

●

多相多组分渗流模拟软件项目

OpenCAEPoro

张晨松，中科院数学院

2023年04月21日，内部交流版

AMSS, Chinese Academy of Sciences

报告内容

01

背景介绍

Application
Background

02

开源项目

Open-Source
Projects

03

数值方法

Numerical
Methods

04

发展规划

Development
Plans



01

背景介绍

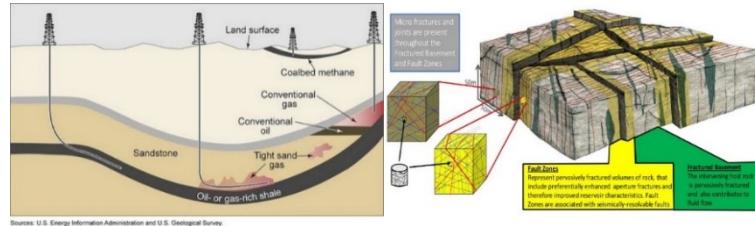
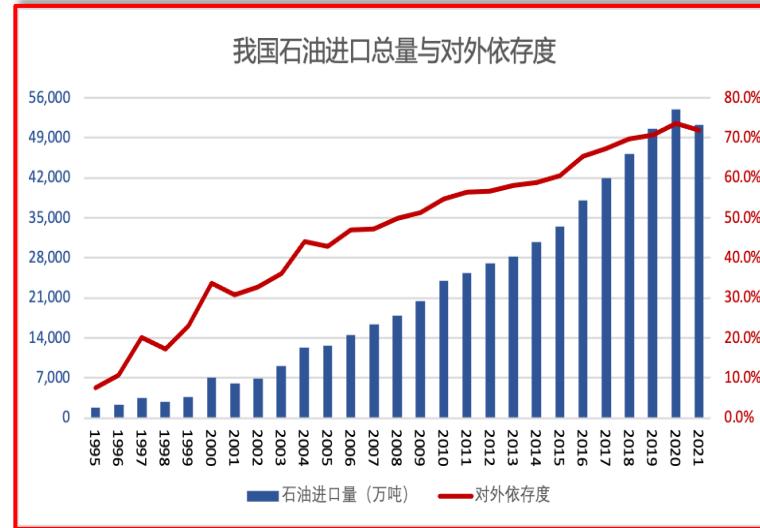
Significance and background of reservoir simulation



多相多组分渗流力学问题

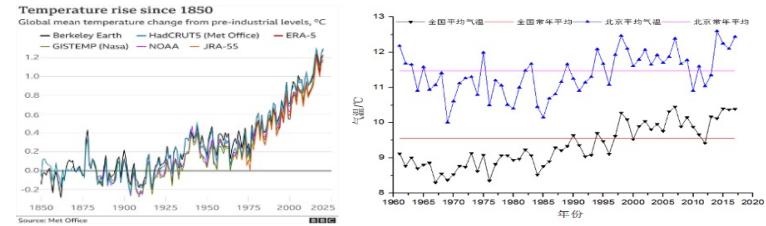


能源困局

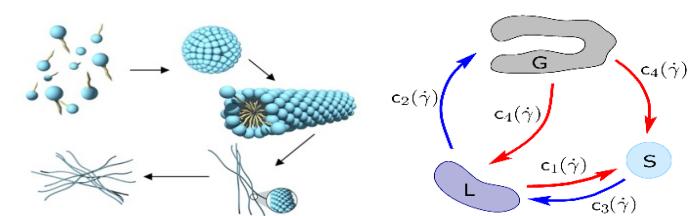
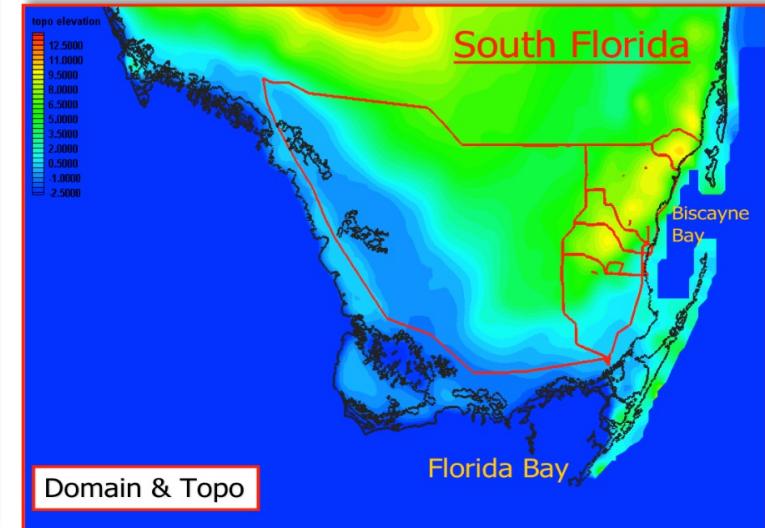


传统油藏、页岩油气、凝析气藏

双碳目标



地热开发、二氧化碳埋存

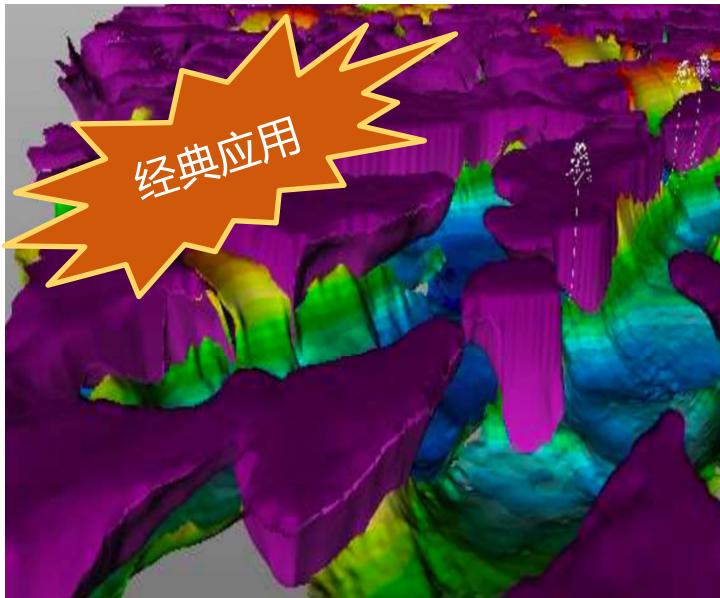


地下水污染处理、核废料埋存

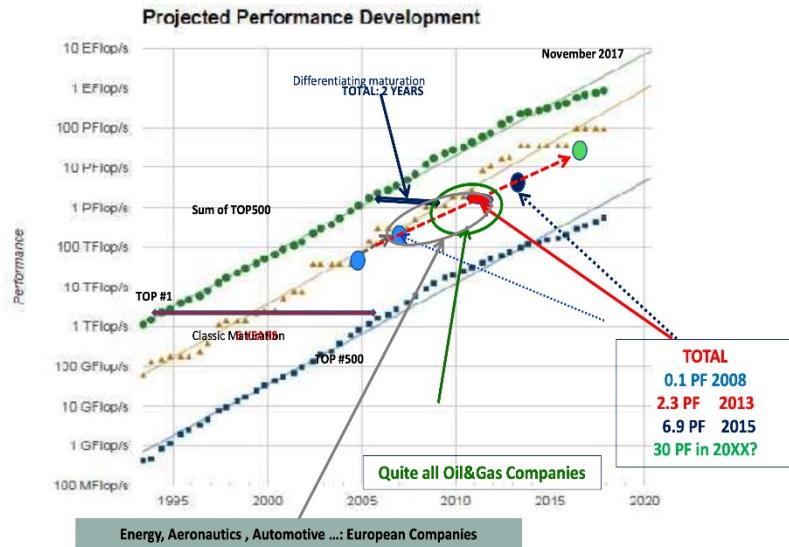
研究目标：为相关应用场景，提供一个开源、现代化、高效、并行模拟软件包



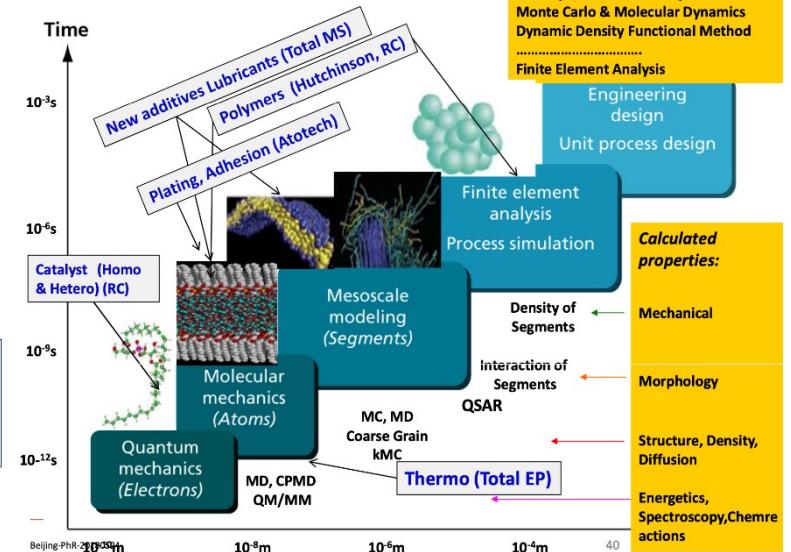
油气开发工程中的应用



TOTAL WELL PLACED INTO HPC PERFORMANCE (TOP 500)



TOTAL APPLICATION: MOLECULAR SIMULATION



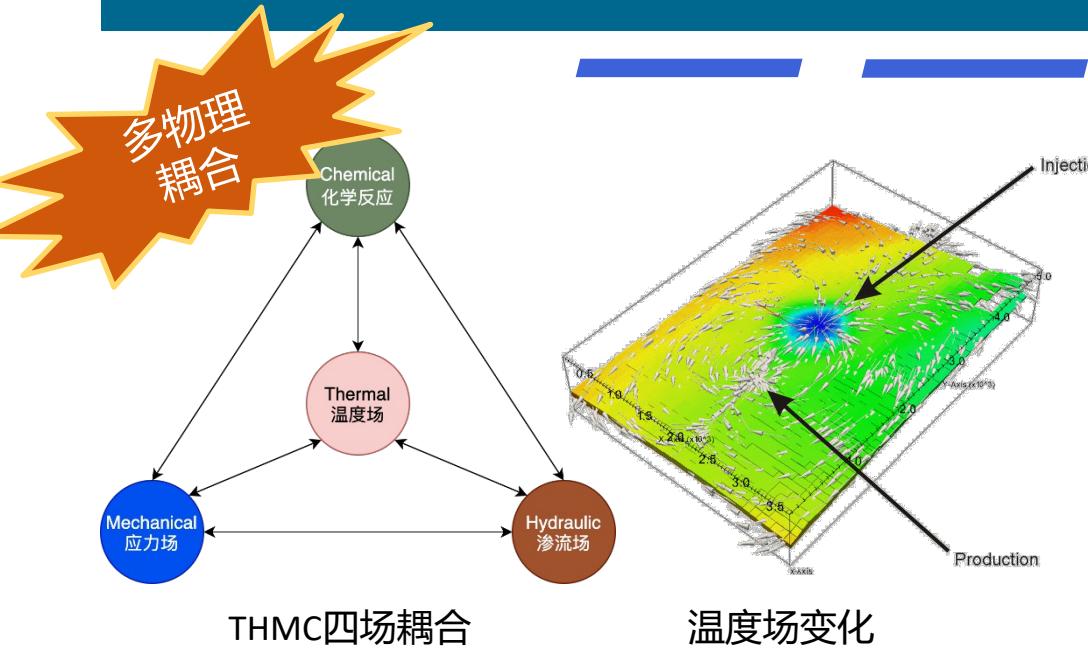
- 难点：多介质、多尺度、多物理、不确定性、高分辨率、.....
- 精细的数值模拟需要更符合物理的模型，更高的空间、时间分辨率，所以常需要大规模并行模拟
- 大规模油气勘探开发数值模拟是超算的主要发展动力之一
- 国际大型石油公司拥有世界一流的HPC计算资源（硬件、软件、人才）



地热能源开发中的应用



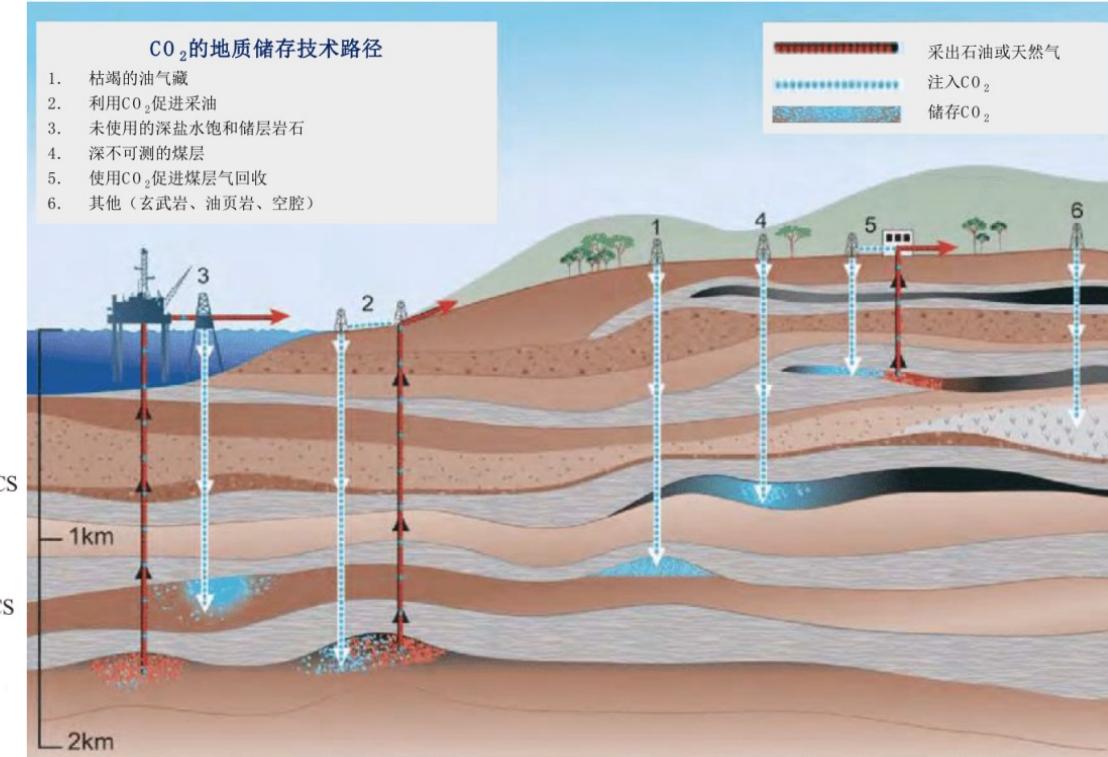
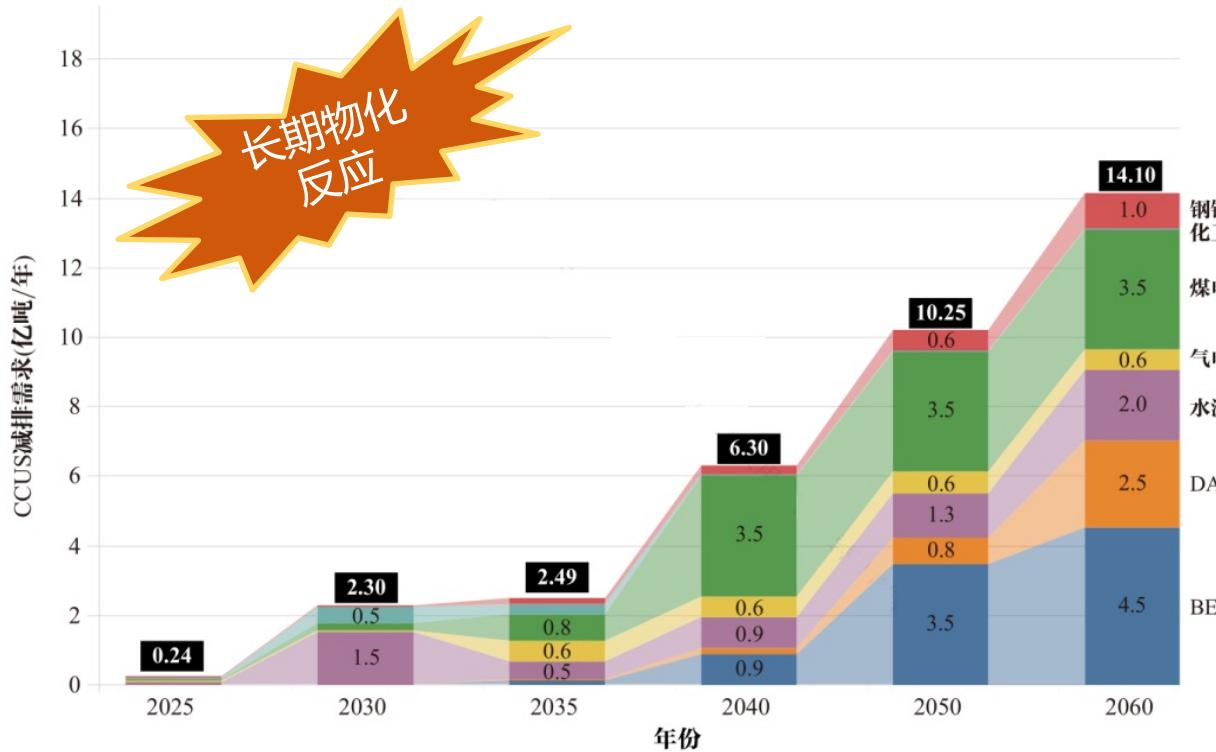
- 2020年9月22日，习近平总书记提出：二氧化碳排放力争于2030年前达到峰值，争取于2060年前实现碳中和；2030年的目标是单位国内生产总值二氧化碳排放量比2005年下降65%以上
- 2021年1月28日，国家发改委能源所发布《2020中国可再生能源展望报告》
- 地热资源是一种清洁环保的非化石能源，也是稳定可靠的本土能源，开发利用不受地缘政治、季节、昼夜、气候等因素影响，可作为基础能源



- 地热开发需要模拟多重介质（如裂隙介质与多孔介质）中的多相、多组分渗流与热量运移（多物理场耦合问题）
- 国外可用于地热模拟的软件包括美国的Tough、德国的OGS 和FEFLOW、加拿大的CMG、瑞典的COMSOL等
- 国内尚无成熟的、完全自主的地热数值模拟软件，针对地热数值模拟的软件主要有中国科学院地质与地球物理研究所研发的地热计算器（调用OGS模块，不能商用）



