10-100 核上1-3 天
 - ❖ 优化发动机运行参数, 遗传算法
 - ❖ 发动机运行参数和模型参数不确定性分析
 - ❖ 多次LES 模拟以获得足够的统计数据
 - 喷雾LES
 - 喷嘴内流动LES



将高性能计算资源用于发动机模拟



科学成就

- 发动机模拟对内存有很高要求
- 加入先进的负荷平衡算法使高性能计算成为可能
- 高时间和空间精度
- 使用基于详细化学机理的燃烧模型

阿贡Fusion 集群



- METIS 是由明尼苏达大学开发的平衡负荷算法
- 在上止点, 若没有METIS, 单核上最大的网格数是 22136, 最小的是0。 使用METIS, 两者分别变为 5953 和 1805

在超级计算机上拓展发动机CFD模拟

来自S. Ciatti的汽油压燃发动机

- 上止点1千万网格
- 固定尺寸网格，无加密
- 运动边界和直喷



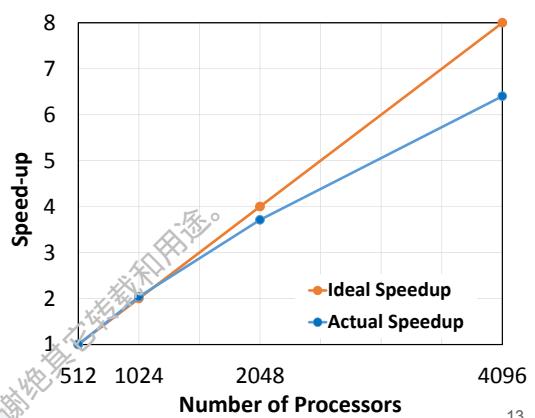
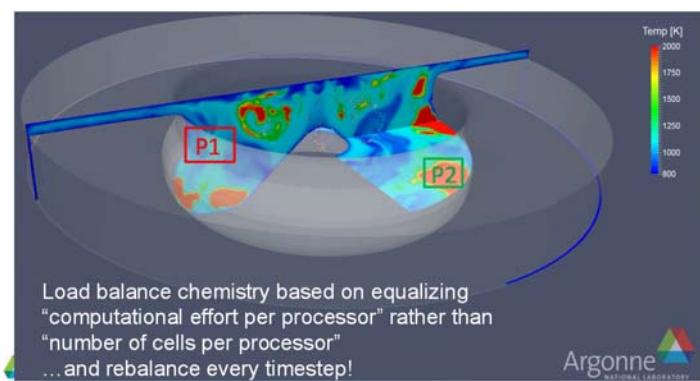
48 racks
1,024 nodes per rack
1.6 GHz 16-way core processor
16 GB RAM per node
384 I/O nodes
240 GB/s, 35 PB storage

That's a total of 768K cores,
768 terabytes of RAM,
and a peak performance of
10 petaflops.

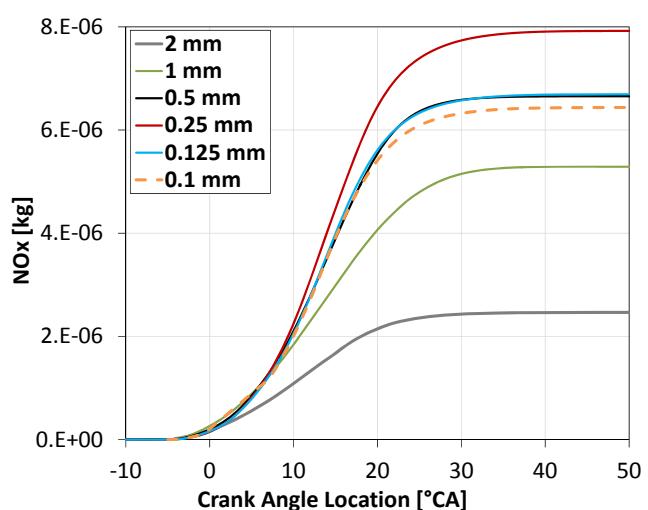
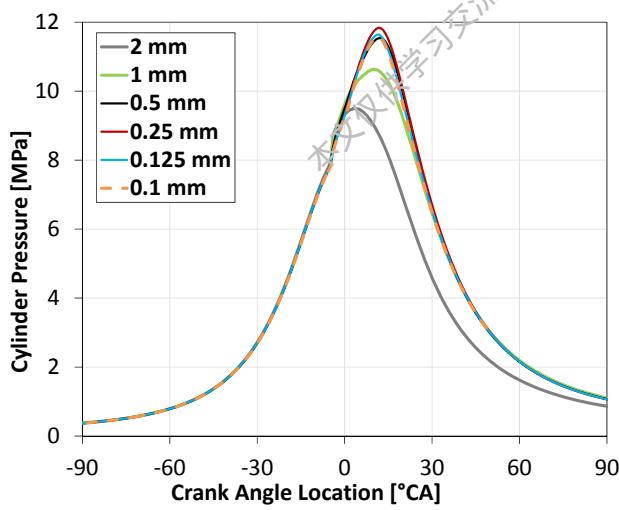
优化后在MIRA上运行：

- 加速重启 (>20x)
- 写重启文件 (500x)
- 加速输出和 post 文件 (1000x)
- 平衡化学反应计算负荷

在MIRA上的拓展性改进对工业界的较小模拟 (24-256 核)也很有用



利用高性能计算资源的柴油机模拟



最小网格(mm)	最大网格数	时间
0.5	2.5 million	14 hours on 64 cores
0.25	9 million	3.5 days on 64 cores
0.125	34 million	13 days on 256 cores
0.1	50 million	14 days on 512 cores

- Caterpillar 单缸机模拟
- 压力，放热率等参数在 0.5 mm 网格收敛
- NOx 在 0.125mm 网格收敛

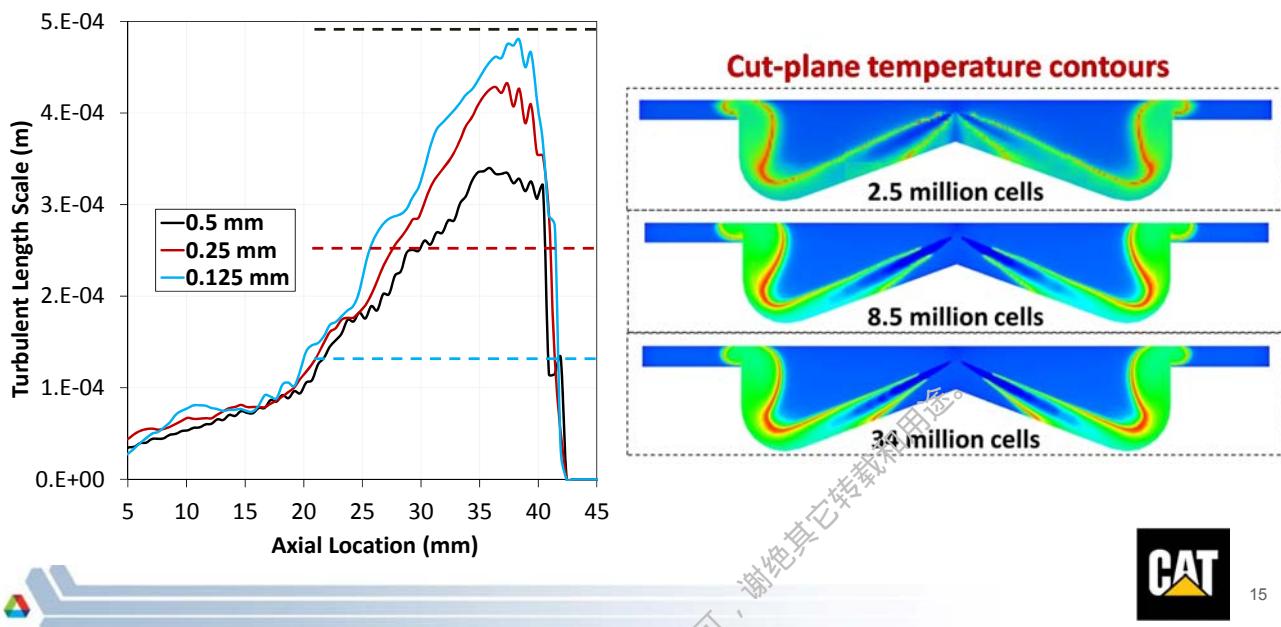
最大型的柴油机模拟!!

多数工业界的发动机计算都在24-64 核上进行



什么导致了网格收敛?