二氧化碳地质储存中的应用



- 二氧化碳地质封存具有存储容量大、存储时间长、成熟技术可迁移、可与二氧化碳利用相结合等优点
- 地质储存面临着长时间封存泄漏的风险，需要大量数值模拟进行风险评估，并进行日常泄漏监测
- CCS和CCUS技术是碳中和为地球物理行业带来的机遇，但碳捕集与封存的代价目前仍很高

参考文献：赵改善《地学新视野》，2021



典型的交叉学科问题



渗流力学

多组分多相流在多孔介质
(孔、洞、裂隙) 中的流动
规律



岩石力学

岩石与流体的物理化学反应，
孔隙变形、裂缝扩展等



油藏工程

油气藏开发工程、油井工程、
水力压裂、生产机制等



计算科学

应用数学、计算数学、科学
计算、并行计算等



软件工程

程序设计、开发、维护、标
准，人机接口等

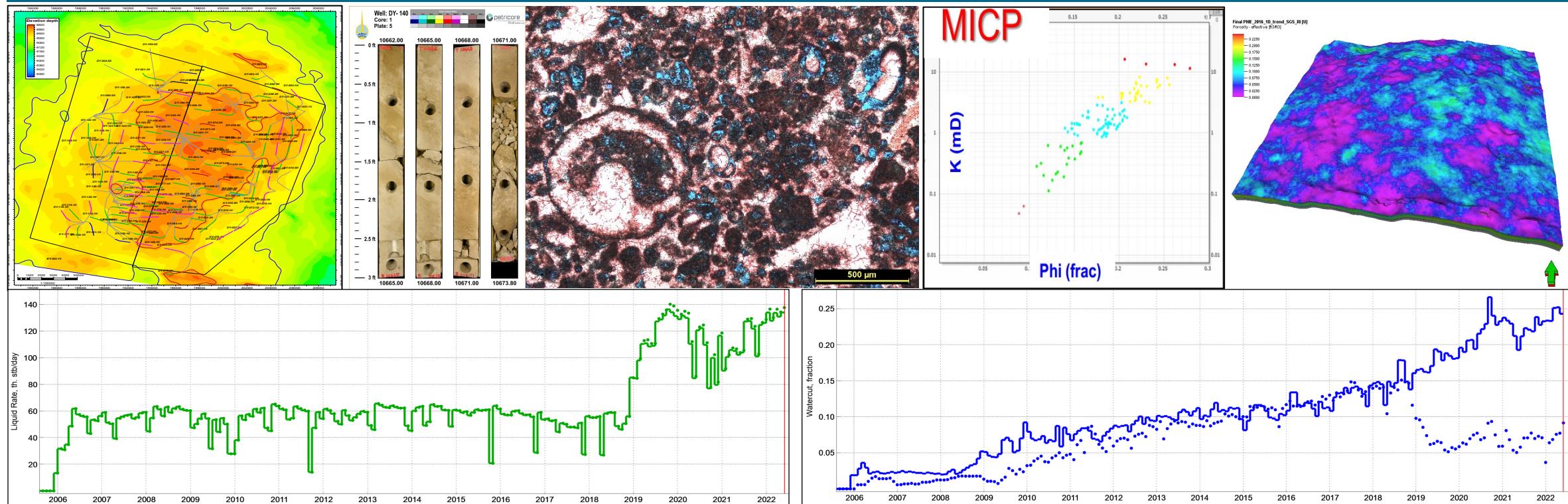




数值模拟中的困难与挑战

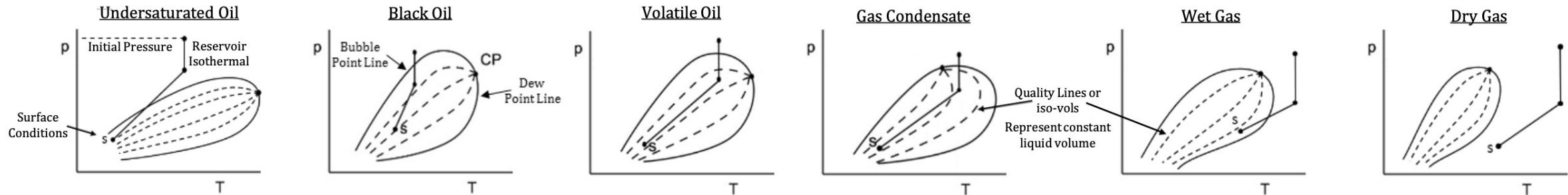


- 中东某碳酸盐岩油藏（魏晨吉、韩如冰，CNPC & ADNOC）：短轴背斜，构造油藏，饱和油藏（发育气顶），原油粘度低，高孔低渗：孔隙类型以粒间孔、粒内孔、粒间溶孔、粒内溶孔为主
- 动态模型对非均质性表征程度不理想，导致常规模型适用性受限：在定产的情况下，全油藏气油比、含水率等关键参数拟合效果差，井底流压数模计算值与实际测试值存在较大偏差





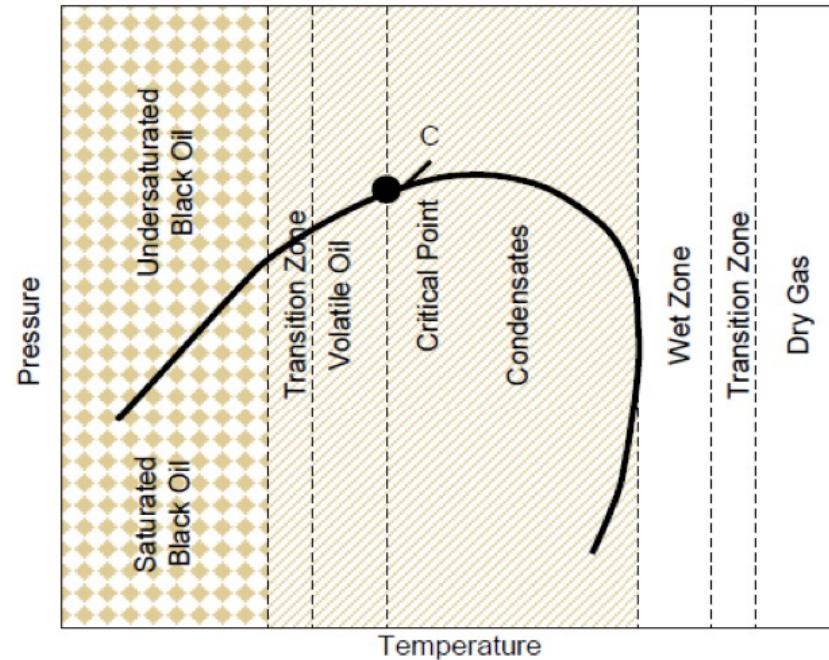
不同性质的多相流体



Laboratory and Field Characteristics

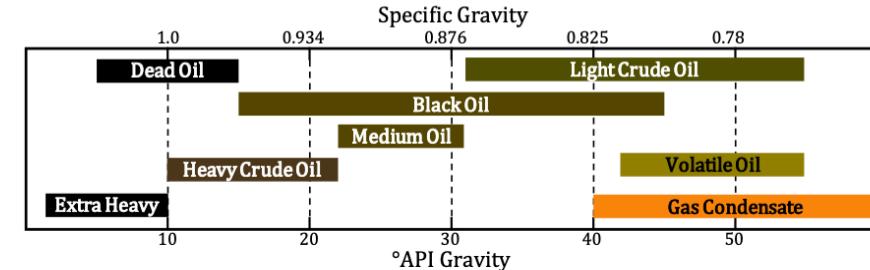
Fluid Type	T^{RC}	Initial GOR scf/STB	Oil Gravity °API	Initial B_o RB/STB	C_{7+} Fraction Mole %	Phase Behavior
Dry Gas	$> T^{crc}$	--	--	--	--	Single phase at all pressures and temperatures
Wet Gas	$> T^{crc}$	$> 50,000$	--	--	--	Gas phase in reservoir at all P & T. Separator within two-phase region.
Gas Condensate	$T^c - T^{crc}$	3300 – 50000	40 – 60	--	< 12.5	All gas initially; As pressure falls below dew point a liquid phase forms
Volatile Oil	$< T^c$	2000 – 3300	42 – 55	1.7 – 3.0	12.5 – 20	T^{RC} close to T^c . Key difference between volatile and black oils is that the gas phase can produce liquid at surface.
Black Oil	$< T^c$	200 – 2000	15 – 45	1.1 – 1.7	25 – 50	As reservoir pressure falls below bubble point, gas phase forms.
Undersaturated Oil	$< T^c$	200 – 2000	15 – 45	1.1 – 1.7	25 – 50	Oil phase in reservoir at all P & T. Separator within two-phase region.
Dead Oil	$< T^c$	--	5 – 15	1.0 – 1.1	> 50	Single phase at all pressures and temperatures.

T^{crc} = cricondentherm



API Classification

Fluid Type	°API Gravity
Light Crude Oil	> 31.1
Medium Oil	22.3 – 31.1
Heavy Crude Oil	10.0 – 22.3
Extra Heavy Oil	< 10.0

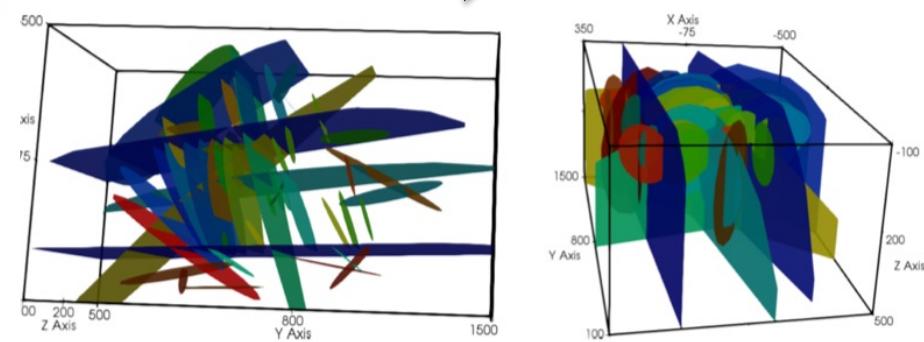
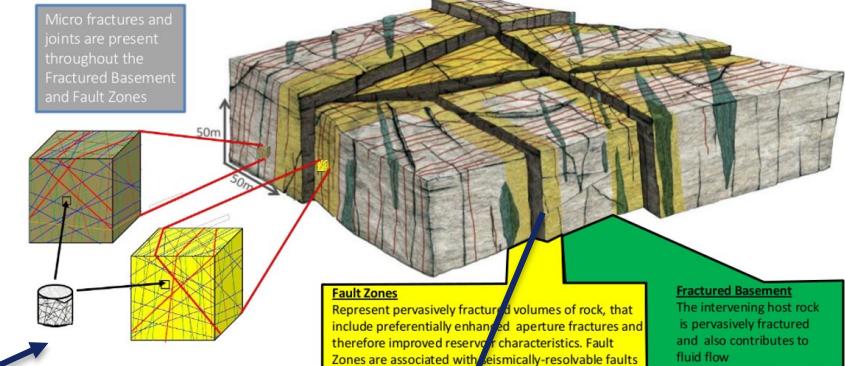
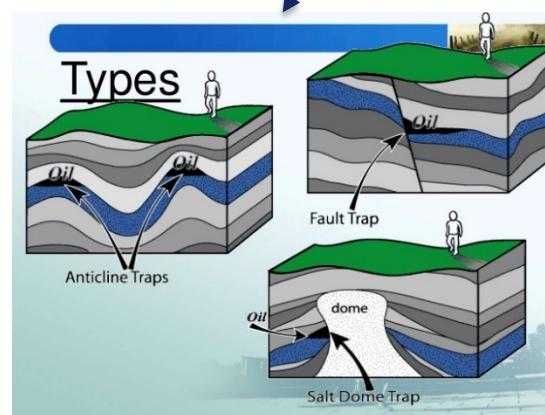
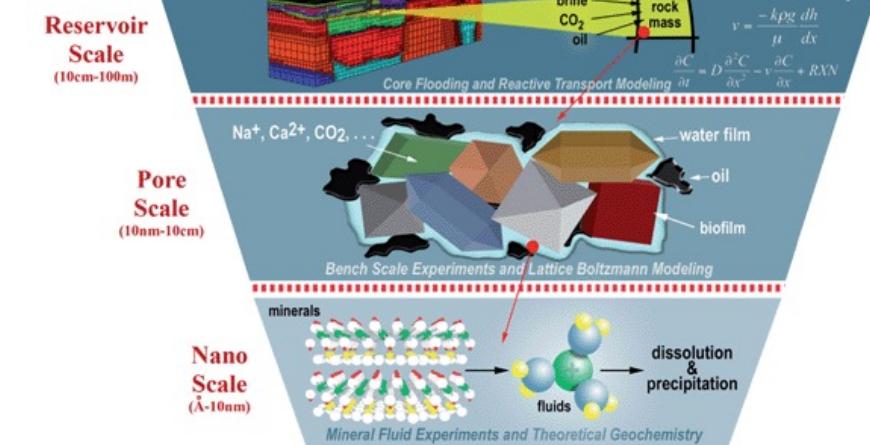
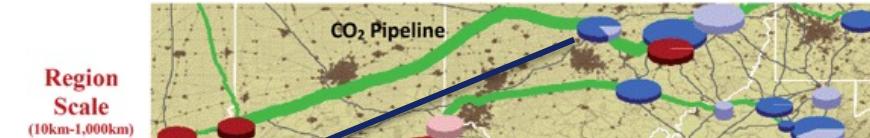
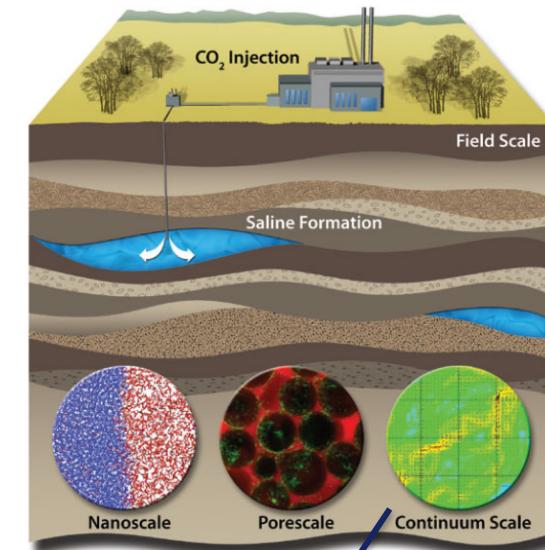


油藏模拟常用模型
适用范围与PT相图

Ref: Thermodynamics and Phase Behavior, J. Riddle, Univ of Texas at Austin



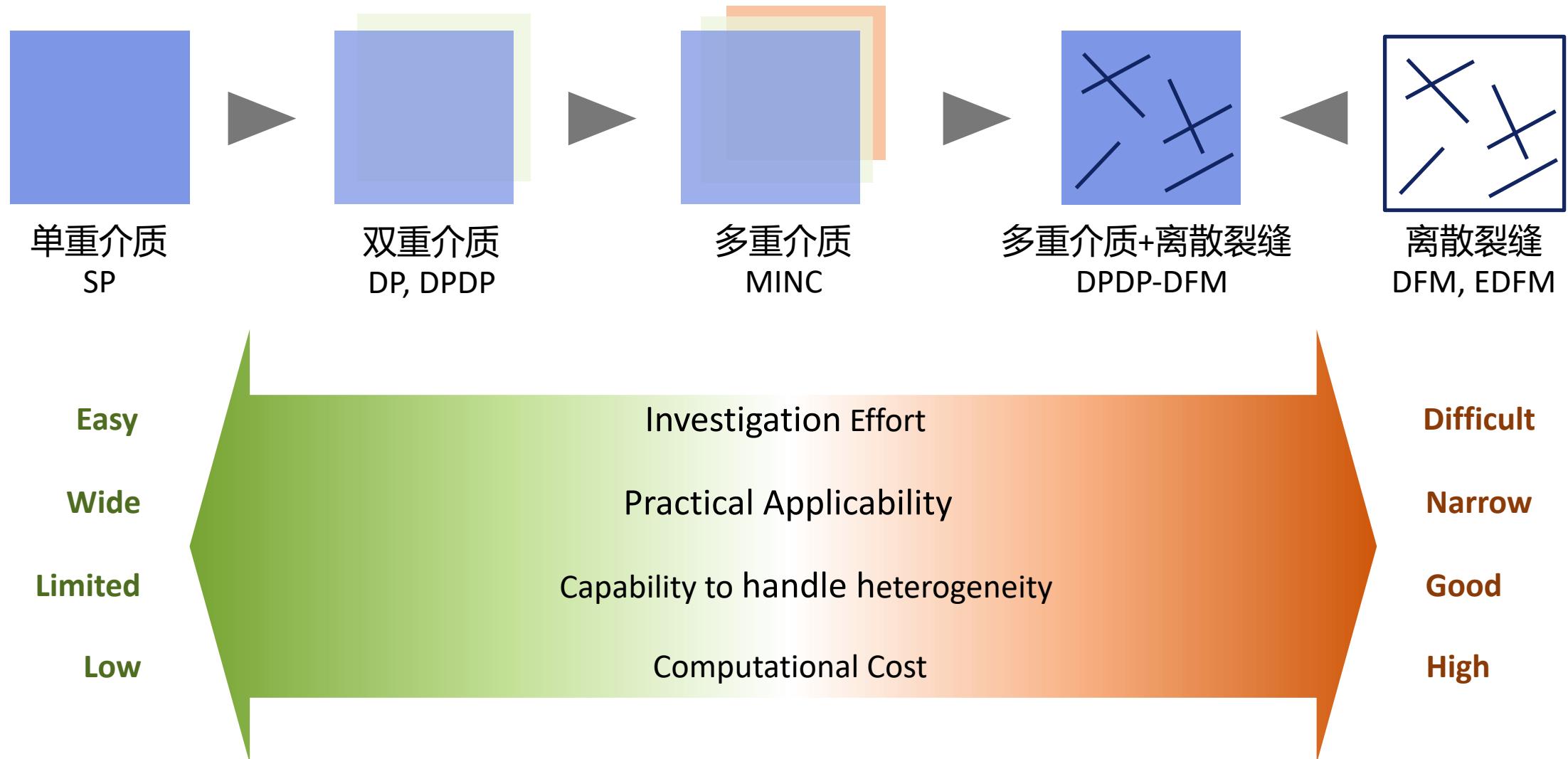
不同尺度的流动模态



来源 : Center for Petroleum & Geosystems Eng, UT Austin

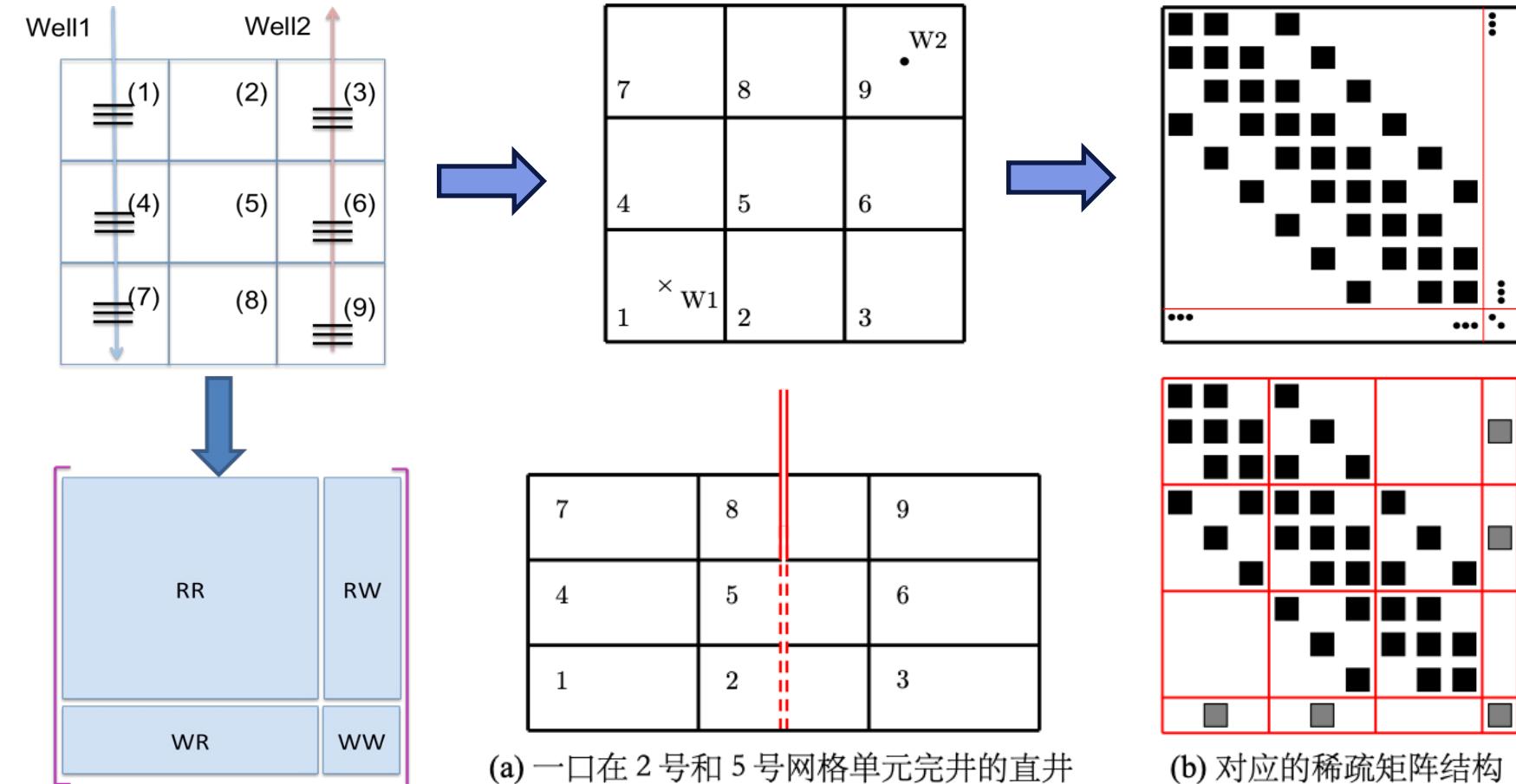
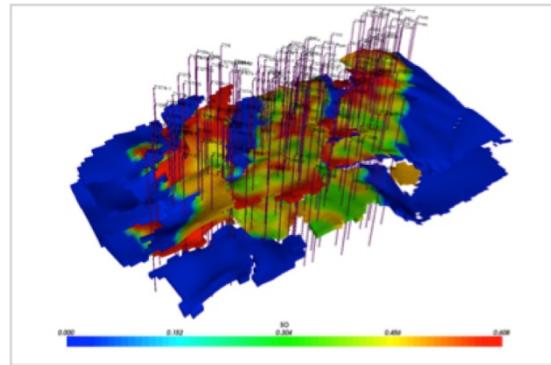


不同特性的介质类型





不同类型的计算网格



- 实际应用中，网格较为复杂：结构网格、PEBI网格、无结构网格、局部加密网格、混合网格等
- 井方程的变量个数与油藏网格块对应的变量个数可能不一致



学术界科研数值模拟软件



CPGE CENTER FOR PETROLEUM & GEOSYSTEMS ENGINEERING

The University of Texas at Austin H. H. Hildebrand Department of Petroleum and Geosystems Engineering Cockrell School of Engineering

About CPGE | Contact Us | People | CPGE News | Feature Stories | Links | Search

Home > Simulators

Simulators

Reservoir Simulators

MPS

The objective of this project is to develop a reservoir simulator with the capability of simulating various recovery processes under one framework. This new simulator is designed to handle miscible gas flooding, chemical flooding, and thermal flooding processes for conventional and unconventional reservoirs. The simulator will also have the capability of executing on parallel computers. The main goal of the project is development of a unified simulator capable of performing simulations for large complex reservoirs operating under various recovery processes.

UTCOMPRS

UTCOMPRS is a three-dimensional, chemical flooding reservoir simulator capable of modelling up to four-phase flow, namely, an aqueous phase, and oleic phase, a microemulsion phase, and a gas phase. An adaptive implicit method (AIM) with switching criteria based on stability analysis is implemented to improve both time-step size selection and performance. Reservoirs can be discretized using Cartesian and Corner-Point grids. A stable third order high resolution scheme is implemented for Cartesian grids, reducing the need for very fine grids and the effects of grid orientation.

[Read more](#)

UTCOMPRS

UTCOMPRS is a three-dimensional, EOS Compositional reservoir simulator capable of modelling up to four-phase flow, namely, an aqueous phase, and oleic phase, a gaseous phase, and a second nonaqueous liquid phase. An adaptive implicit method (AIM) with switching criteria based on stability analysis is implemented to improve both time-step size selection and performance. Reservoirs can be discretized using Cartesian, Corner-Point or Unstructured grids. Stable high resolution schemes are also implemented for both Cartesian and Unstructured grids, reducing the need for very fine grids and the effects of grid orientation.

[Read more](#)

CSM Center for Subsurface Modeling

Introduction | Source code | Documentation | Build | Run

Integrated Parallel Accurate Reservoir Simulator

The diagram illustrates the Integrated Parallel Accurate Reservoir Simulator (IPARS) architecture. It shows a central "Boundary conditions" block connected to "Wells", "Solvers", and "Black Oil" blocks. "Solvers" are further divided into "Compositional" and "Black Oil 2". "Wells" interact with "Boundary conditions" and "Solvers". "Boundary conditions" also connect to "Keyword Input" (including "Table Lookup" and "WWW interface"), "Memory Management", "Parallel Processing", "Platforms", and "Visualization". "Solvers" interact with "Two-Phase", "Two-Phase Impes", "Single Phase Implicit", "Single Phase Sequential", "Multiblock", "Multiphysics", "Geomechanics", "DG Impes", "Air-Water", "Geomechanics + Flow", and "Flow + Reactive Transport". "Two-Phase", "Two-Phase Impes", "Single Phase Implicit", "Single Phase Sequential", "Multiblock", "Multiphysics", "Geomechanics", "DG Impes", "Air-Water", and "Geomechanics + Flow" are interconnected. "Flow + Reactive Transport" is shown separately. "Parallel Processing" and "Platforms" are part of the "Memory Management" and "Parallel Processing" stack.

Stanford SCHOOL OF EARTH, ENERGY & ENVIRONMENTAL SCIENCES SUPRI-B: Reservoir Simulation

HOME ABOUT PEOPLE ACADEMICS RESEARCH AFFILIATES PUBLICATIONS

Research

We work in virtually all aspects of reservoir simulation, and our research program is constantly evolving to meet the changing needs of the industry, the wider community, and the interests of students.

The research areas include:

- AD-GPRs**: Multiscale Methods, Optimization, Parallel Computing, Reactive Transport, Stochastic PDEs.
- Compositional Simulation**: Fracture Modeling.
- Geomechanics**: Geomechanics + Flow, Flow + Reactive Transport.
- Pore-Scale Simulation**: Cyclic spin problem, Darcy's law problem.

BERKELEY LAB Bringing Science Solutions to the World

TOUGH

Home Software Licensing & Download Research Papers News and Events User Support

TOUGH: Suite of Simulators for Nonisothermal Multiphase Flow and Transport in Fractured Porous Media

The TOUGH ("Transport Of Unsaturated Groundwater and Heat") suite of software codes are multi-dimensional numerical models for simulating the coupled transport of water, vapor, non-condensable gas, and heat in porous and fractured media. Developed at the Lawrence Berkeley National Laboratory (LBNL) in the early 1980s primarily for geothermal reservoir engineering, the suite of simulators is now widely used at universities, government organizations, and private industry for applications to nuclear waste disposal, environmental remediation problems, energy production from geothermal, oil and gas reservoirs as well as gas hydrate deposits, geological carbon sequestration, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and mechanical processes in permeable media. The TOUGH suite of simulators is continually updated, with new equation-of-state (EOS) modules being developed, and refined process descriptions implemented into the TOUGH framework (see the overview of the TOUGH development history). Notably, EOS property modules for mixtures of water, NaCl, and CO₂ has been developed and is widely used for the analysis of geologic carbon sequestration processes.

TOUGH and its application have been the subject of more than 500 peer-reviewed journal articles, conference proceedings, and project reports. TOUGH and its various modules are documented in a series of manuals.

PFLOTRAN

About Bitbucket Installation Documentation Parallel Performance Development Team Publications

PFLOTRAN

A Massively Parallel Reactive Flow and Transport Model for describing Subsurface Processes

Los Alamos National Laboratory | Oak Ridge National Laboratory | OFM Research | OpenGeoSim | Pacific Northwest National Laboratory | Sandia National Laboratories

PFLOTRAN is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries. PFLOTRAN has been developed from the ground up for parallel scalability and has been run on up to 2¹⁸ processor cores with problem sizes up to 2 billion degrees of freedom. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. The reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or the less robust operator splitting method.

OPM The Open Porous Media Initiative

HOME FLOW UPSCALING RESIGHT TOOLBOX DATASETS GALLERY DOCUMENTATION DOWNLOAD

GALLERY

Here, we would like to share with you some of the many cases we have studied with OPM software. This way, we seek to highlight features and capabilities that are not described in tutorials.

RECENT OPM NEWS

- Flow manual for the 2021.10 release available November 17, 2021
- OPM Release 2021.10 November 10, 2021
- Flow manual for the 2021.04 release available June 17, 2021
- OPM RELEASE 2021.04 May 5, 2021
- Commercial support for OPM Flow! January 27, 2021

ALL OPM NEWS

The OPM news archive.

Use of flow diagnostics tool from MBST to identify and visualize volumetric connections within the Manz field. OPM offers the basic solvers needed to compute these diagnostics, and work is in progress to develop similar capabilities for visual analysis in Resight.

02

开源项目

Open-source software development projects



OpenCAEPoro软件开发团队



当前版本贡献者

- 张晨松，中科院数学院
- 李仕哲，中科院数学院
- 沈博芊，中科院数学院
- 赖 婷，湘潭大学
- 冯春生，湘潭大学
- 赵 梨，湘潭大学
- 张林杰，湘潭大学
- 刘生豪，湘潭大学
- 程晓行，深圳大数据研究院
- 张 炼，深圳大数据研究院

早期版本贡献者

- 乔长河，滨州州立大学
- 张鸿轩，滨州州立大学
- 齐浩然，滨州州立大学
- 胡潇喆，Tufts University
- 关文超，中山大学
- 李 政，湘潭大学
- 王锦东，北京大学
- 王 慧，湘潭大学



<https://github.com/OpenCAEPlus/OpenCAEPoro>



OpenCAEPoro软件设计目标



- 方便与其它模型的耦合作用
 - 方便组分间的化学反应
 - 方便更换EOS模型
 - 方便支持不同网格类型
 - 方便更换闪蒸计算算法
 - 方便发展新型隐式/半隐式方法
 - 方便发展新型离散方法
 - 方便发展新型求解方法
 - 方便进行底层的性能优化
-
- 适应分布式异构并行环境
 - 增强接口灵活性，配合嵌套分布式并行调用
 - 由任意解法器调用任意解法器作为预条件
 - 对接底层稀疏数学库
 - 增强程序的可读性和可维护性
 - 重新设计报错信息
 - 重新设计单元测试和回归测试
 - 增加必要的文档
 - 利用C++减少冗余代码



OpenCAEPoro软件设计思想

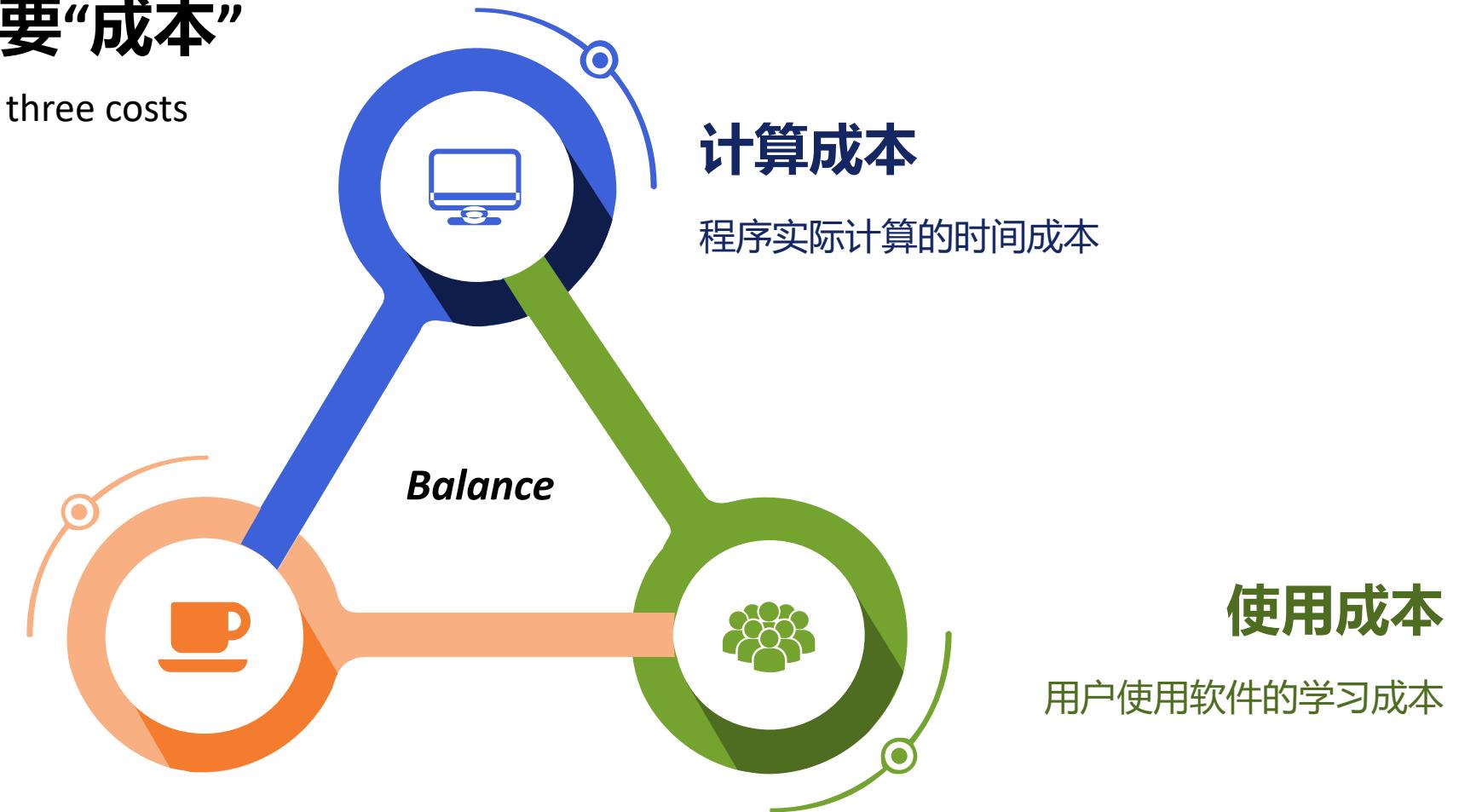


平衡三个主要“成本”