- **湍流尺度:**
 - 在粗网格 (0.5 mm) 上比网格尺寸小, 因此没有完全求解
 - 在细网格 (0.125 mm) 上比网格尺寸大, 因此可以完全求解
- **湍流时间尺度在0.25 mm收敛**



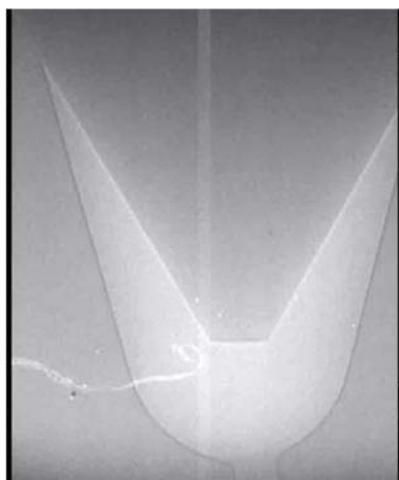
喷嘴内流动

1. M. Battistoni, Q. Xue, S. Som, "LES of Spray Transients: Start and End of Injection Phenomena," *Oil and Gas Science Technology*, 2015
2. M. Battistoni, D.J. Duke, A.L. Kastengren, A.B. Swantek, F.Z. Tilocco, C.F. Powell, S. Som, "Effect of Non-Condensable Gas on Cavitating Fuel Nozzles," Special Issue (invited) titled "Sprays in Automotive Applications" *Atomization and Sprays*, 25(6): 453-483, 2015
3. Q. Xue, M. Battistoni, C.F. Powell, D.E. Longman, S. Quan, E. Pomraning, P.K. Senecal, D.P. Schmidt, S. Som, "An Eulerian CFD Model and x-ray radiography for coupled nozzle flow and spray in internal combustion engines," *International Journal of Multi-phase Flows* 70, 77-88, <http://dx.doi.org/10.1016/j.ijmultiphaseflow.2014.11.012>, 2015
4. Q. Xue, M. Battistoni, S. Som, S. Quan, P.K. Senecal, E. Pomraning, D. Schmidt, "Eulerian CFD modeling of coupled nozzle flow and spray with validation against x-ray radiography data," *SAE International Journal of Fuels and Lubricants*, 7(2):2014, doi:10.4271/2014-01-1425
5. K. Saha, Y. Li, S. Quan, P.K. Senecal, M. Battistoni, S. Som, "Modeling of internal and near-nozzle flow of a GDI Fuel injector," *Proceedings of the ASME 2015 Internal Combustion Engine Division Fall Technical Conference*, ICEF2015-1112, November 2015

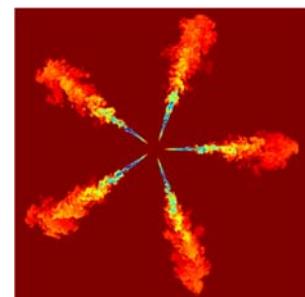
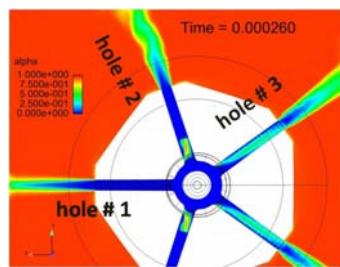
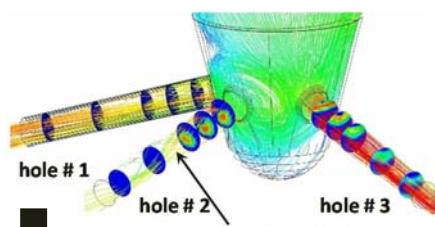
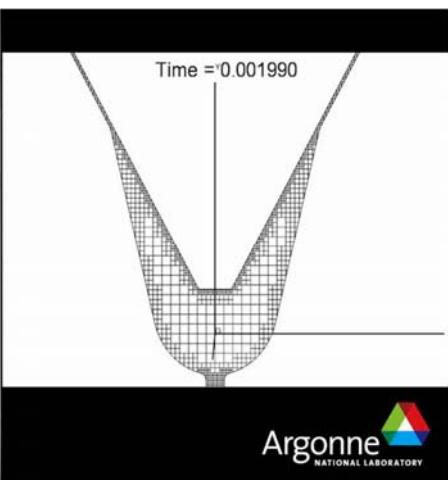


喷嘴内合喷嘴-喷雾耦合模拟

X-ray 相衬成像



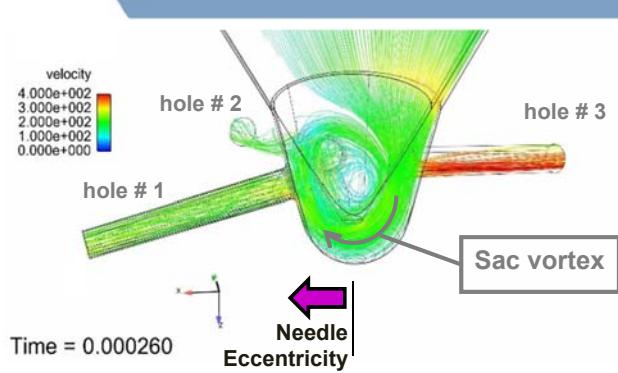
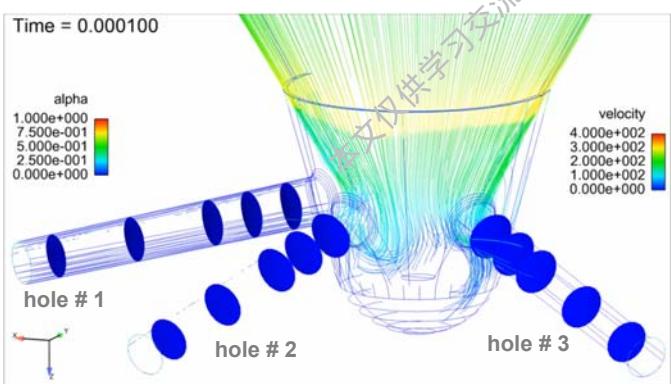
CFD 模拟



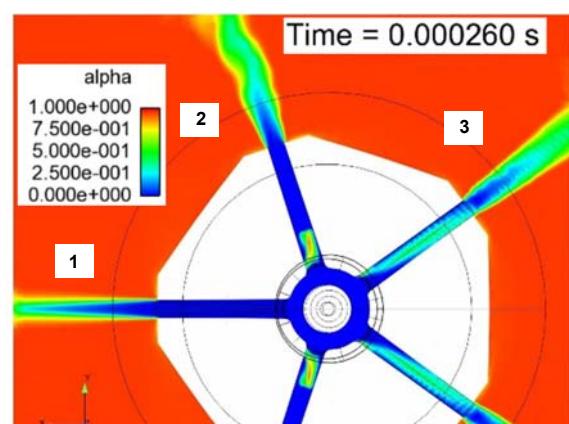
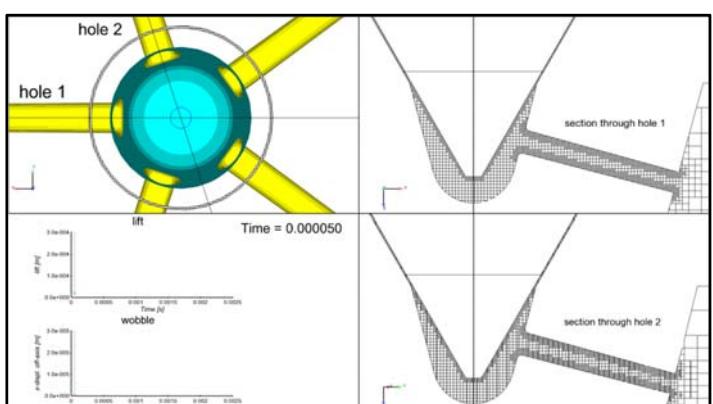
- 可以捕捉针阀偏向移动导致的油束-油束间差异
- 喷嘴-喷雾耦合
- 可以捕捉针阀偏向移动导致的周期性差异