Balancing between three costs

开发成本

程序开发与优化的人工成本



计算成本

程序实际计算的时间成本

使用成本

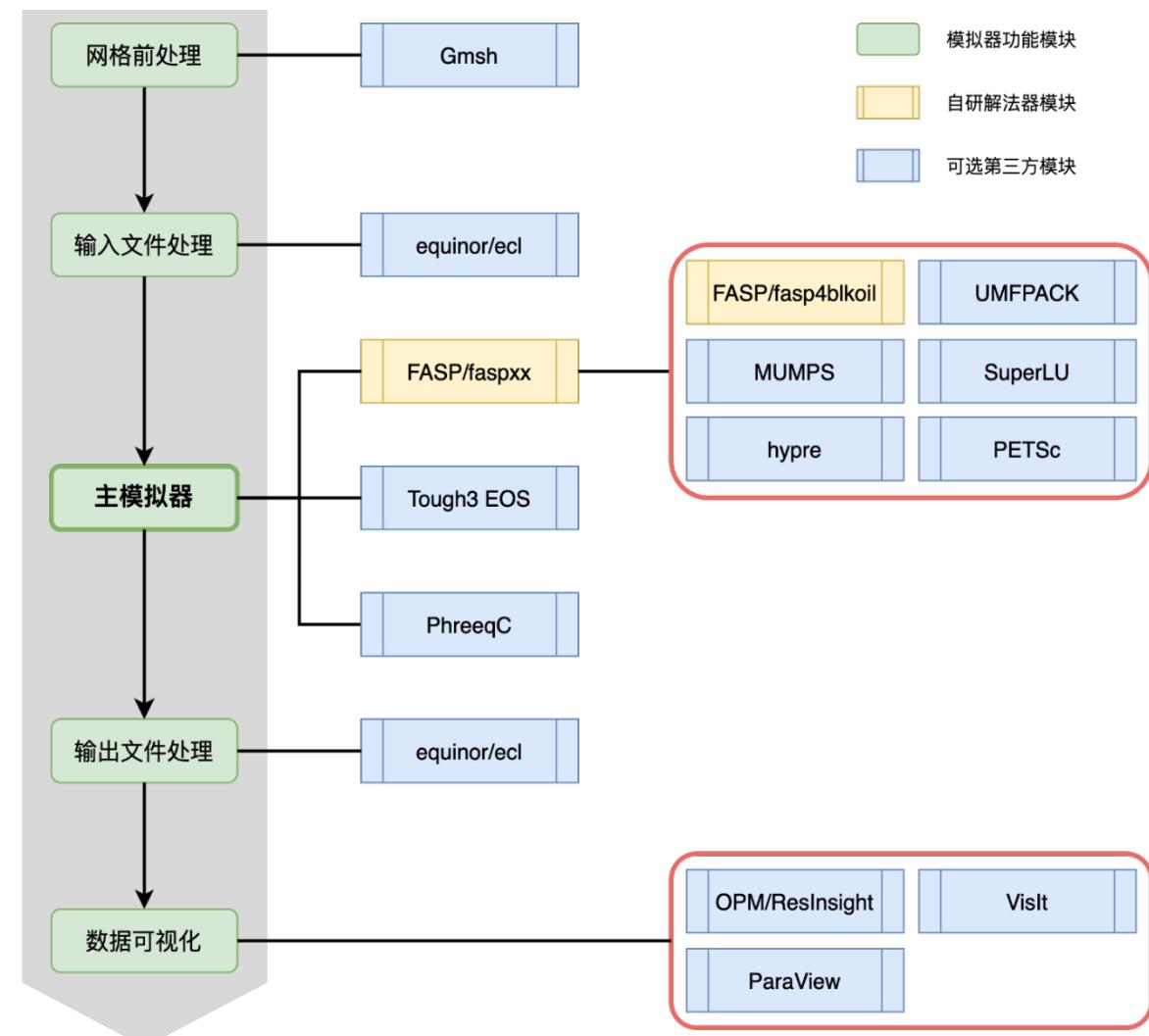
用户使用软件的学习成本



OpenCAEPoro软件整体结构

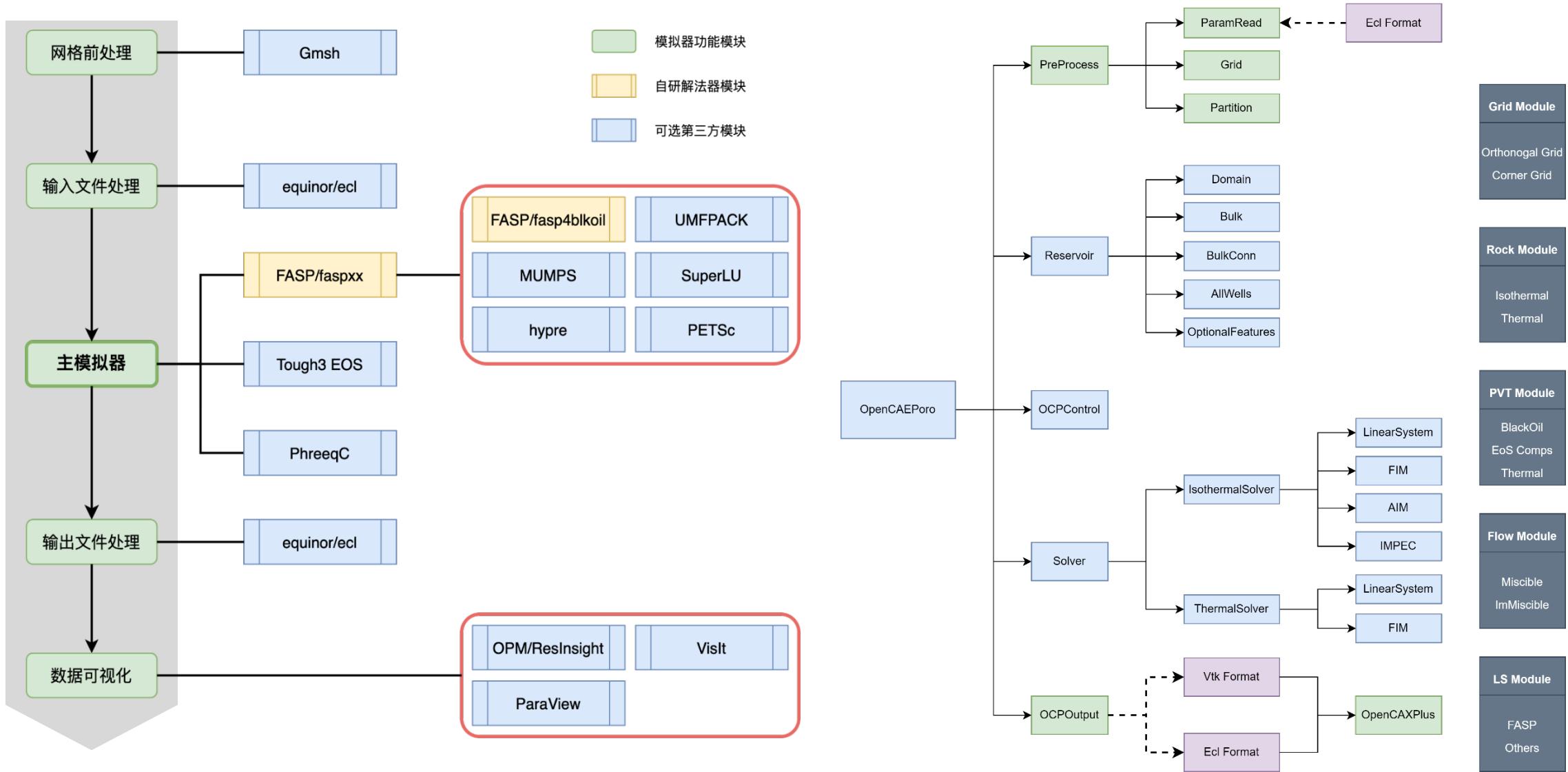


组分模型并行数值模拟



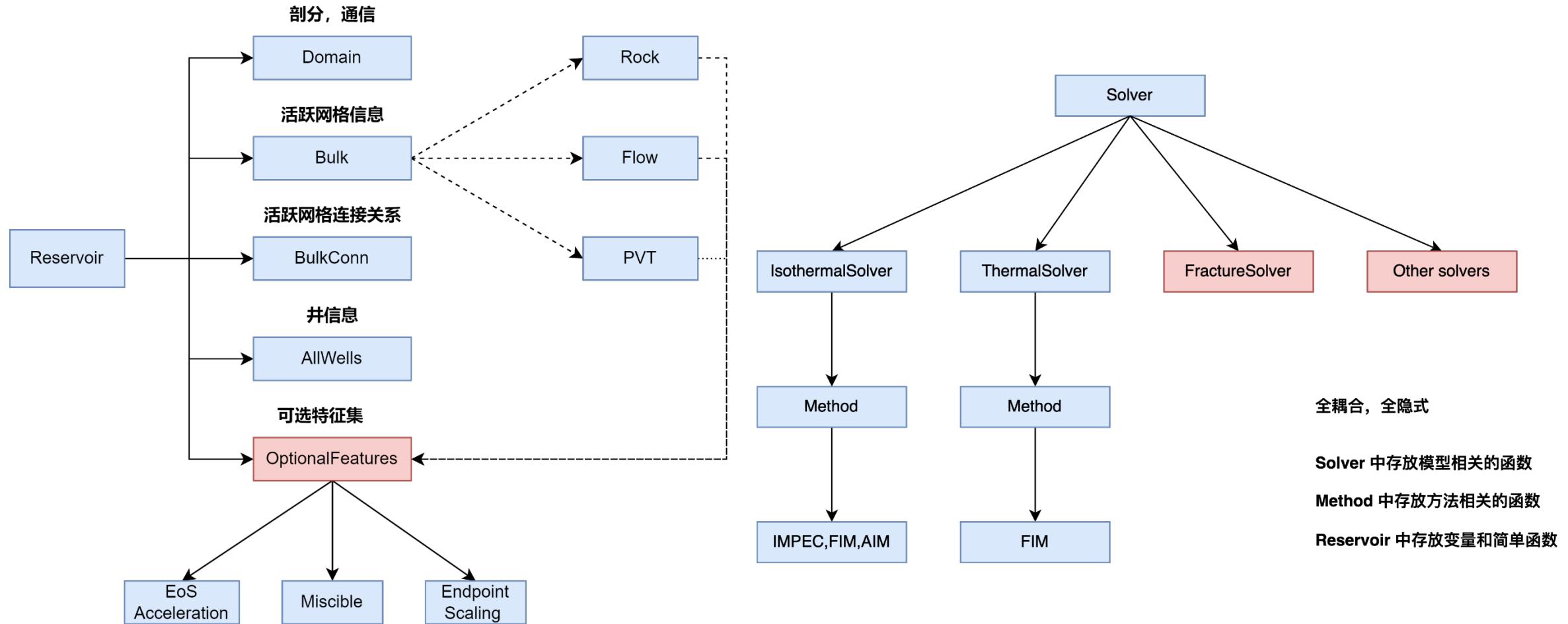


OpenCAEPoro软件整体结构



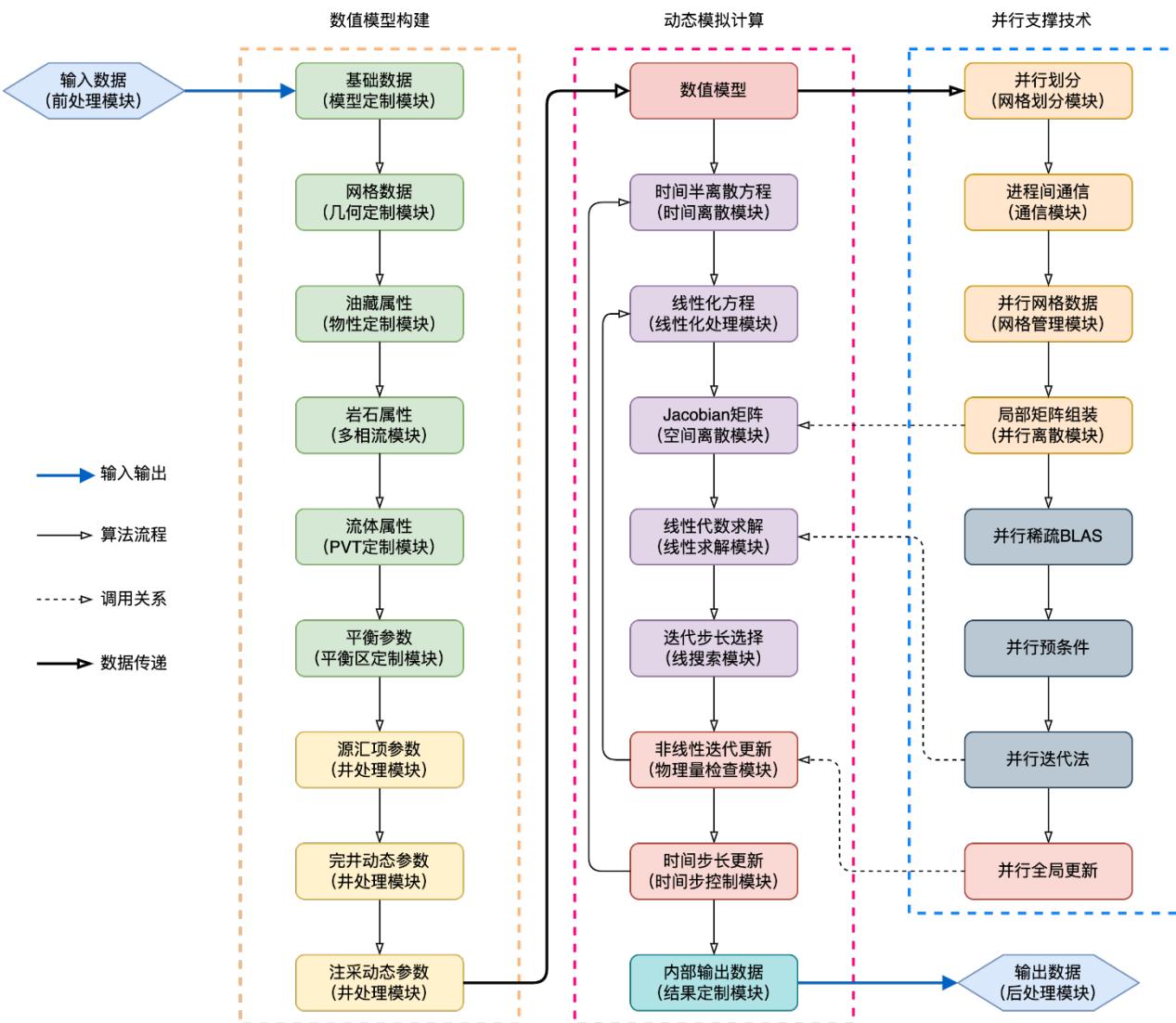


OpenCAEPoro主要数据结构





分布式并行程序设计



将网格划分成若干个部分 (子区域)

进程有自己的数据及邻居的部分数据

进程之间在需要的时候可以交换数据

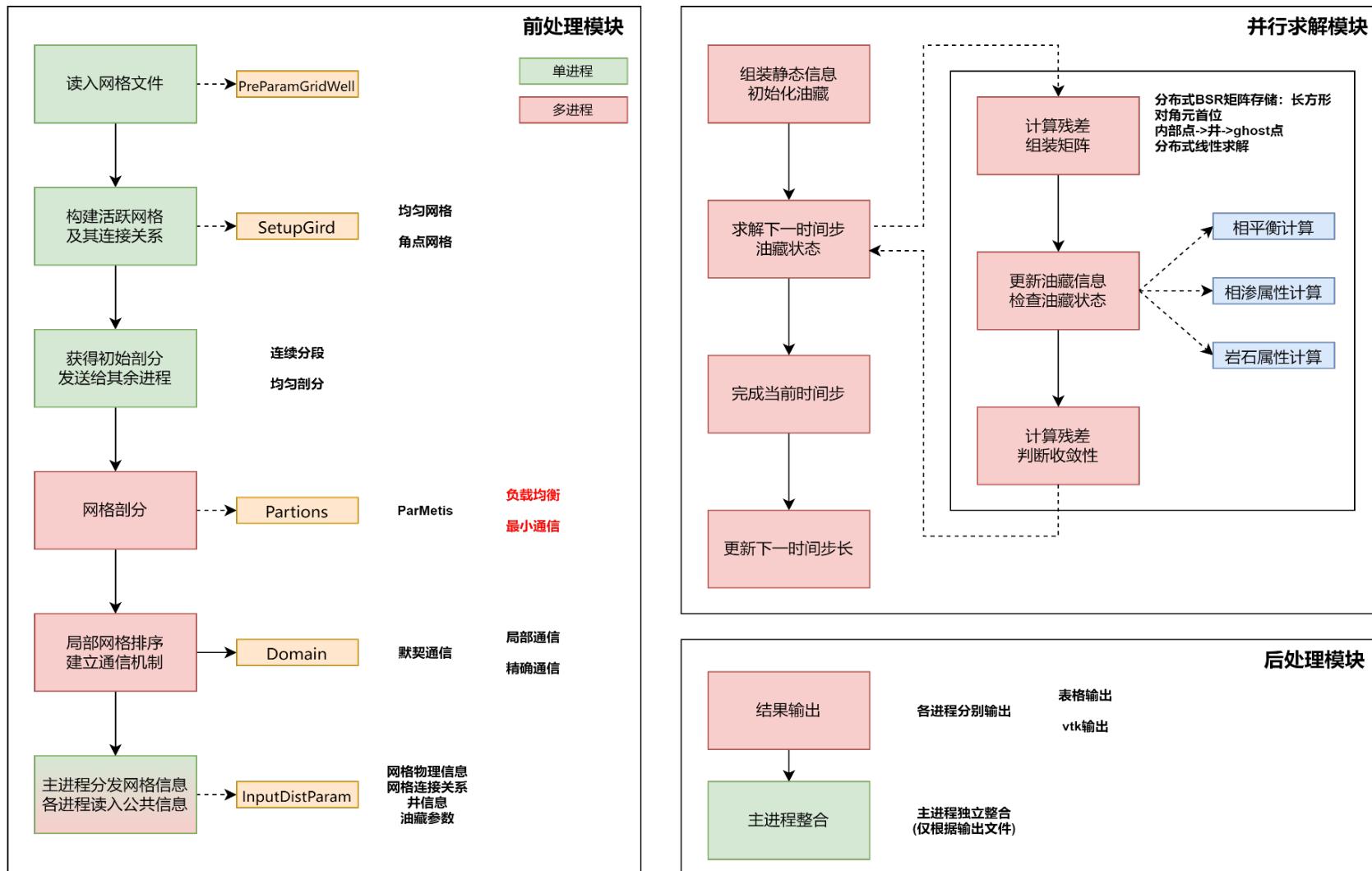
形成Jacobian系统分布式矩阵和右端项

调用并行线性解法器求解Jacobian系统

结束迭代，对解向量进行并行更新



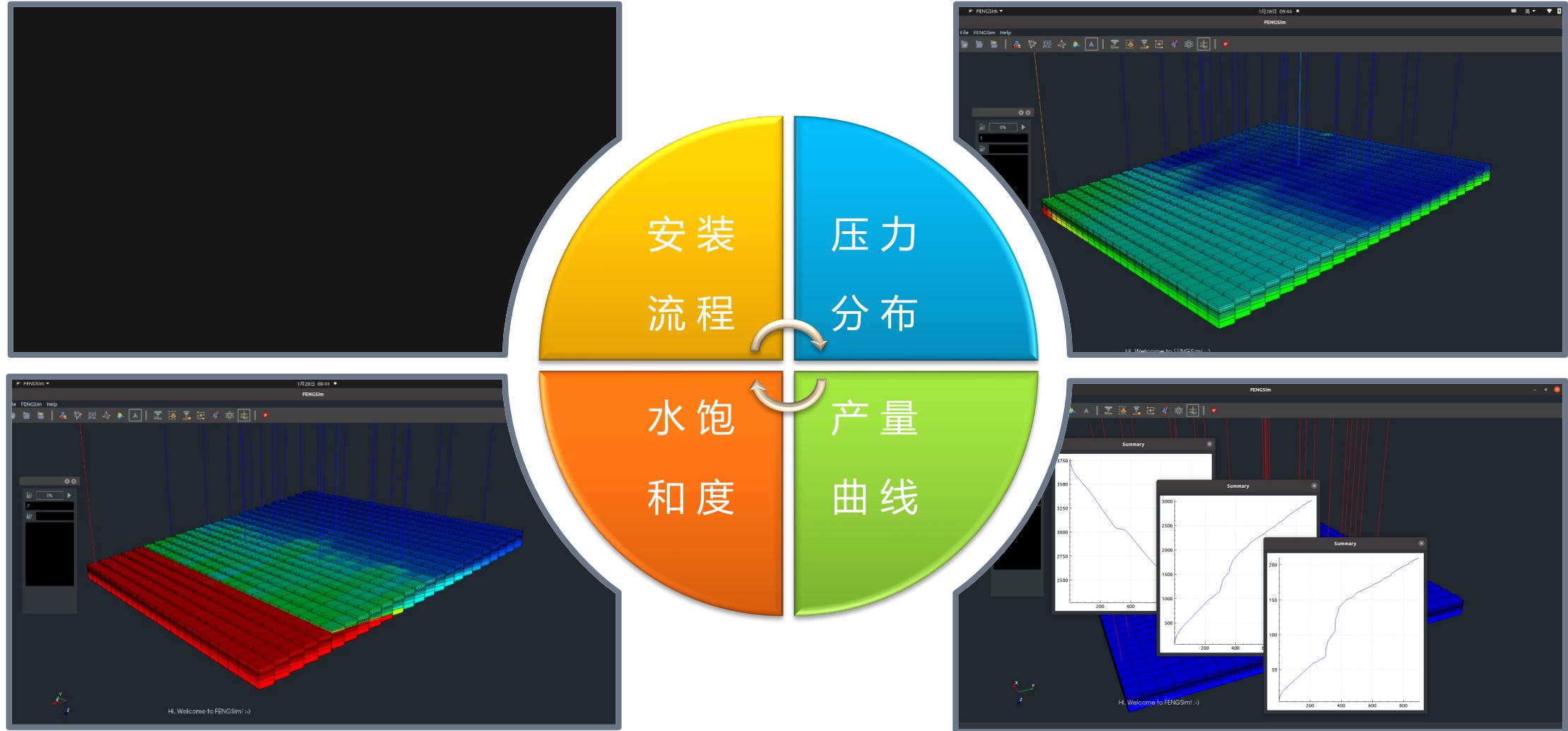
分布式并行模拟流程



1. 串行地读取输入文件是潜在的瓶颈所在，这一块也是绝大部分软件所缺失的。但更大的问题在于串行地对一般网格的前处理——得到网格信息和连接关系，需要进一步分析和研究。
2. 在模拟过程中，油藏的状态不断发生变化，每个网格上的计算量以及网格间的联通强弱也在不断发生变化，难以在整个模拟过程中始终保持各进程的负载均衡或是达到具有某种优势的网格部分，随着进程数的增加负载不平衡的影响会逐渐趋于主导地位。
3. 解法器的并行效率是整个模拟过程能否高效并行的关键。

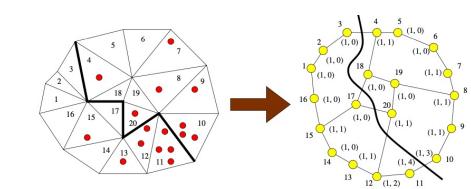


后处理工具包

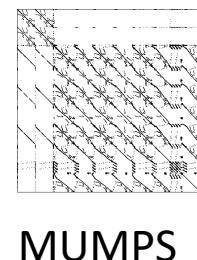




基于SDK的图形用户界面



Metis/ParMetis



UMFPack



Open MPI



团队的开源项目

已形成三个稳定的、互补
的开源开发团队

支撑线性解法器算法开发、
测试与应用的算法库

FASp



面向多相多组分渗流力学
应用的并行数值模拟器

支撑CAX应用软件研发的
开发工具集





测试算例设计



- 串并行实现

串行、OpenMP, GPU, MPI

- 模型方程

黑油模型、组分模型

- 多相流体

单相、两相、三相

- 算法框架

FIM、IMPEC、Improved IMPEC

- 离散网格

正交网格、角点网格

- 测试问题

理论模型、SPE标准算例、实际油田算例

正确性

稳健性

稳定性

收敛性

高效性

可用性



国际油藏工程师协会标准算例



TABLE 17.1—SPE COMPARATIVE SOLUTION PROJECT PROBLEMS

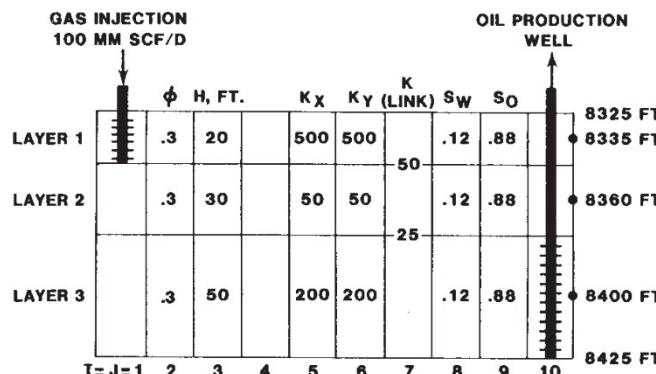
SPE1	Three-phase black oil 10×10×3 300-block grid 3,650-day depletion with gas injection
SPE2	Three-phase black oil 10×1×15 150-block r-z grid 900-day single-well coning depletion
SPE3	Nine-component retrograde gas 9×9×4 324-block grid 5,480-day cycling and blowdown
SPE4	Cyclic steam injection and steam displacement of heavy oils
SPE5	Six-component volatile oil 7×7×3 147-block grid 20-year WAG injection
SPE6	Three-phase black oil Single-block and cross-sectional dual porosity with drainage and gas and water injection cases
SPE7	Three-phase black oil 9×9×6 486-block grid with horizontal wells Eight 1,500-day injection-production cases
SPE8	Two-phase gas-oil black oil 10×10×4 400-block grid Comparison of 2,500-day 400-block grid results with 20-block unstructured and locally refined grid results
SPE9	Three-phase black oil 24×25×15 9,000-block 25-well grid with geostatistical description 900-day depletion
SPE10	Model 1: Two-phase gas-oil case with a 2,000-block 100×1×20 grid and gas injection to 2,000 days Model 2: Two-phase water-oil case with a 1.12-million block 60×220×85 grid and water injection to 2,000 days Both models have geostatistical descriptions

- 1) Odeh, A.S. 1981. Comparison of Solutions to a Three-Dimensional Black-Oil Reservoir Simulation Problem. *J Pet Technol* 33 (1): 13–25. SPE-9723-PA.
- 2) Weinstein, H.G., Chappelar, J.E., and Nolen, J.S. 1986. Second Comparative Solution Project: A Three-Phase Coning Study. *J Pet Technol* 38 (3): 345–353. SPE-10489-PA.
- 3) Kenyon, D. 1987. Third SPE Comparative Solution Project: Gas Cycling of Retrograde Condensate Reservoirs. *J Pet Technol* 39 (8): 981–997. SPE-12278-PA.
- 4) Aziz, K., Ramesh, A.B., and Woo, P.T. 1987. Fourth SPE Comparative Solution Project: Comparison of Steam Injection Simulators. *J Pet Technol* 39 (12): 1576–1584. SPE-13510-PA.
- 5) Killough, J.E. and Kossack, C.A. 1987. Fifth Comparative Solution Project: Evaluation of Miscible Flood Simulators. Presented at the SPE Symposium on Reservoir Simulation, San Antonio, Texas, 1–4 February. SPE-16000-MS.
- 6) Firoozabadi, A. and Thomas, L.K. 1990. Sixth SPE Comparative Solution Project: Dual-Porosity Simulators. *J Pet Technol* 42 (6): 710–715, 762–763. SPE-18741-PA.
- 7) Nghiem, L., Collins, D.A., and Sharma, R. 1991. Seventh SPE Comparative Solution Project: Modelling of Horizontal Wells in Reservoir Simulation. Presented at the SPE Symposium on Reservoir Simulation, Anaheim, California, 17–20 February 1991. SPE-21221-MS.
- 8) Quandalle, P. 1993. Eighth SPE Comparative Solution Project: Gridding Techniques in Reservoir Simulation. Presented at the SPE Symposium on Reservoir Simulation, New Orleans, Louisiana, 28 February–3 March 1993. SPE-25263-MS.
- 9) Killough, J.E. 1995. Ninth SPE Comparative Solution Project: A Reexamination of Black-Oil Simulation. Presented at the SPE Reservoir Simulation Symposium, San Antonio, Texas, USA, 12–15 February. SPE 29110.
- 10) Christie, M.A. and Blunt, M.J. 2001. Tenth SPE Comparative Solution Project: A Comparison of Upscaling Techniques. *SPE Res Eval & Eng* 4 (4): 308–317. SPE-72469-PA.

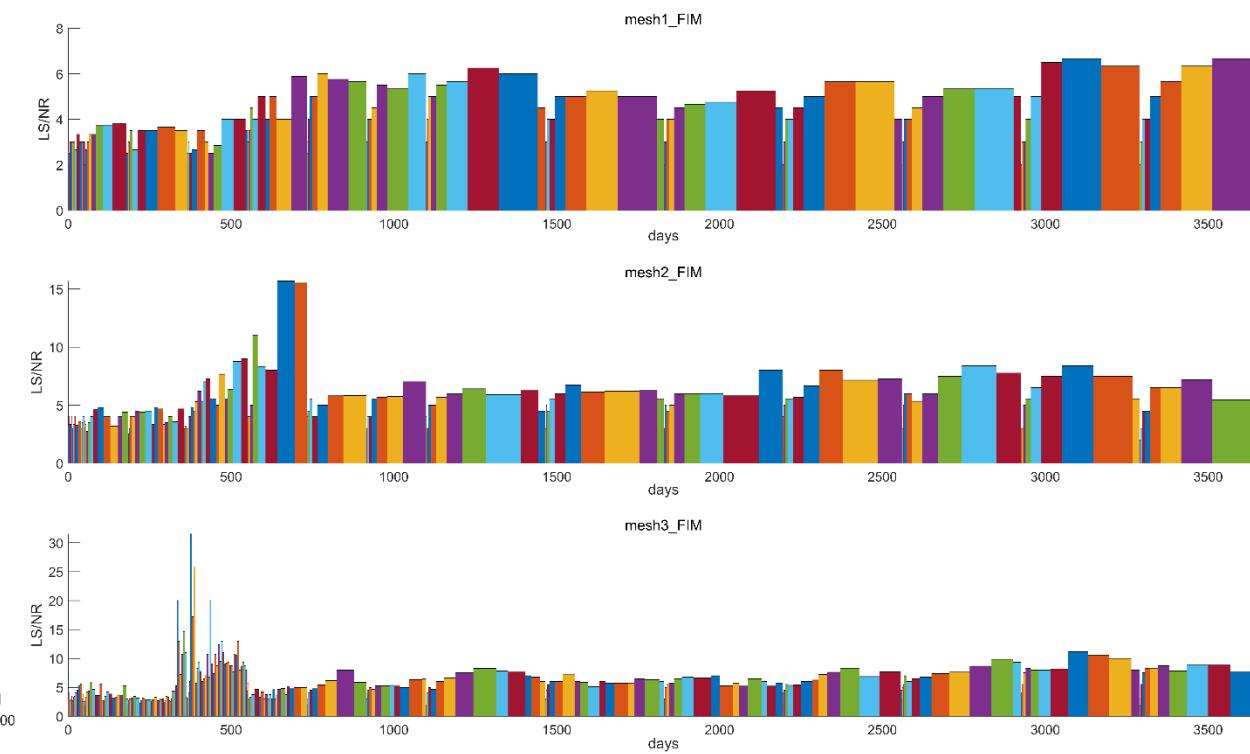
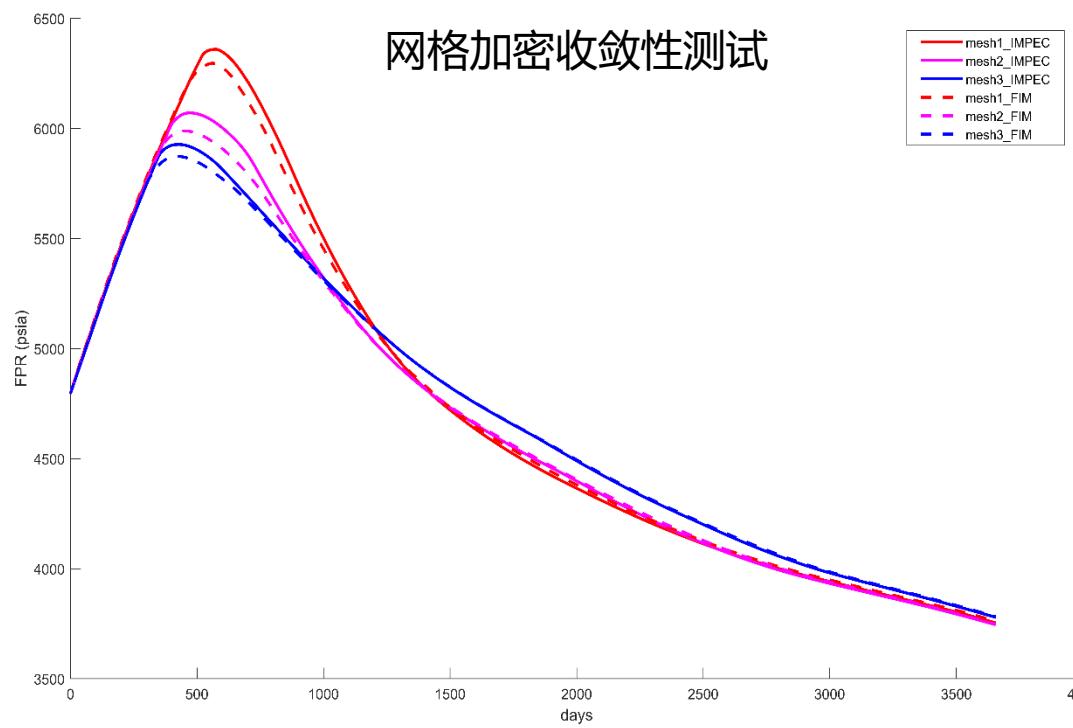
https://petrowiki.spe.org/Reservoir_simulation



SPE1A标准算例：网格收敛性

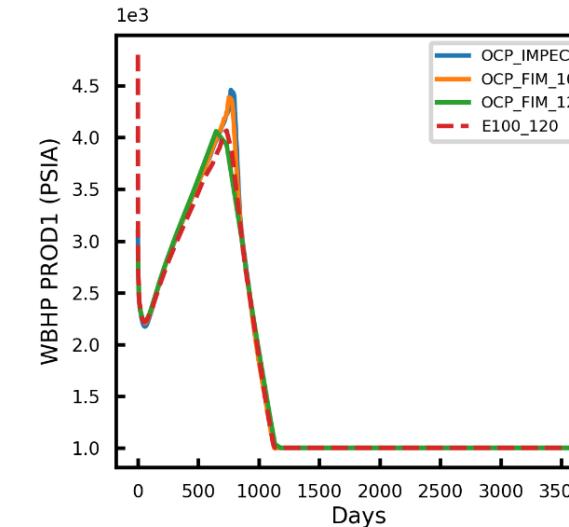
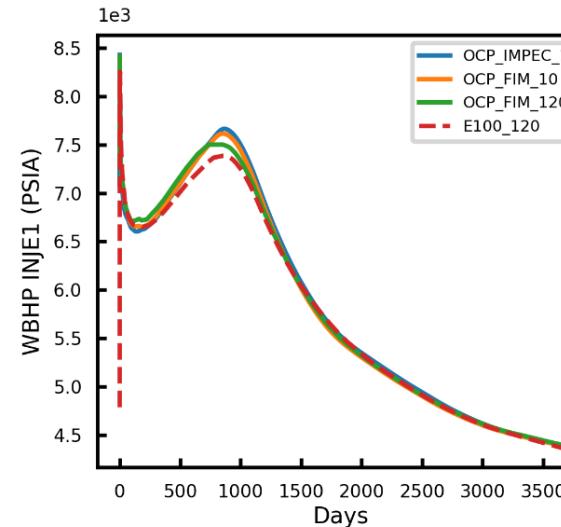
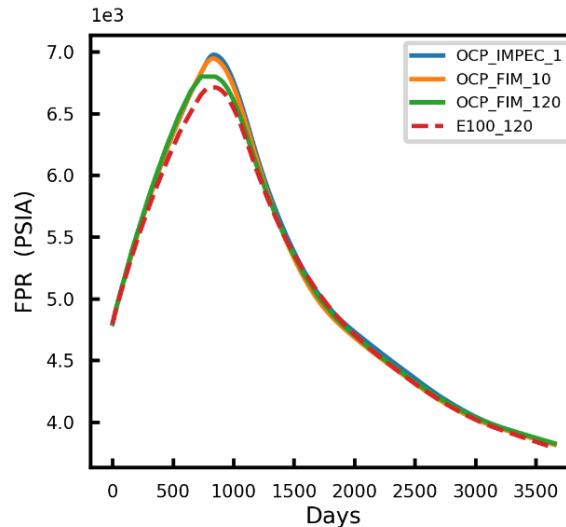


基于SPE1A标准算例构造：油田区域的水平方向为边长1000ft的正方形，垂向厚度为100ft。初始状态下，参考深度（8400ft）的油压为4800psia，初始油饱和度0.88，初始水饱和度0.12；平衡状态油水界面为8500ft，油气界面为7000ft
(mesh1 : 20×20×10 , mesh2 : 40×40×20 , mesh3 : 80×80×40)