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油束-油束间差异

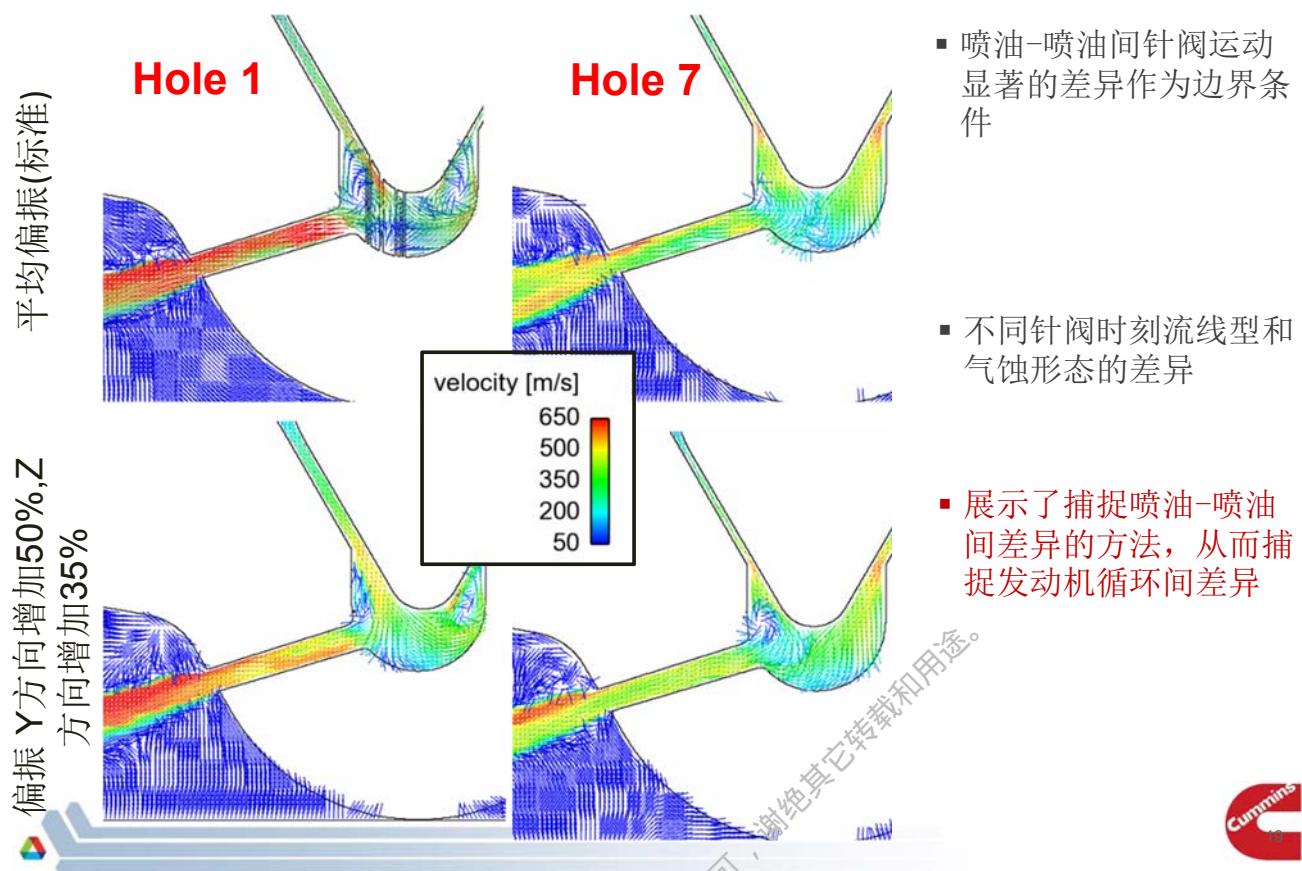


- 孔#2流出的涡流型油束
- 孔#3一半的截面被堵住



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喷油-喷油间的偏振=>发动机循环间差异

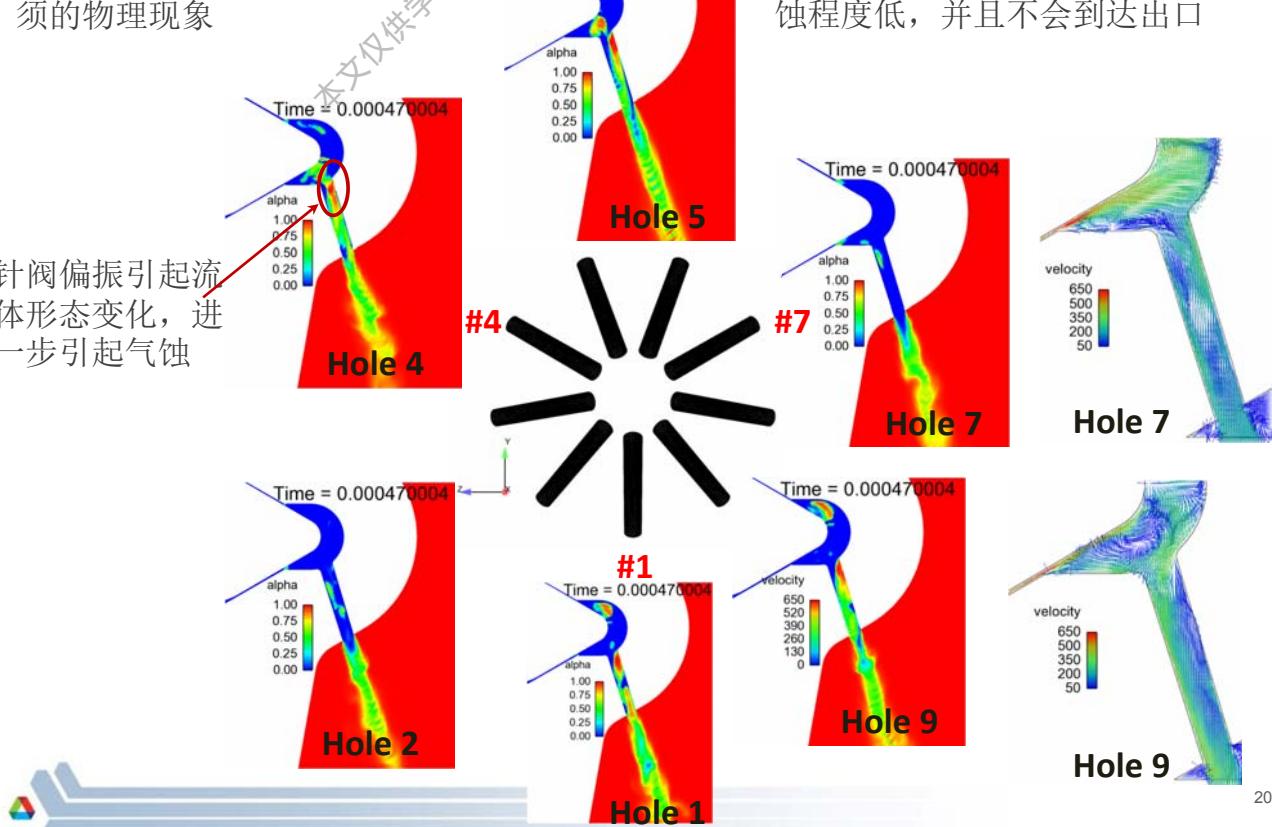


低针阀升程时孔-孔间差异

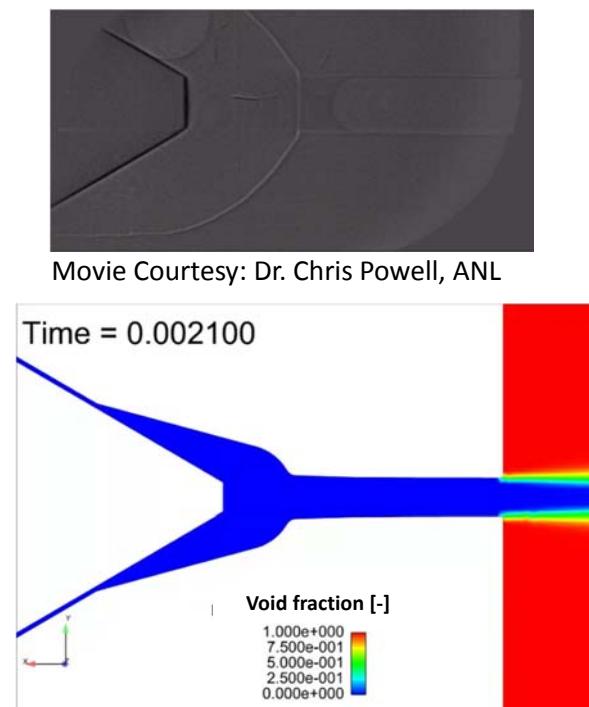
单孔或sector模拟不能捕捉必须的物理现象

针阀偏振引起流体形态变化，进一步引起气蚀

偏振使气蚀更明显。没有偏振，气蚀程度低，并且不会到达出口



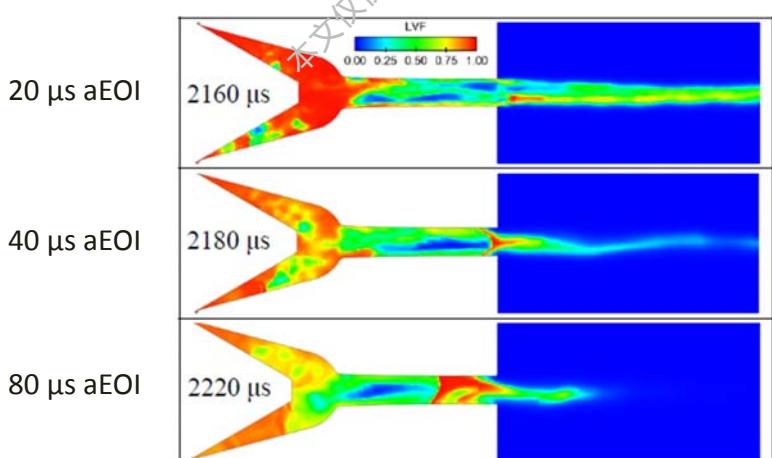
针阀瞬态：喷油末期



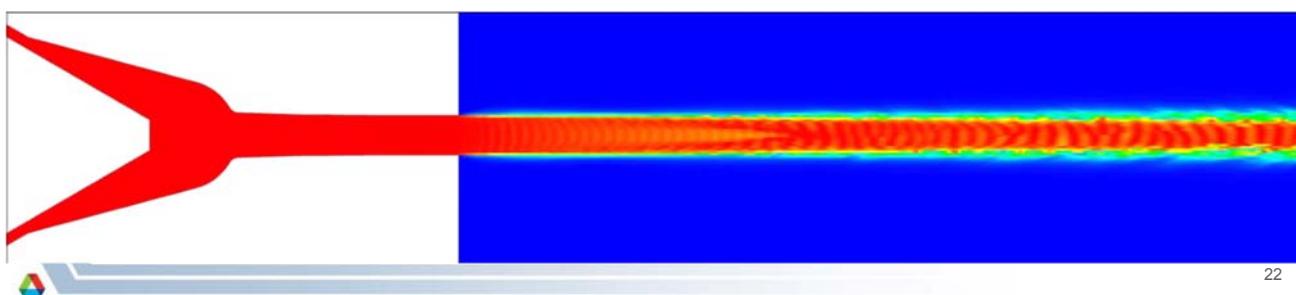
- 首次高精度模拟
- 最小网格 $5\text{ }\mu\text{m}$, 超过2千万网格
- 最小时间步长 $1\text{ E-}9$
- 模拟解释了被吸入喷嘴内气体的物理本质

喷油末期的油滴“泄露”

大涡模拟捕捉油滴“泄露”