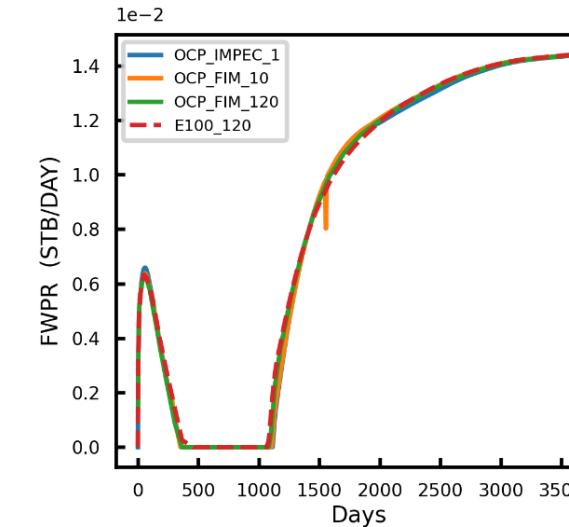
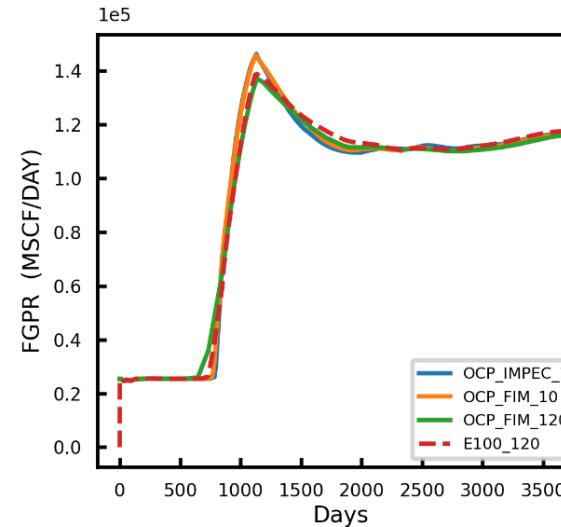
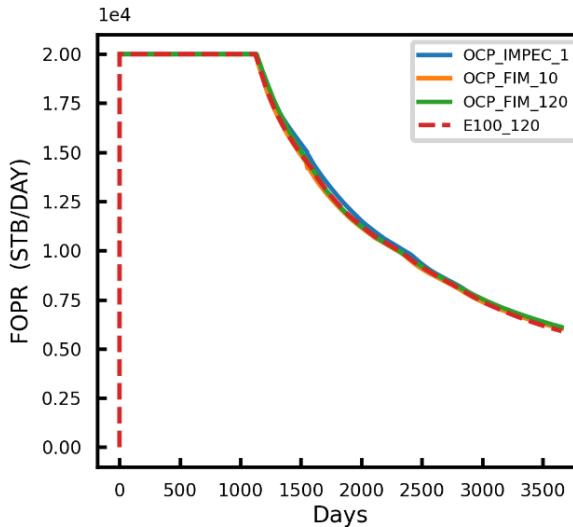
SPE1A标准算例：非混相注气驱



Grid: 10x10x3

Well: 2

Year: 10



IMPEC

NR: 5622 (+28)

LS: 8681 (+55)

LTime: 0.87s (55%)

Total: 1.57s

FIM(120)

NR: 154 (+2)

LS: 2281 (+34)

LTime: 0.17s (65%)

Total: 0.26s



SPE7标准算例：三相水平井

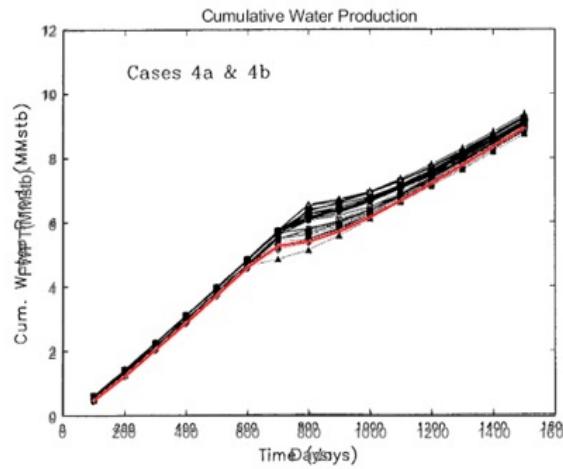


Figure 22: Cumulative water production for Case 4a (solid) and 4b (dashed)

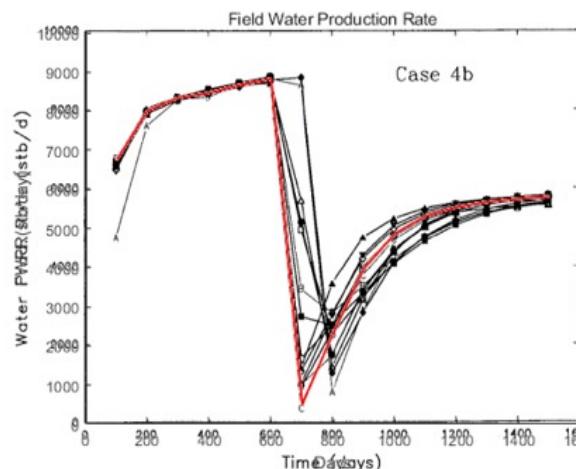


Figure 21: Water production rate for Case 4b

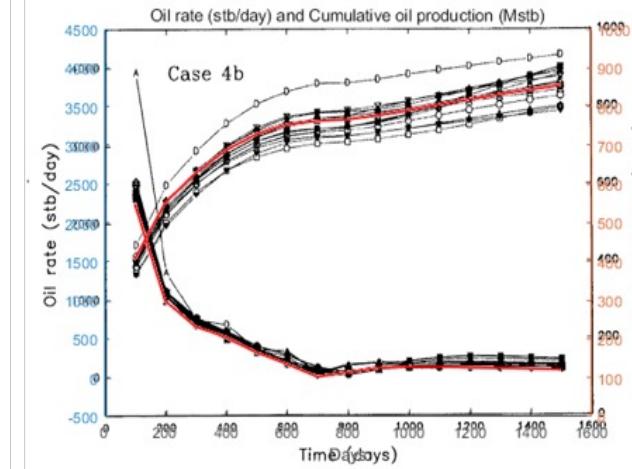


Figure 19: Oil rate (solid) and cumulative oil production (dashed) for Case 4b

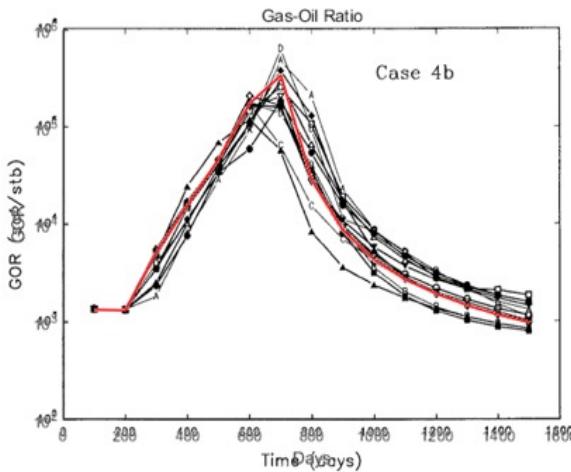


Figure 24: Gas-oil ratio for Case 4b

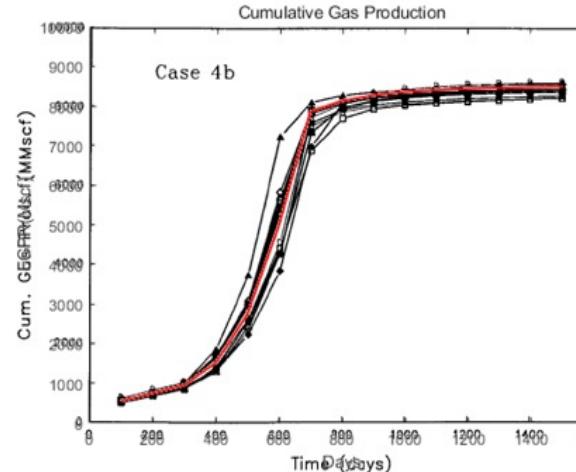


Figure 26: Cumulative gas production for Case 4b

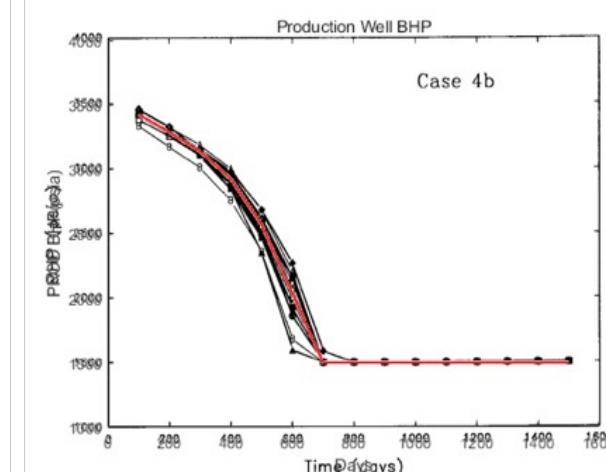
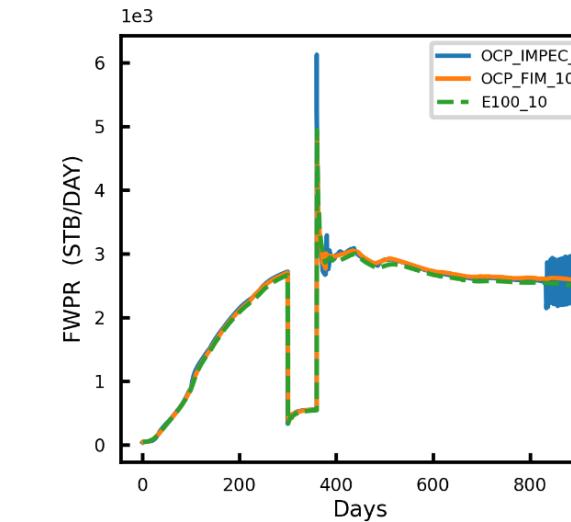
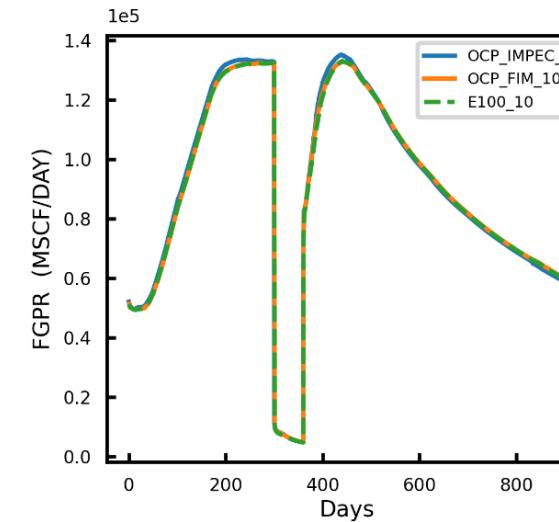
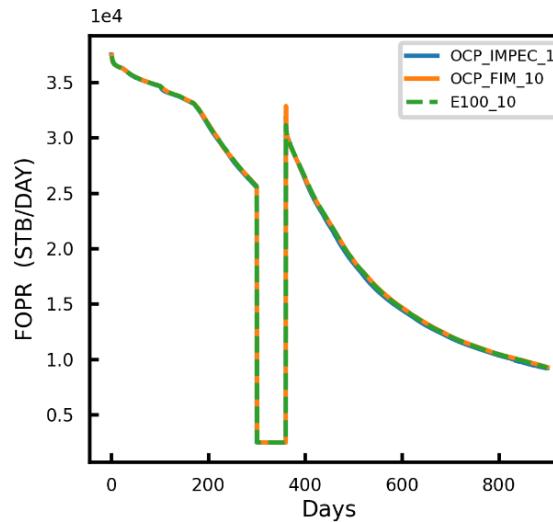
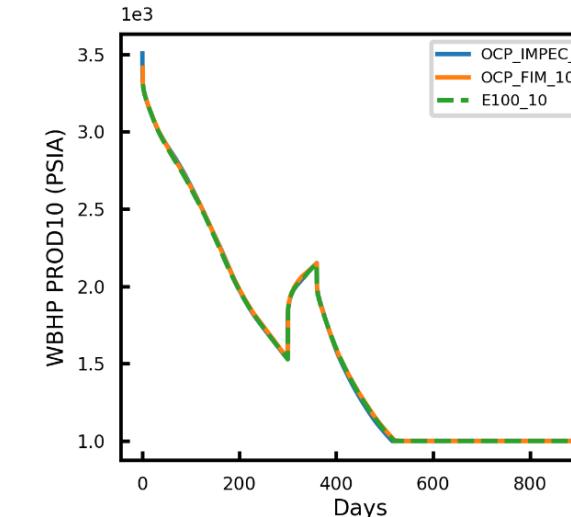
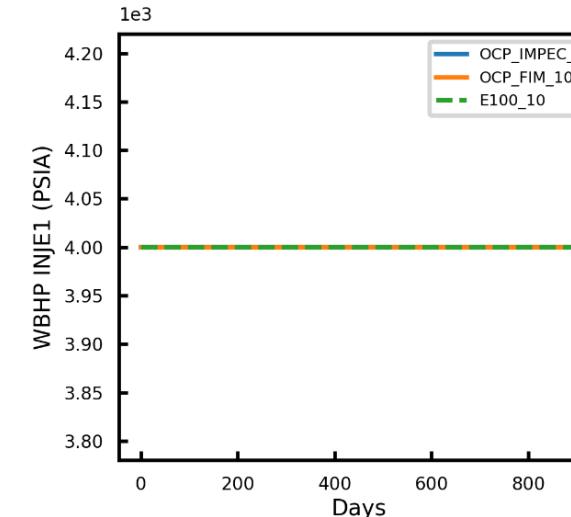
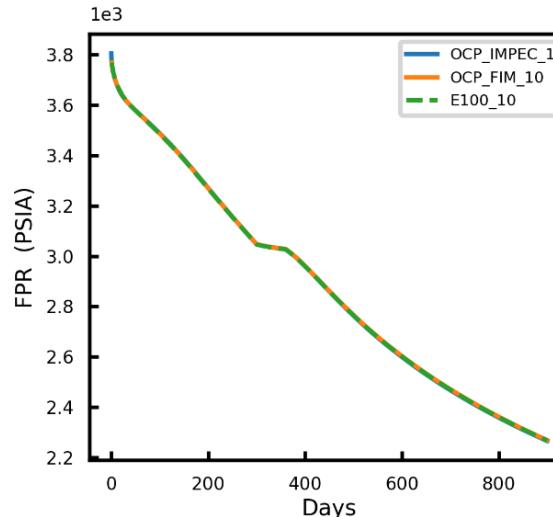


Figure 28: Bottom-hole pressure for Case 4b

Grid: 9x9x6
Well: 12
Day: 1500



SPE9标准算例：三相问题



Grid: 24*24*15

Well: 26

Day: 900

IMPEC

NR: 7508 (+12)

LS: 9962 (+64)

LTime: 61s (57%)

Total: 93.5s

FIM

NR: 211 (+92)

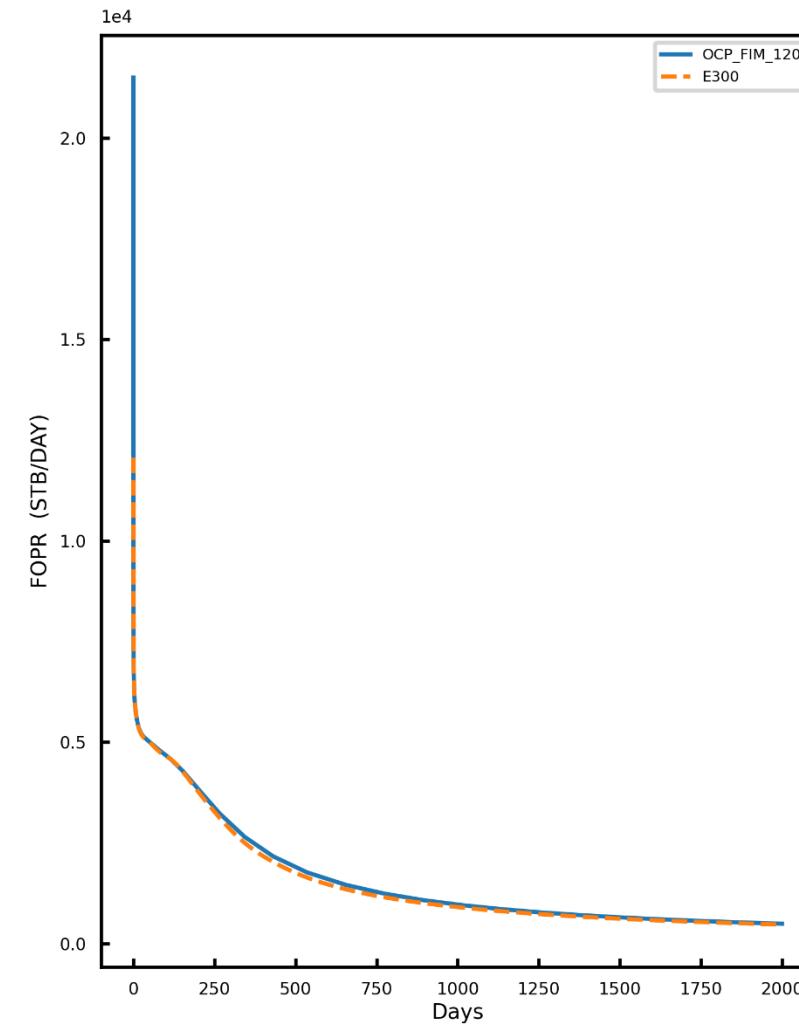
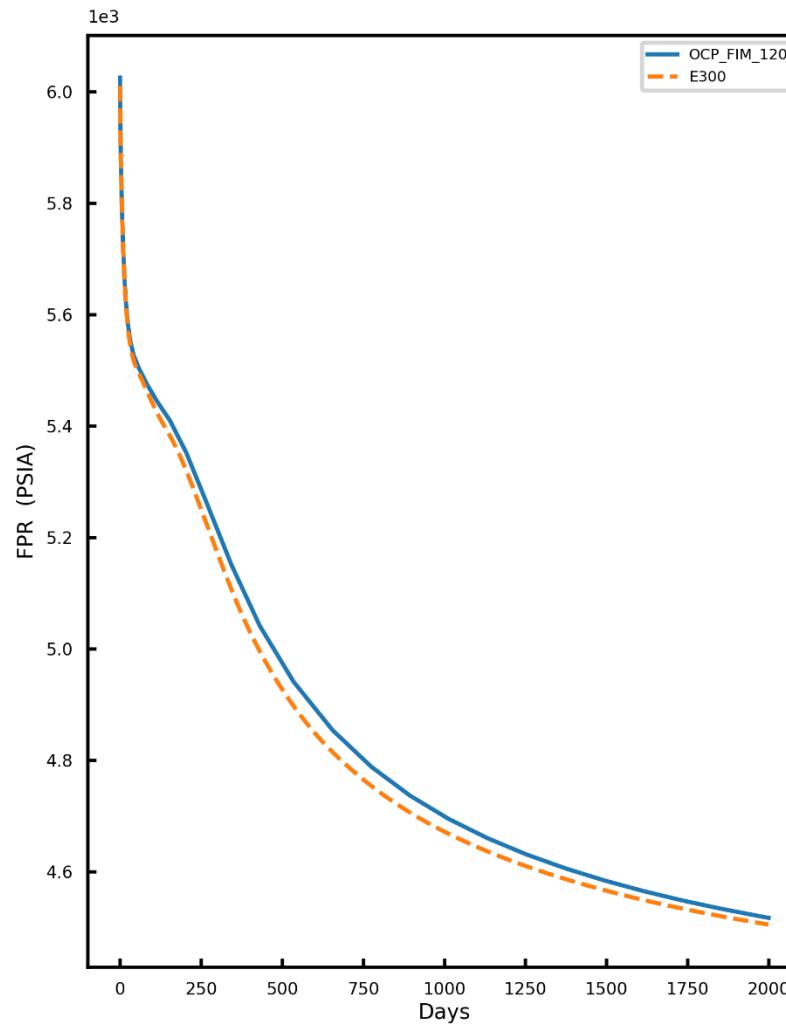
LS: 3033(+1108)