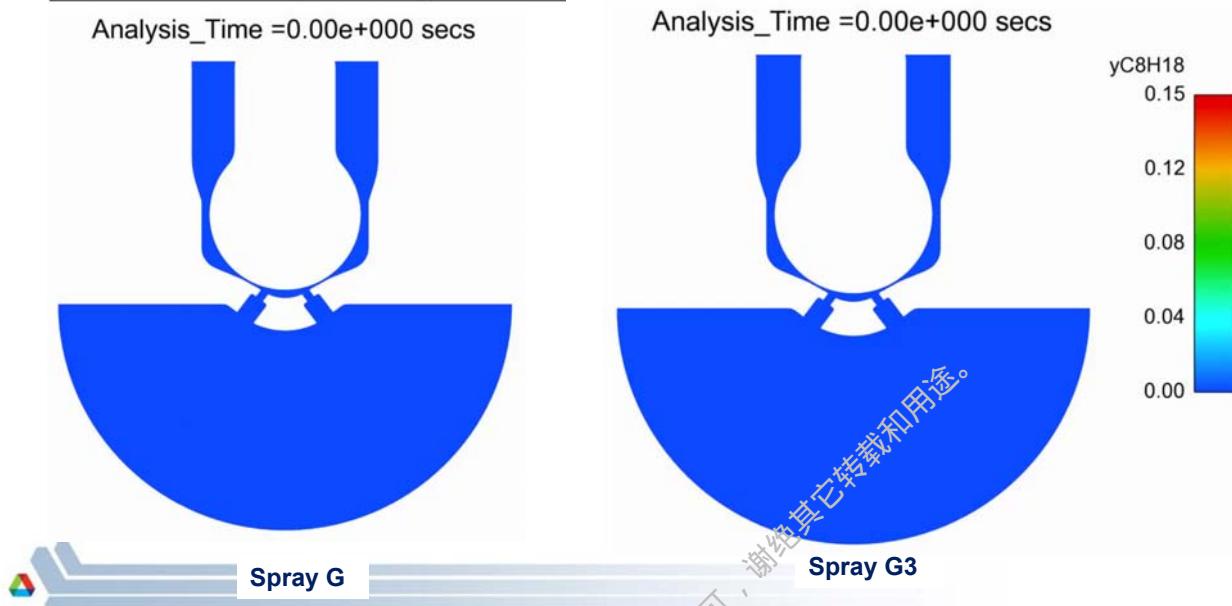
- 油滴“泄露”增加排放因为燃烧不充分
- 很难测量油滴“泄露”量
- 展示了应用LES模型捕捉单孔喷嘴油滴“泄露”（包含针阀偏振）
- 方法正确预测油滴对喷射压力和背压的敏感性



汽油直喷系统的闪沸

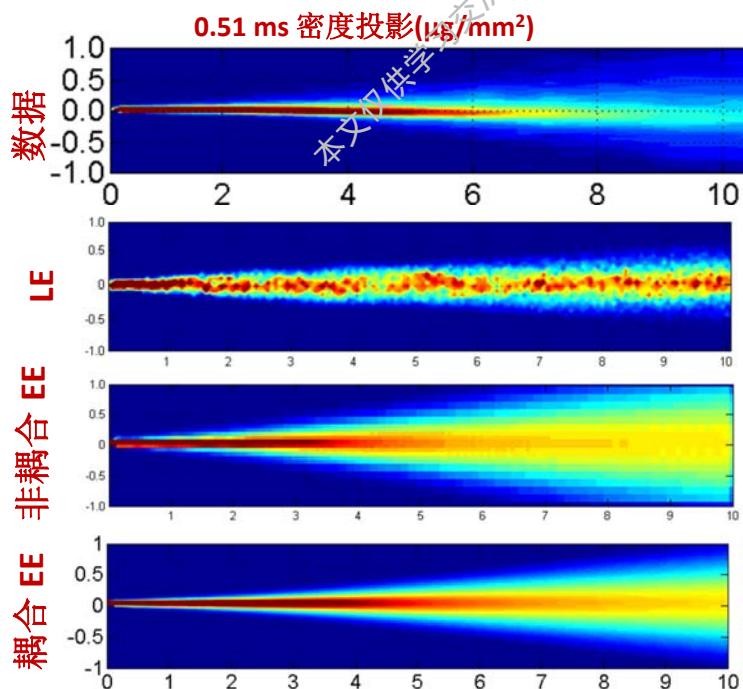
Parameters	Spray G	Spray G3
Inj. Press.(MPa)	20	20
Chamber Press.(kPa)	600	100
Chamber Temp.(K)	573	293
Fuel Temp.(K)	363	413
Chamber Fluid	N ₂	N ₂

强烈的闪沸=> 油束间相互作用

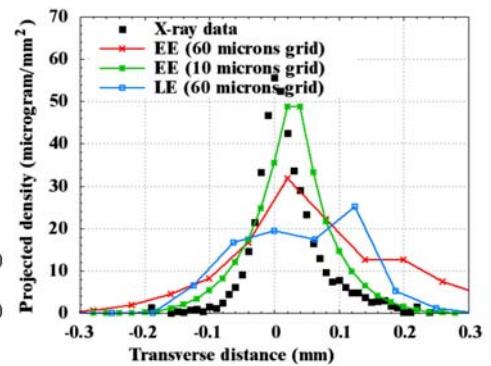


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欧拉和拉格朗日方法对比



- ❖ 耦合的欧拉-欧拉模型是非耦合欧拉-欧拉的3倍时长
- ❖ 对相同解析度，耦合的欧拉-欧拉模型是拉格朗日-欧拉模型5倍时长



- ❖ 在喷嘴附近，欧拉-欧拉模型优于拉格朗日-欧拉
- ❖ 拉格朗日模型：62.5μm 最小网格；blob 喷射模型；30万 parcels
- ❖ 如果喷油规律已知并且没有气蚀，非耦合欧拉-欧拉与耦合欧拉-欧拉效果类似



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LES湍流模拟

1. Z. Wang, A. Swantek, R. Scarcelli, D. Duke, A. Kastengren, C. Powell, **S. Som**, R. Reese, K. Freeman, Y. Zhu, "LES Modeling of Diesel and Gasoline Sprays with Validation Against X-ray Radiography data," *SAE International Journal of Fuels and Lubricants*, doi:10.4271/2015-01-0931, 2015
2. Y. Pei, **S. Som**, E. Pomraning, P.K Senecal, S.A. Skeen, J. Manin, L. Pickett, "Large Eddy Simulation of a Reacting Spray Flame with Multiple Realizations under Compression Ignition Engine Conditions," *Combustion and Flame*; 000: 1-14, 2015
3. P.K. Senecal, E. Pomraning, Q. Xue, **S. Som**, S. Banerjee, B. Hu, K. Liu, J. Deur, "Large Eddy simulation of vaporizing sprays considering multi-injection averaging and grid-convergent mesh resolution," *Journal of Engineering for Gas Turbine and Power* 136 (11), 111504: 1-13, 2014
4. Q. Xue, **S. Som**, P.K. Senecal, E. Pomraning, "Large Eddy Simulation of Fuel Spray Under Non-Reacting IC Engine Conditions," *Atomization and Sprays* 23(10), 925-955, 2013
5. B. Hu, S. Banerjee, K. Liu, D. Rajamohan, J.M. Deur, Q. Xue, **S. Som**, P.K. Senecal, E. Pomraning, "Large Eddy Simulation of a turbulent non-reacting spray jet (Spray H)," *Proceedings of the ASME 2015 Internal Combustion Engine Division Fall Technical Conference*, ICEF2015-1033, November 2015



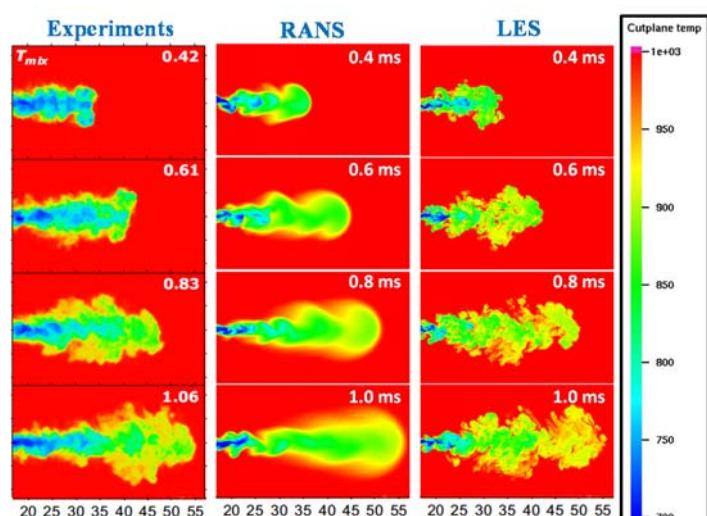
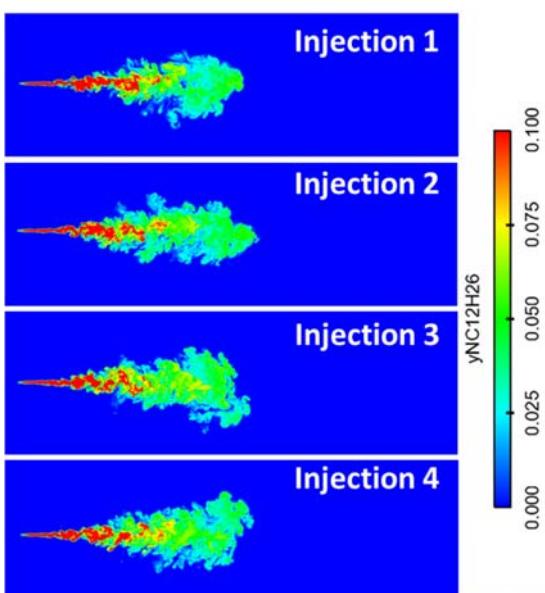
<http://www.verifi.anl.gov/>

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LES湍流模拟

模拟设置

- 针对内燃机模拟开发 Dynamic structure LES 模型
- 高时间和空间精度导致较少的模拟（参数假设）

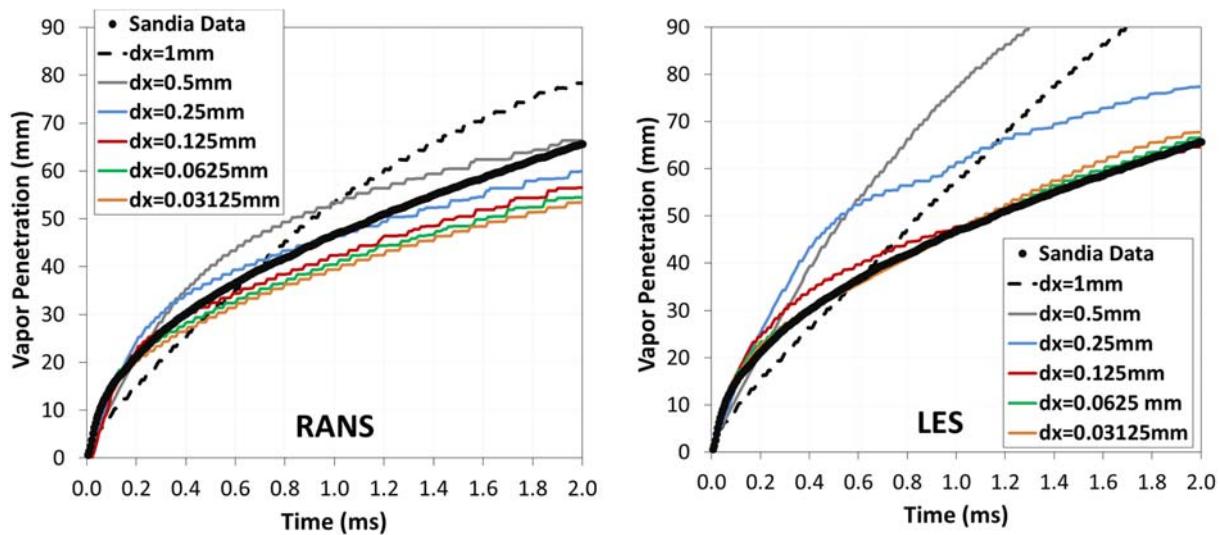


项目影响

- LES 模型能捕捉流场结构，而RANS则不能
- LES 也能捕捉循环间差异

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简化 (RANS) vs. 高精度 (LES) 湍流模型

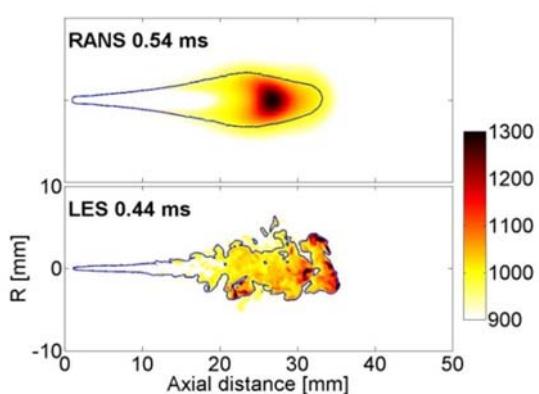


- RANS 结果在网格收敛的情况下不能捕捉实验数据。
- LES (Dynamic structure 模型) 结果能捕捉实验数据
- 这是因为LES 求解更多的流体结构，因此能更好预测燃油-空气混合
- 实验数据来自 Sandia National Laboratory ECN Spray A

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LES用于喷雾和燃烧模拟

- 我们将 LES 喷雾模拟与 CONVERGE 燃烧求解器 SAGE 结合
- ✓ 大量与 Engine Combustion Network 数据验证



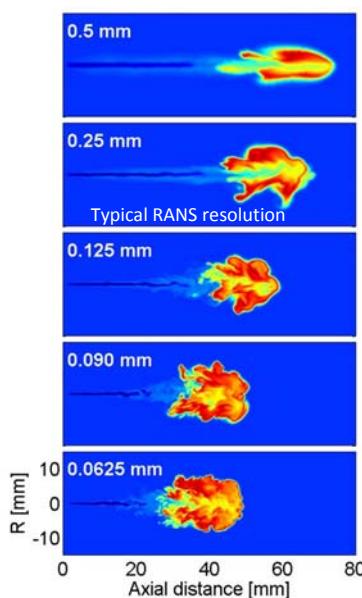
- LES高时间和空间精度导致较少的模拟
- LES 模型能捕捉RANS不能的流体结构
- LES 捕捉自燃现象
- LES 还能捕捉循环间差异

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LES的网格精度和多次 喷射模拟

不同LES喷射对应的温度分布
@ 62.5 μm

不同网格对应的温度分布



- 网格收敛性接近 62.5 μm
- 每一次喷射在200核上需 3 周，大于 2千5百万网格

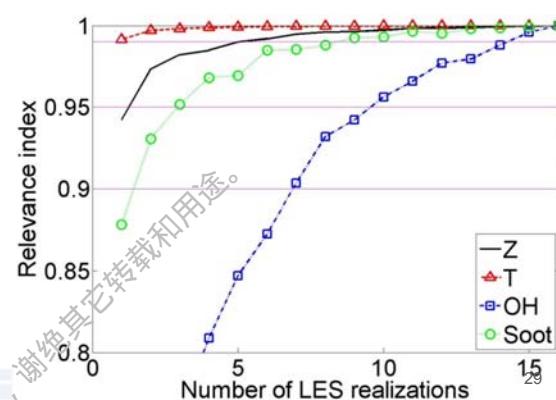


工业界的问题: 多少次LES喷射才能达到统计学上的收敛数据?

- 温度: 2
- 混合物分数(Z): 5
- 炭烟: 8

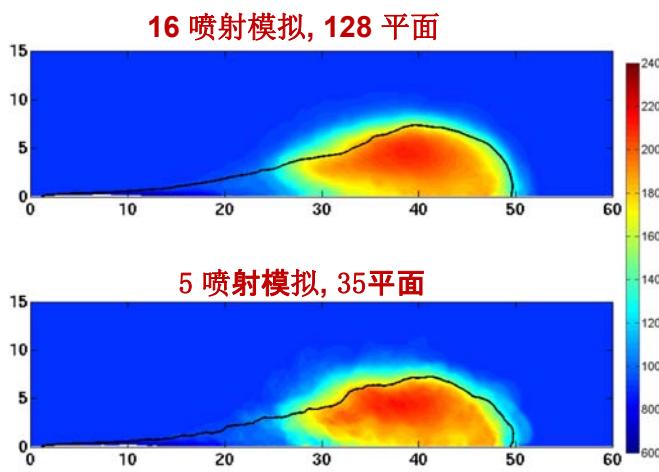
$$\text{相关性指} = \frac{\langle \vec{\phi}_i, \vec{\phi}_b \rangle}{\| \vec{\phi}_i \| \| \vec{\phi}_b \|}$$

“i” 任意一次喷射
“b” 总喷射次数

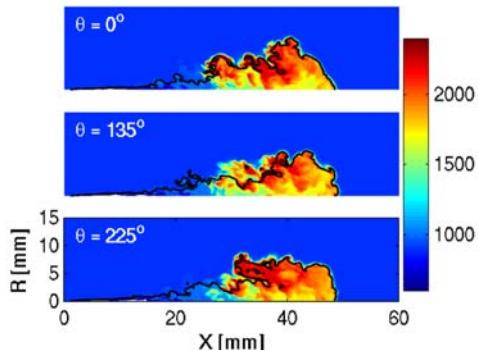


使用方位角平均来减少计算成本

- 我们能否利用轴对称性来减少喷射模拟的次数?



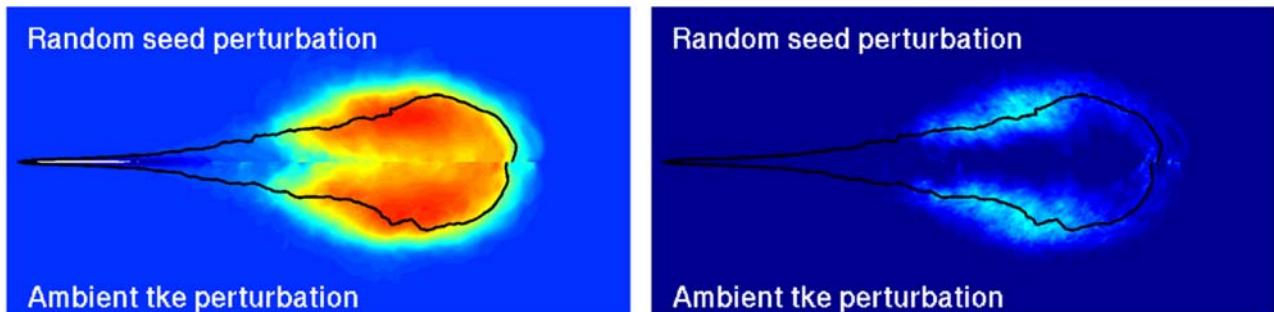
对5次喷射模拟使用方位角平均显著减少计算成本!