LTime: 9.3s (51%)

Total: 18.4s



SPE10标准算例：油水两相

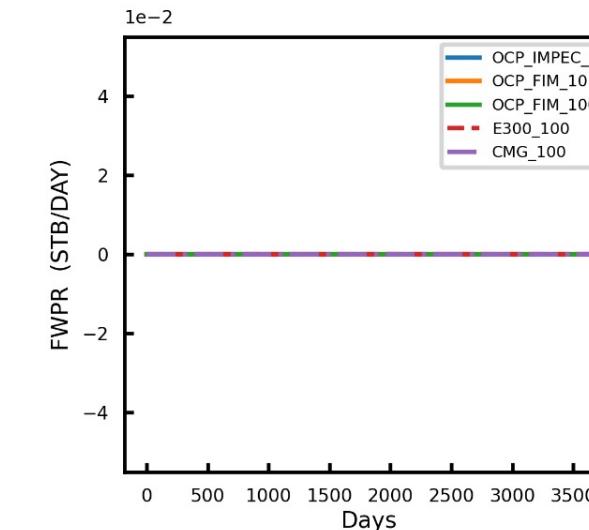
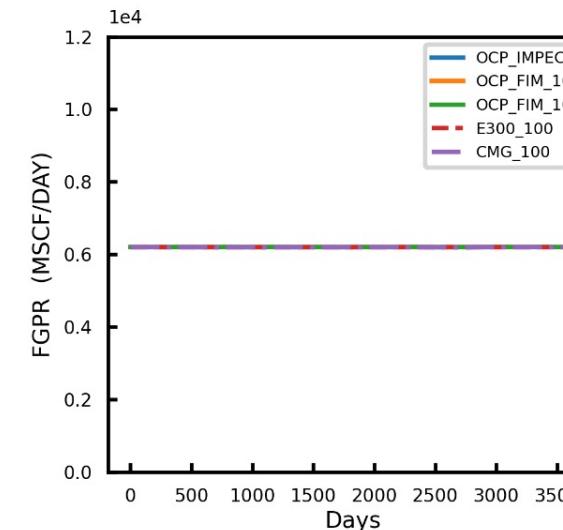
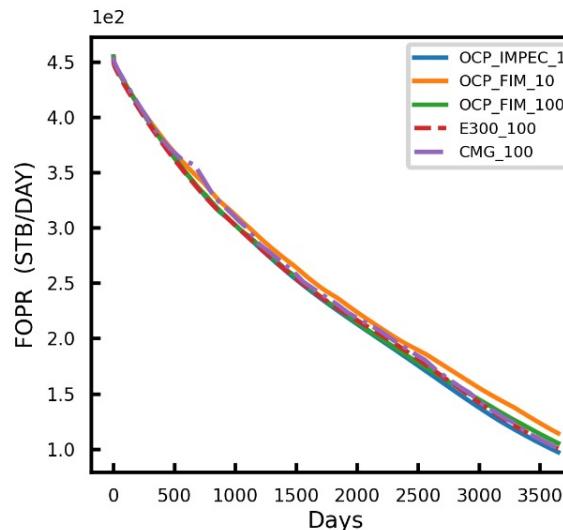
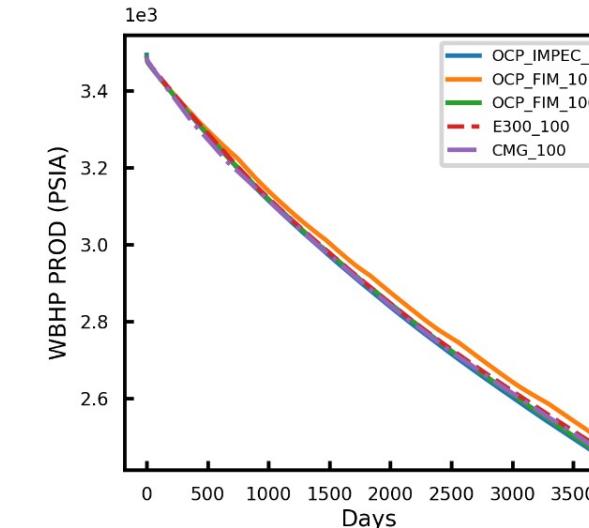
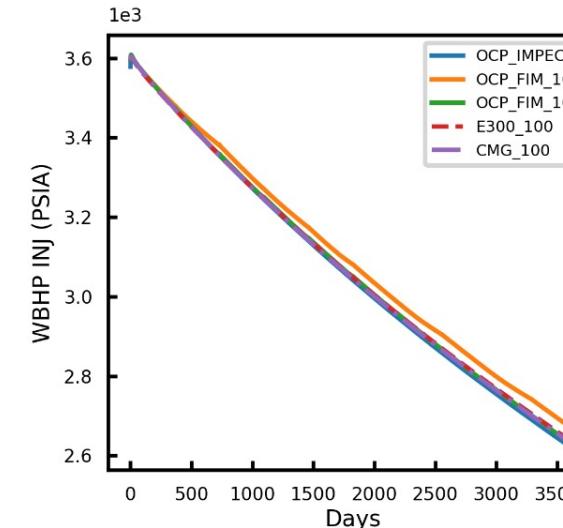
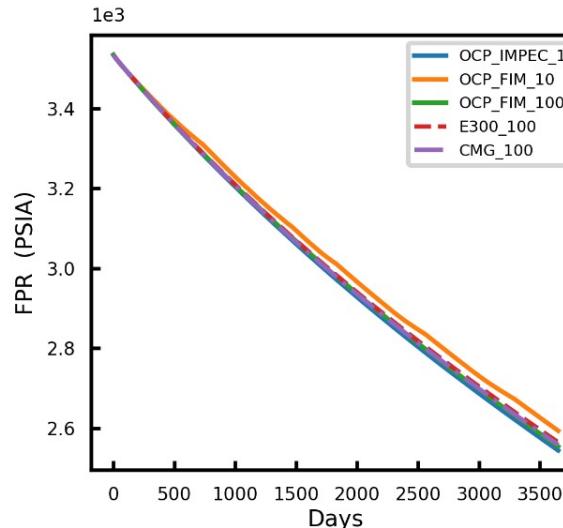


Grid: 60*220*85
Well: 5
Day: 2000

OpenCAEPoro
NR: 218(+6)
LS: 1344(+51)
LStime: 1435s(74%)
Total: 1939s



SPE3标准算例：十组分回注



Grid: 9*9*4

Well: 2

Year: 10

IMPEC

NR: 3652 (+0)

LS: 7307 (+0)

LTime: 1s (2.9%)

Total: 37.8s

FIM(100)

NR: 158 (+1)

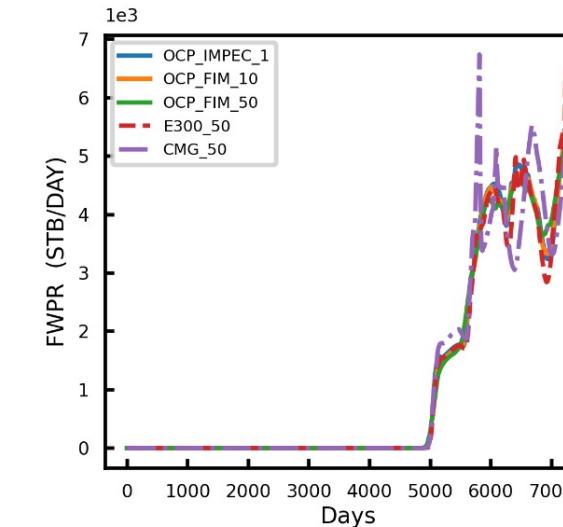
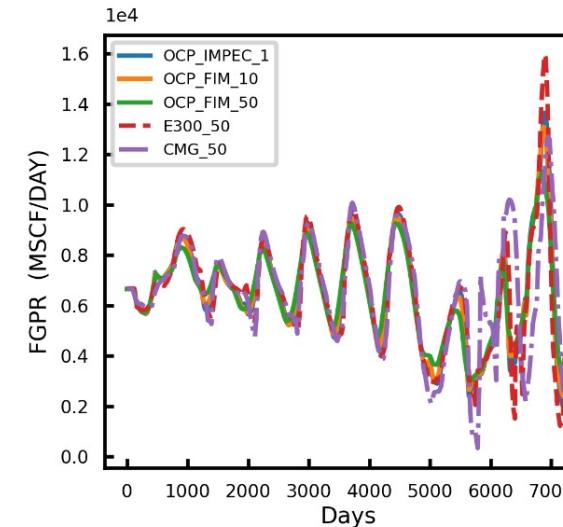
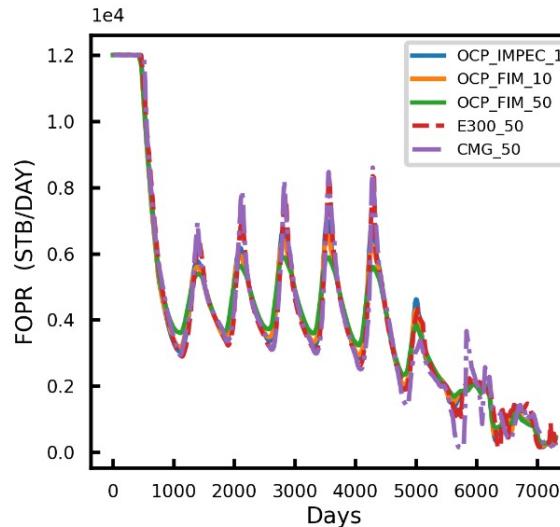
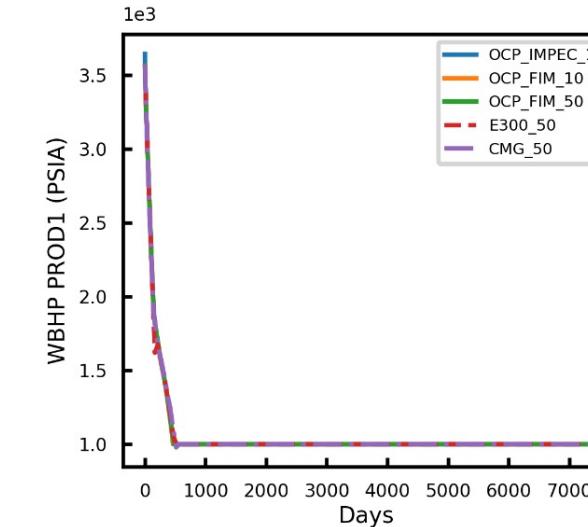
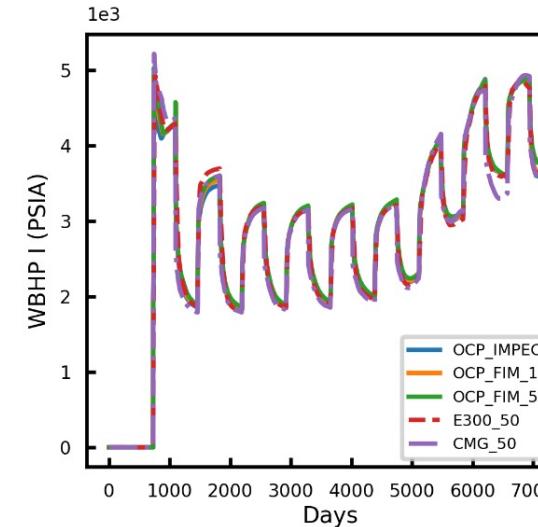
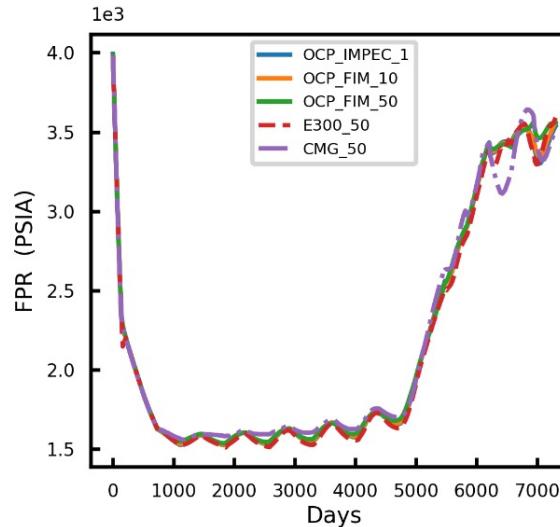
LS: 246 (+2)

LTime: 1.5s (51%)

Total: 3.0s



SPE5标准算例：七组分挥发油



Grid: 7*7*3

Well: 2

Year: 20

IMPEC

NR: 10834 (+62)

LS: 17371 (+124)

LTime: 1.2s (8%)

Total: 15.3s

FIM(50)

NR: 860 (+45)

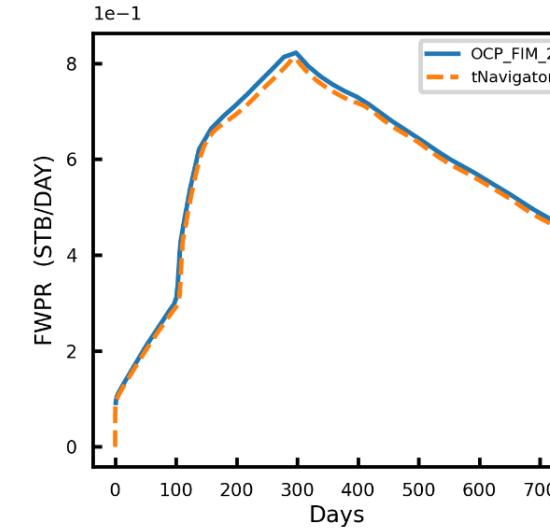
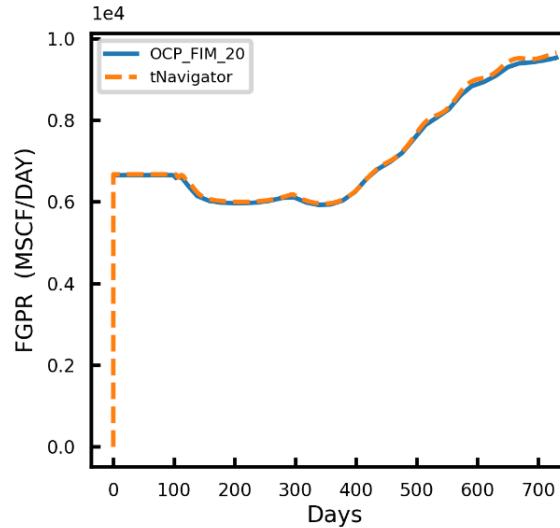
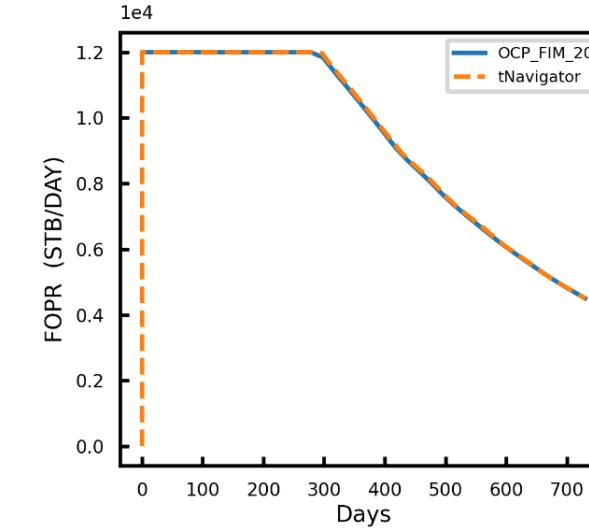
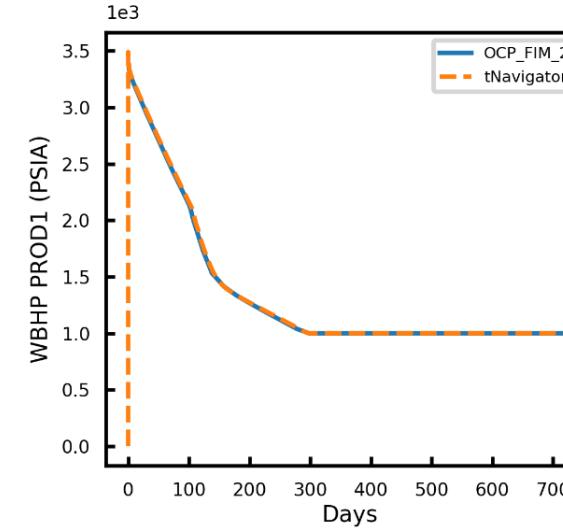
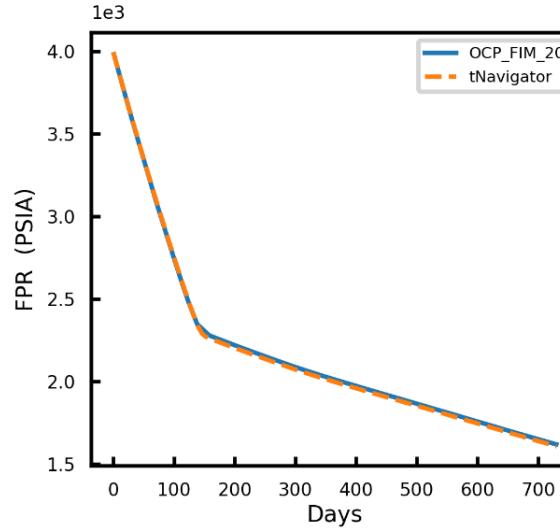
LS: 2766 (+185)

LTime: 7.4(83%)

Total: 8.9s



SPE5标准算例：网格加密



Grid: 70*70*30

Well: 1

Year: 2

FIM

NR: 214 (+19)