- 对16次喷射模拟的每一次都在 128个平面上用方位角平均
- 由相关性分析可知
 - 最少的喷射模拟次数
 - 最小的平面数

扰乱环境湍流强度

通常我们扰乱随机数种子来获得不同LES喷射间的差异

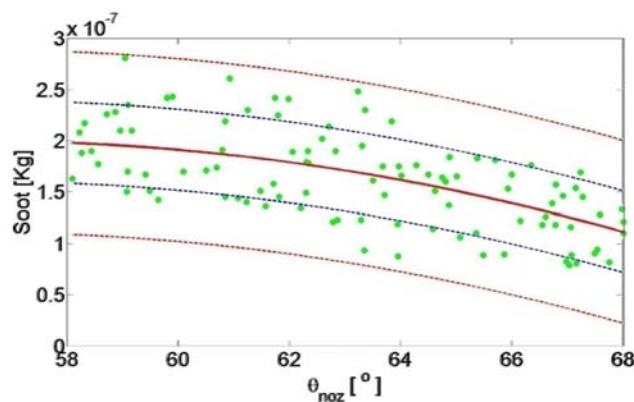


- 上半区: 根据**随机数种子**扰动平均
- 下半区: 根据**环境湍流强度**扰动平均
- 对环境湍流强度扰动, 模拟了5次喷射, 环境湍流强度为 $0.1, 0.6, 1.2, 5.0$ and $10 \text{ m}^2/\text{s}^2$
- 扰动环境湍动能产生相似的平均温度和OH质量分数。

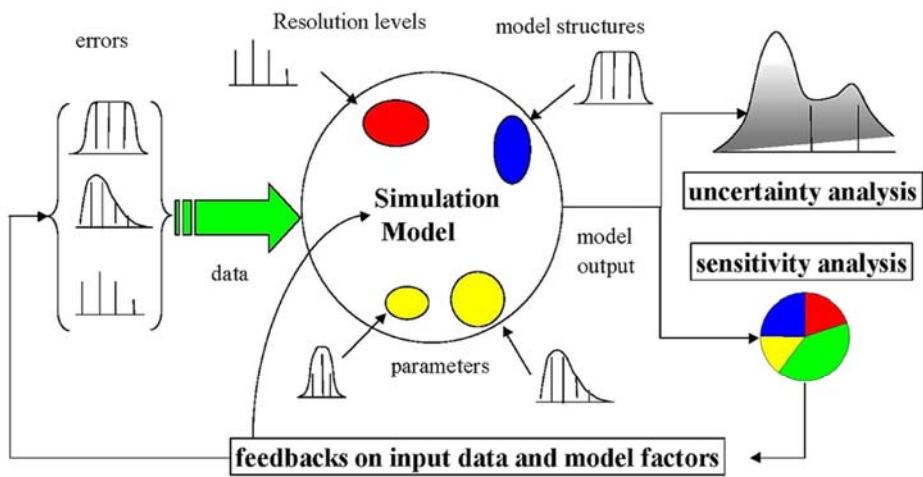
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不确定性分析

1. Y. Pei, M.J. Davis, L.M. Pickett, S. Som, "Engine Combustion Network (ECN): uncertainty quantification of Spray A for different combustion vessels," *Combustion and Flame*; 162: 2337-2347, 2015
2. Y. Pei, R. Shan, S. Som, T. Lu, D.E. Longman, M.J. Davis, "Global sensitivity analysis of a diesel engine simulation with multi-target functions," SAE Paper No. 2014-01-1117, April 2014



敏感性分析

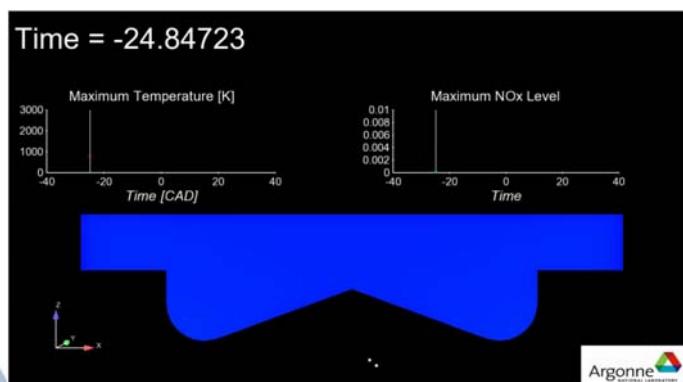


- 不确定性有很多来源:
 - 实验
 - 参数预估
 - 模型结构
- 通过模型传递
- 他们的相对重要性通过敏感性分析量化
 - 设计实验
 - 获得更精确预测

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发动机参数不确定性分析

- CAT 单缸机闭循环模拟
- 32 不确定变量 (实验和模拟) 可能影响模拟结果
- 所有的变量在不确定性的范围内使用蒙特卡洛采样同时，随机被扰动
- 全局敏感性分析(GSA) 帮助理解某一不确定参数对目标的影响
- GSA 代码由阿贡化学工程部Dr. M.J. Davis开发

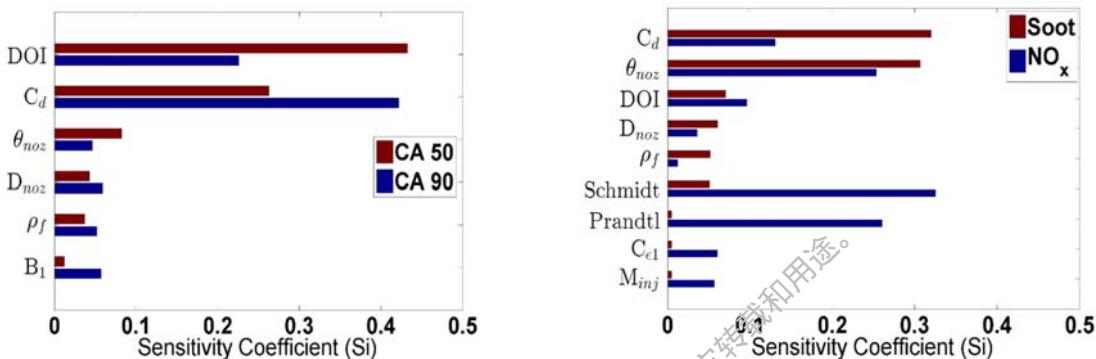


Variable	Description	Baseline	Min.	Max.
T_{piston}	piston wall temperature [K]	553	538	568
T_{cylinder}	cylinder wall temperature [K]	433	423	443
T_{head}	Cylinder head temperature [K]	523	508	538
RPM	engine speed [RPM]	1500	1495	1505
SR	Swirl Ratio	0.98	0.95	1.00
Schmidt	Schmidt number	0.78	0.70	0.90
Prandtl	Prandtl number	0.9	0.8	1.0
I_{turb}	initial turbulence intensity [m^2/s^2]	1.6	1.0	2.0
L_i	initial length scale [mm]	11.2	5.0	15.0
M_{res}	residual mass [mg]	0.05	0.02	0.10
$T_{\text{c,cr}}$	fuel critical temperature [K]	657	645	659
ρ_f	Normalized fuel density	1.00	0.95	1.05
HOV_f	Normalized fuel heat of vaporization	1.0	0.9	1.1
VP_f	Normalized fuel vapor pressure	1.0	0.9	1.1
μ_f	Normalized fuel viscosity	1.0	0.7	1.3
Parcosei	total parcels injected	1.0E+6	1.0E+5	2.0E+6
B_0	KH breakup length constant	0.60	0.55	0.65
B_1	KH breakup time constant	7	5	15
Parcnew	new parcel cut off	0.05	0.03	0.07
$C_{\text{RT},0}$	RT time constant	1.0	0.5	2.0
C_{RT}	RT size constant	0.1	0.1	1.0
D_{noz}	nozzle diameter [microns]	169	164	174
θ_{noz}	nozzle orientation angle [degrees]	63	58	68
C_d	discharge coefficient	0.70	0.65	0.85
θ_{cone}	spray cone angle [degrees]	9	7	15
SOI	start of injection [°CA]	-7.7	-8.2	-7.2
DOI	duration of injection [°CA]	25.7	23.7	27.7
M_{inj}	total fuel mass injected [mg]	13.00	12.35	13.65
T_{inj}	injected fuel temperature [K]	312.9	307.0	317.0
D_{diffus}	fuel mass diffusivity constant [m^2/s]	3.7E-6	1.9E-6	5.6E-6
$C_{\text{diss},1}$	dissipation constant 1	1.42	1.35	1.50
$C_{\text{diss},2}$	dissipation constant 2	1.68	1.60	1.76

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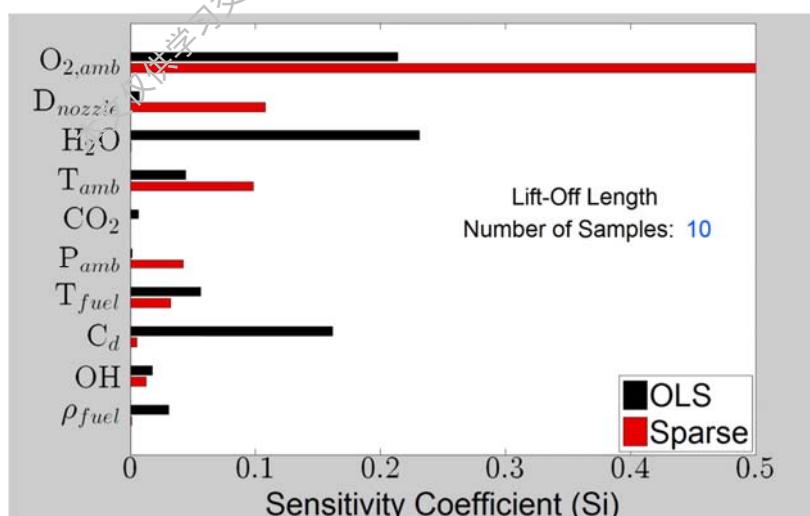
变量对目标的敏感性

- 每个转速-符合点100个模拟，用稀疏算法取得统计上收敛的结果
 - 每个算例在48核上40–50小时
 - 最大网格数：2百万（最小网格0.25 mm）
- 相对一次只能扰动一个变量的强力计算，GSA显得更有效
 - ✓ 能捕捉变量间和变量对目标的非线性相互影响
 - ✓ 计算高效



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收敛性排序：最小二乘 vs. Sparse



➤ 最小二乘 vs. 稀疏技术 对lift-off length:

- 900 K 条件下分析340个算例
- 前10排名如图所示，剩下的7个敏感性小于0.01
- 收敛后，两种方法的排序是相同的
- 取得合理的收敛的排序：
 - 最小二乘和稀疏技术60次
 - 稀疏技术30次能得出合理排序

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应用于低温燃烧概念开发

1. Z. Wang, R. Scarcelli, S. Som, S.S. McConnell, N. Salman, Y. Zhu, K. Freeman, K. Hardman, R.A. Reese, P.K. Senecal, M. Raju, S.D. Gilver, "Multi-dimensional modeling and validation of combustion in a high-efficiency dual-fuel light-duty engine," SAE Paper No. 2013-01-1091, April 2013
2. Y. Zhu, N. Salman, K. Freeman, R. Reese, Z. Wang, R. Scarcelli, S. Som, "Numerical study of the combustion characteristics of a turbocharged DI gasoline engine with diesel micro pilot ignition and cooled EGR," *Proceedings of the ASME 2013 Internal Combustion Engine Division Fall Technical Conference*, ICEF2013-19170, October, 2013
3. J. Kodavasal, C. Kolodziej, S. Ciatti, S. Som, "CFD Simulation of Gasoline Compression Ignition," *Journal of Energy Resource Technology*; 137(3):032212-032212-13, JERT-15-1029, 2015



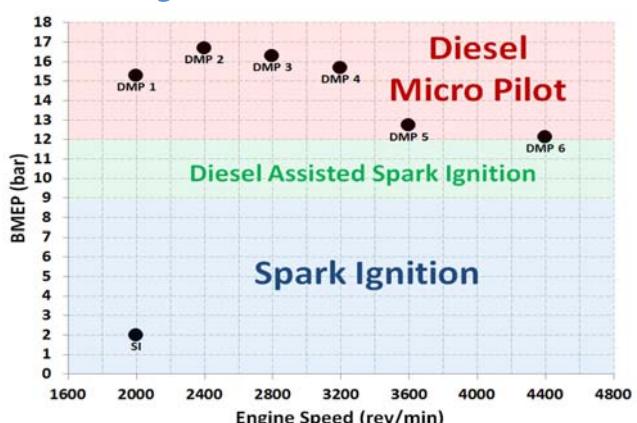
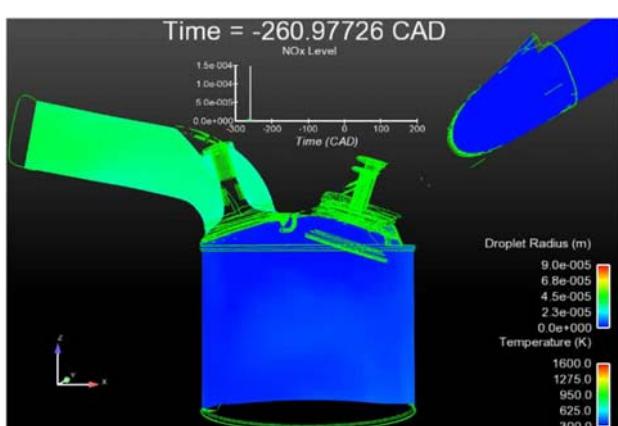
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Dual - Fuel Combustion with Chrysler LLC.

项目影响

- 为克莱斯勒开发在SI, DASI, 和 DMP 间灵活转换的燃烧策略
- 双燃料策略: 柴油作为点火能量, 汽油直喷贡献主要放热



科学成就

- 用基于遗传算法的优化取得发动机运行和排放的优势
- NOx 和 炭烟排放均有降低
- 模拟帮助实验发现最优的运行参数

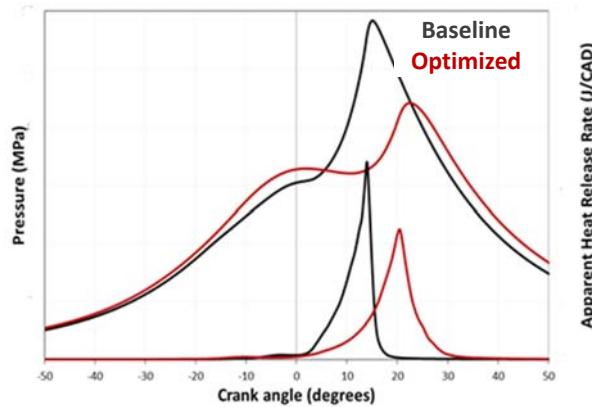
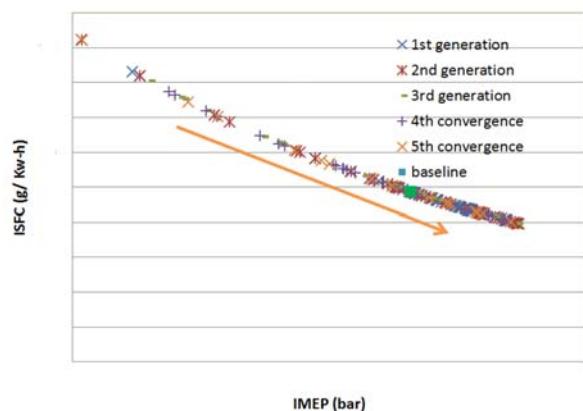


Argonne contributors: Z. Wang, R. Scarcelli, S. McConnell

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优化的结果

50代(每代8个模拟):总共400个模拟
每个模拟在48核上用40-50小时
最大网格数:3百万



Parameters	Baseline	Optimized
EGR ratio (%)	35.3	↓
ICL (° CA ATDC)	461.8	↓
DMP ratio (%)	13.4	↓
Diesel SOI (° CA BTDC)	19.5	↑

Argonne contributors: Z. Wang, R. Scarcelli, S. McConnell



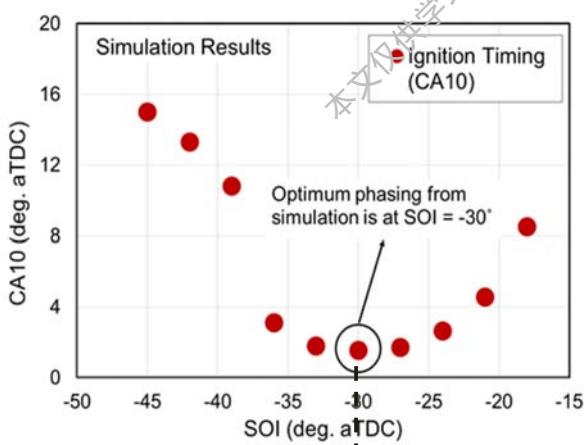
优化显示:

- 更高进气压力
- 较早和更早的柴油喷射

导致:

- 滞燃的燃烧相位
- 更长的燃烧持续期

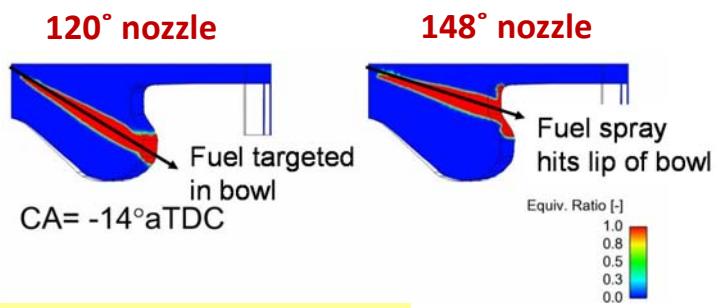
优化汽油压燃发动机



- 优化阿贡汽油压燃发动机
- 推迟SOI，滞燃期缩短因为燃油分层更加明显
- 但是，滞燃期的缩短比停留时间的缩短少(因为SOI推迟)
- 因此，当SOI迟于“最优点”后，自然推迟直到失火

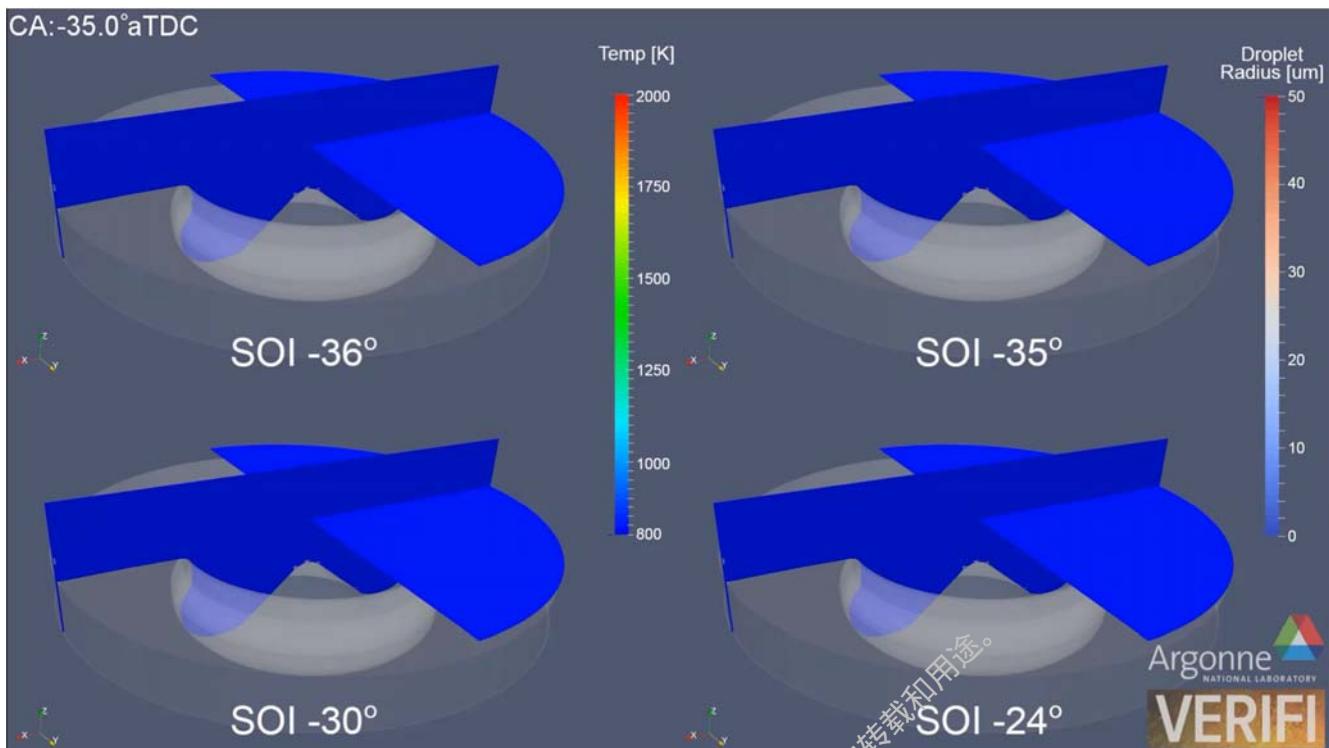
- 喷射角度是获得良好燃烧效率的关键

更多的燃油在挤气间隙，
更多地热损失和更低的
反应活性
对自然动力学合适的停留时间快
速减少



Experimental data from Argonne: S. Ciatti, C. Kolodziej

用高性能计算优化汽油压燃发动机喷油时刻



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结论

- 高性能计算让5年前都不可行的计算成为可能
 - 不久的将来发动机模拟的变革
- 一百万核小时(集群上)是常规的并且可以提供独特性的结果。展示的案例:
 - 优化, 不确定性分析
 - 多循环模拟, 特别是用LES
 - 喷嘴内流体LES模拟
- 模拟比实验更快, 但是取决于应用, 他们能提供实验不能提供的数据, 例如, 敏感性分析, 不确定性量化
- 我们为工业界伙伴修正了针对发动机模拟的“最优策略”
- 为了利用下一代计算架构(千万亿级别和更高), 把计算拓展到1000多核是非常重要的
 - 高的时间和空间上精度, 现今湍流, 湍流燃烧模型, 详细反应机理, 稳定的多相流模型
 - 这些模拟产生大量数据, 需要高效的数据挖掘来协助“工程”等级的简单模型的开发

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High Performance Computing Enabling a Paradigm Shift in Engine CFD



Dr. Sibendu Som

Principal Mechanical Engineer - Argonne National Laboratory
Computational Fellow – University of Chicago

CONVERGE USER GROUP MEETING

November 2015



Key Steps For GSA

- Simulations varying all variables over uncertainty ranges simultaneously
 - Fit the response (ignition delay, liquid length, etc) to the uncertainties
- $$t_{ign}(\{u_i\}) = t_0 + \sum A_i(u_i) + \sum \sum B_{ij}(u_i, u_j) + \dots, u_i \text{'s : uncertainties}$$
- $$A_i(u_i) = \sum_{k=1}^4 a_{ik} u_i^k$$
- The fit of the response to the uncertainties leads to a variance associated with each variable (partial variance: V_i)
 - Calculate sensitivity coeffs., $S_i = V_i/V, \sum S_i \cong 1$, (V : total variance)

Eulerian Mixture & Cavitation Model

Mixture Model equations (homogeneous multi-phase model)

Continuity: $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0$

Momentum: $\frac{\partial \rho \vec{v}}{\partial t} + (\nabla \cdot \rho \vec{v}) \vec{v} = -\nabla p + \nabla \cdot \bar{\tau} + \rho \vec{f}$

Species: $\frac{\partial \rho Y_i}{\partial t} + (\nabla \cdot \rho Y_i) \vec{v} = \nabla \cdot (\rho D_i \nabla Y_i) + S_i$

(plus: Energy, Turbulence)

mixture density: $\rho = \sum_{i=1}^n \alpha_i \rho_i$

volume & mass fractions: $\alpha_i \rho_i = Y_i \rho$

void fraction: $\alpha_g = \frac{Y_g / \rho_g}{\sum Y_i / \rho_i}$

Mass transfer: Homogeneous Relaxation Model (HRM) ^{1,2}

The model accounts for non-equilibrium heat transfer phenomena, using an empirical correlation

Hypothesis: finite rate of relaxation to equilibrium

$$\frac{dY_v}{dt} = \frac{Y - \bar{Y}_v}{\Theta}$$

Exponential relaxation of the vapor quality Y to the equilibrium table value \bar{Y}_v over a timescale Θ .

$$\bar{Y}_v = \frac{h - h_l}{h_v - h_l} \quad \Theta = \Theta_0 \alpha^a \psi^b \quad \psi = \left| \frac{p_{sat} - p}{p_{crit} - p_{sat}} \right|$$

Mixture: 1. liquid + 2. vapor + 3. air

1. Schmidt, D. P., et al., *Int. J. of Multiphase Flow*, 2012
2. Bilicki and Kestin, *Proc. Roy. Soc. Lond. A.*, 1990

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Further Details About Eulerian Mixture Model

- VOF method used to model the internal nozzle two-phase flow with cavitation description closed by the homogeneous relaxation model
- Eulerian single velocity field approach by Vallet et al. (2001) is implemented for near-nozzle spray simulations
 - Large scale flow features dominate rather than the small scale structures under the high Reynolds and Weber number conditions
- This approach considers the liquid and gas phases as a complex mixture with a highly variable density to describe the dense spray region
 - Mean density is obtained from Favre-averaged liquid mass fraction: $\frac{1}{\bar{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1 - \tilde{Y}}{\rho_g}$
- The liquid mass fraction is transported with a model for the *turbulent liquid diffusion flux into the gas*: $\frac{\partial \tilde{\rho} \tilde{Y}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{Y}}{\partial x_i} = -\frac{\partial \widetilde{\rho u'_i Y'}}{\partial x_i} - \tilde{\rho} \tilde{Y}_{evap}$
- Closure for the liquid mass transport is based on a turbulent gradient flux model:

□ Void fraction (α) = $\begin{cases} 0 & \text{if the computational cell is filled with pure liquid} \\ 1 & \text{if the computational cell is filled with pure gas} \\ (0, 1) & \text{if the computational cell is filled with both liquid and gas} \end{cases}$

$$\widetilde{\rho u'_i Y'} = \frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}}{\partial x_i}$$

Core Capabilities & Collaborations

Large variety of engine platforms and fuels

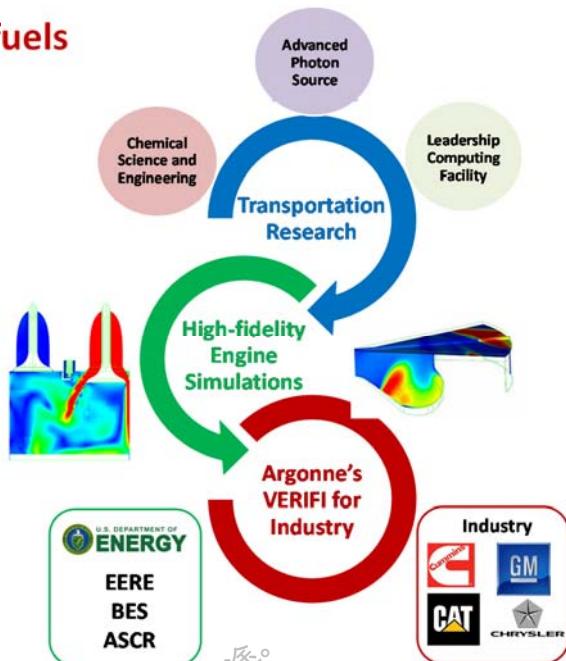
- Light- and heavy-duty engines
- CI – SI – LTC – Dual-fuel
- Gasoline – Diesel – Biofuels
- Gasoline Compression Ignition

Model Development

- Nozzle internal flow
- Sprays
 - Lagrangian models
 - Eulerian models
- Detailed chemistry
- Mechanism reduction
- RANS and Large Eddy Simulations
- Cyclic variability
- Turbulence chemistry interaction
- Optimization
- Uncertainty Analysis

Computational resources

- Clusters and Super-Computer Facility



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