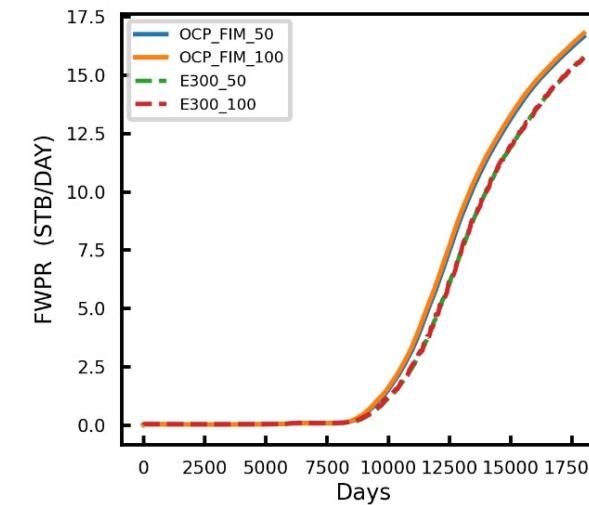
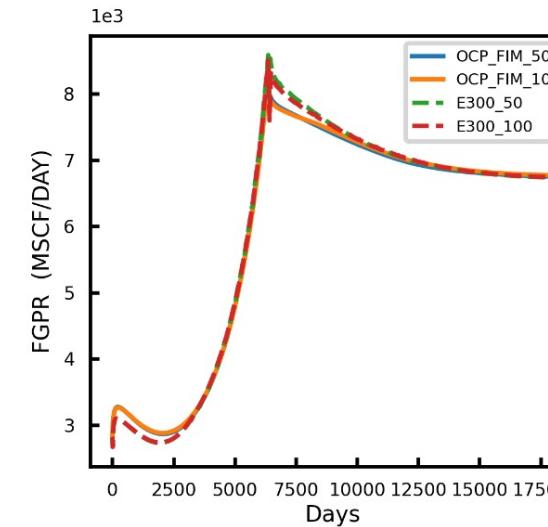
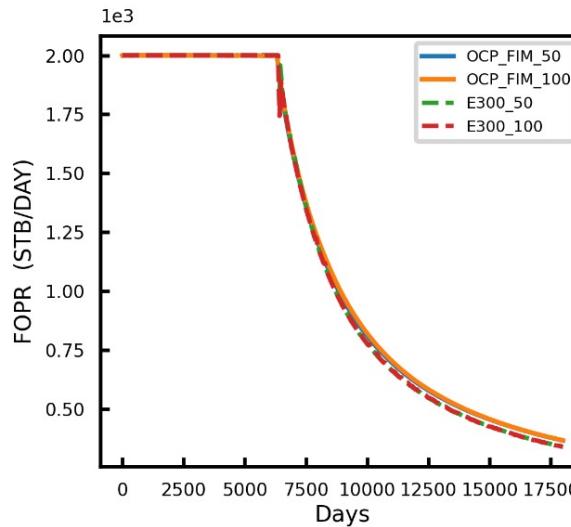
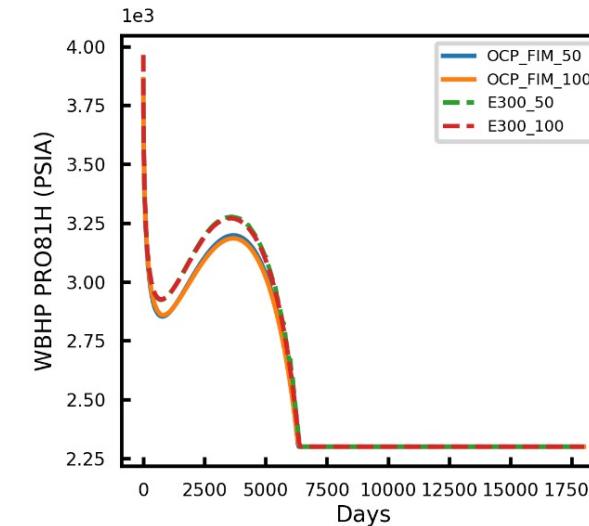
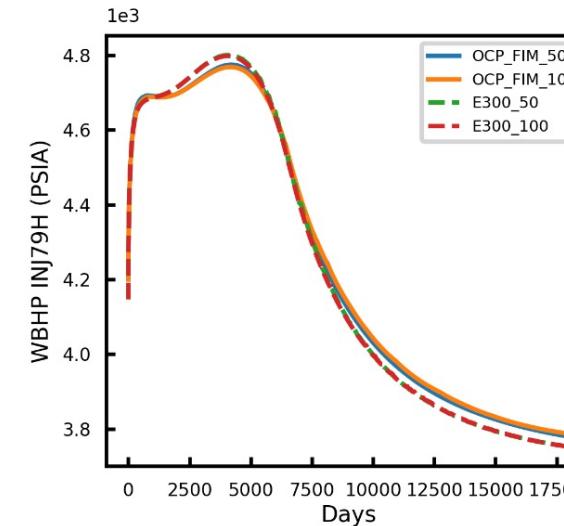
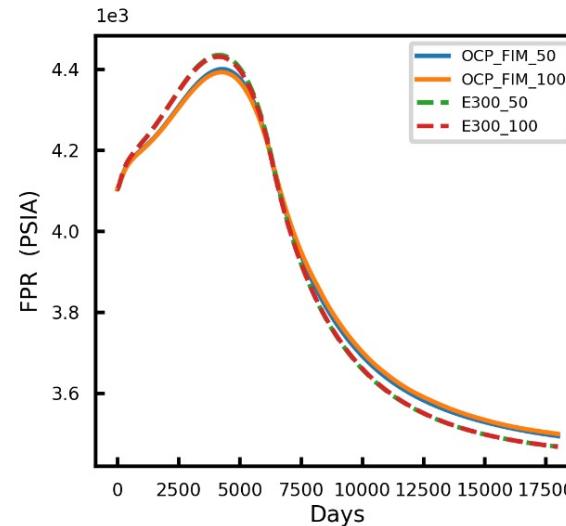
LS: 798 (+75)

LStime: 429s (50%)

Total: 855.7s



ZB-CO₂实际算例：三口井



Grid: 16x15x75

Well: 3

Year: 50

FIM(100)

NR: 757 (+66)

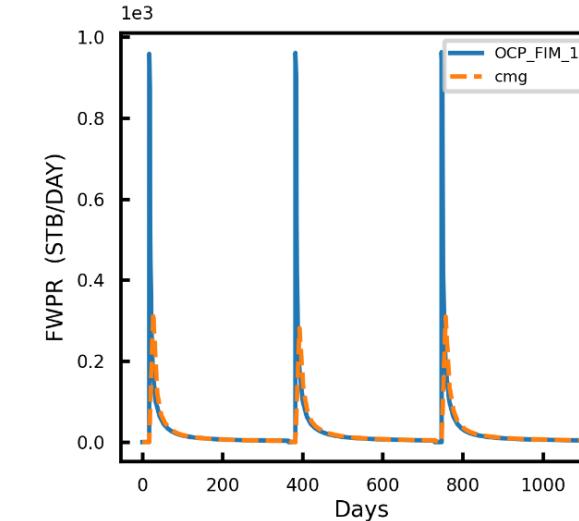
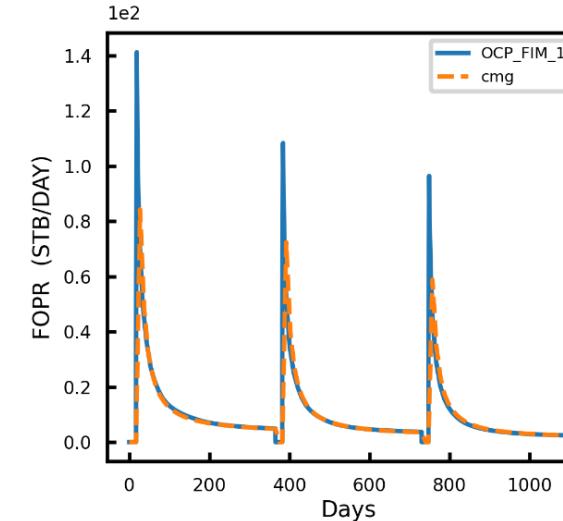
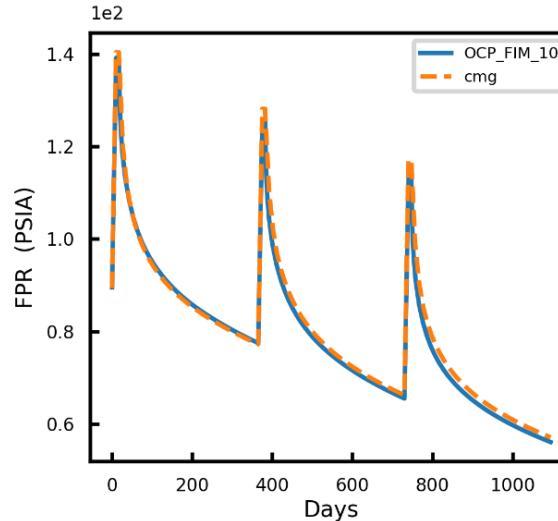
LS: 1385 (+129)

LStime: 197s (45.8%)

Total: 430s



SPE4标准算例：非等温、交替注采



Grid: 13*1*4

Well: 1

Year: 3

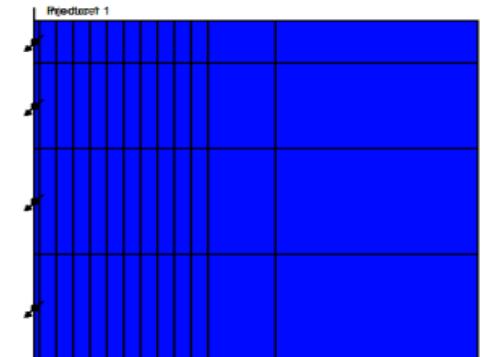
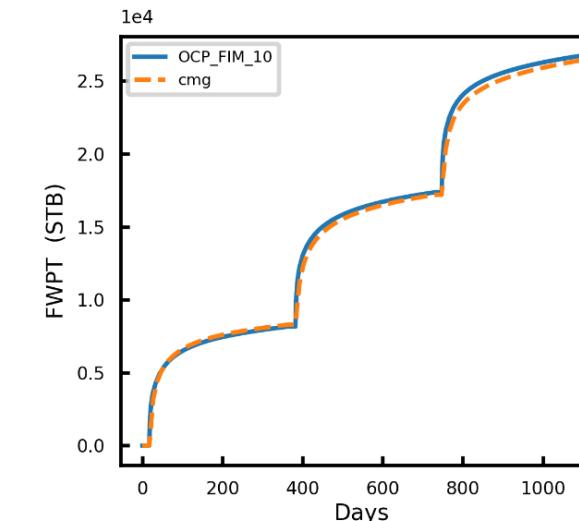
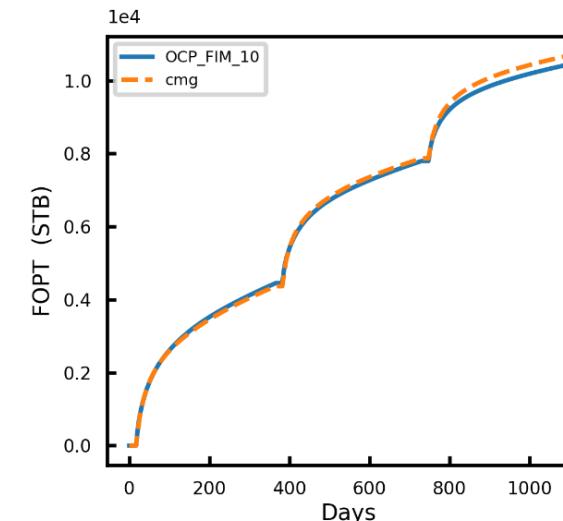
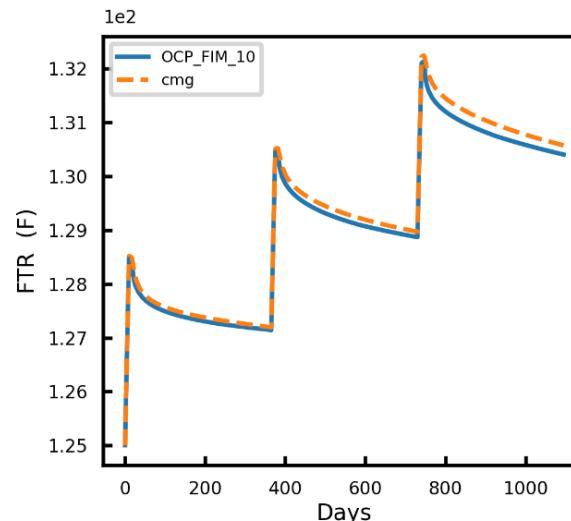
FIM

NR: 399 (+32)

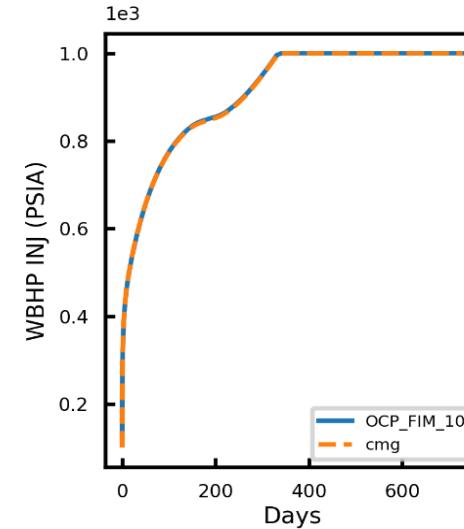
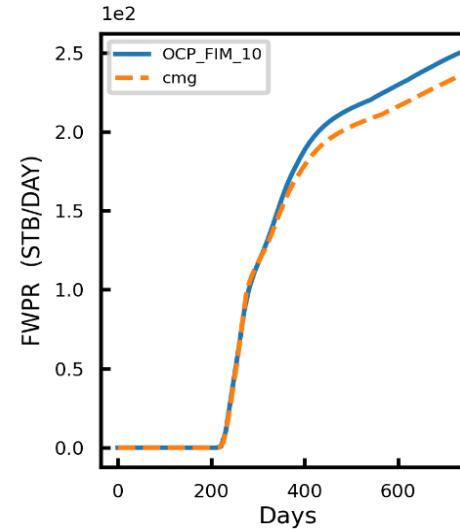
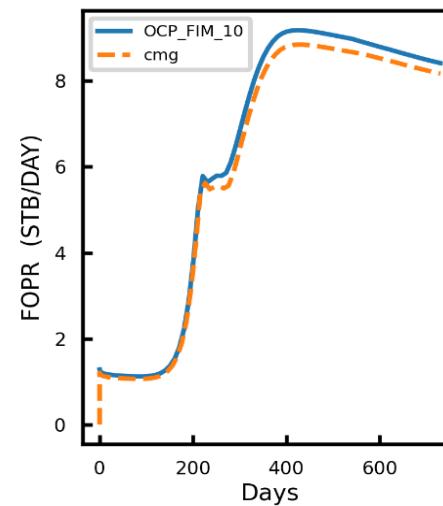
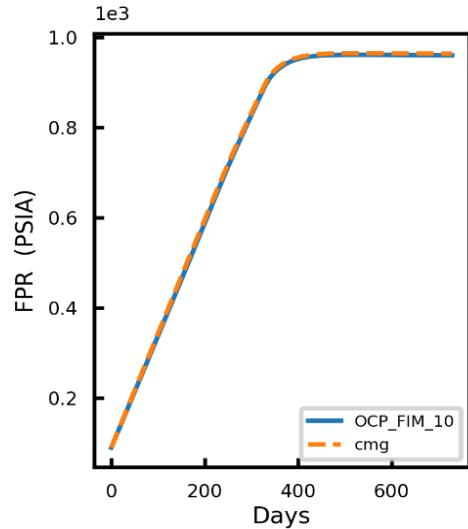
LS: 2936 (+258)

LStime: 0.03 (36%)

Total: 0.08s

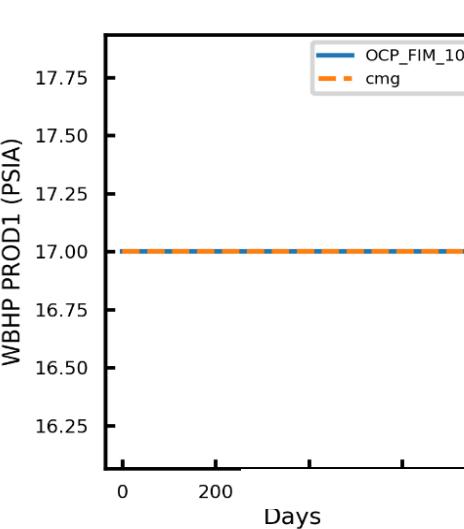
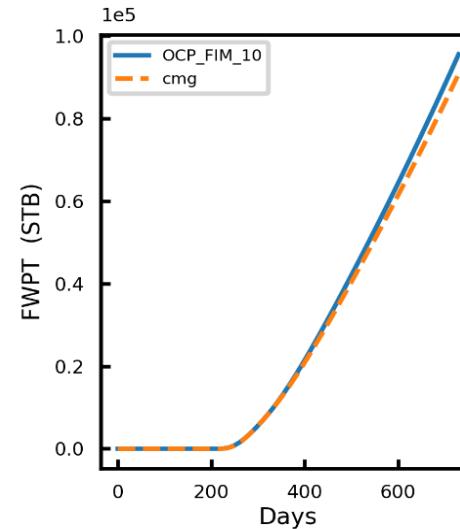
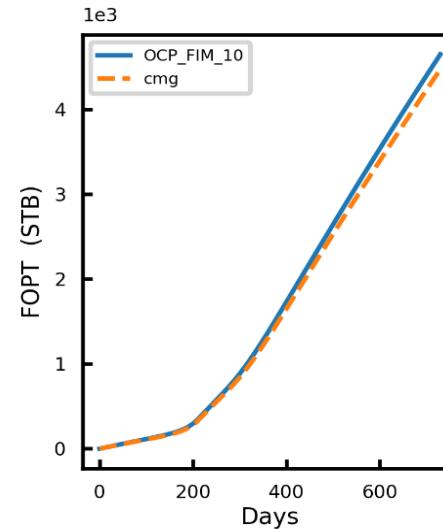
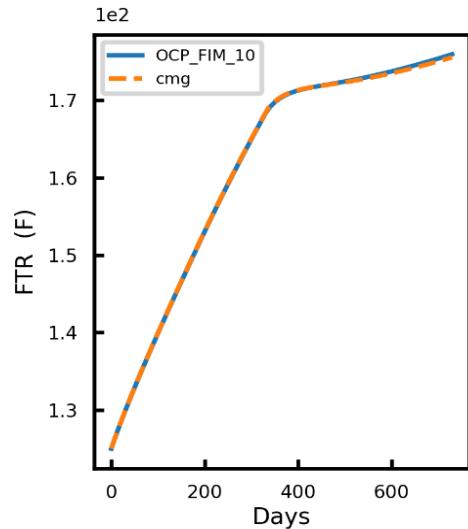


SPE4-M1算例：非等温、一注一采



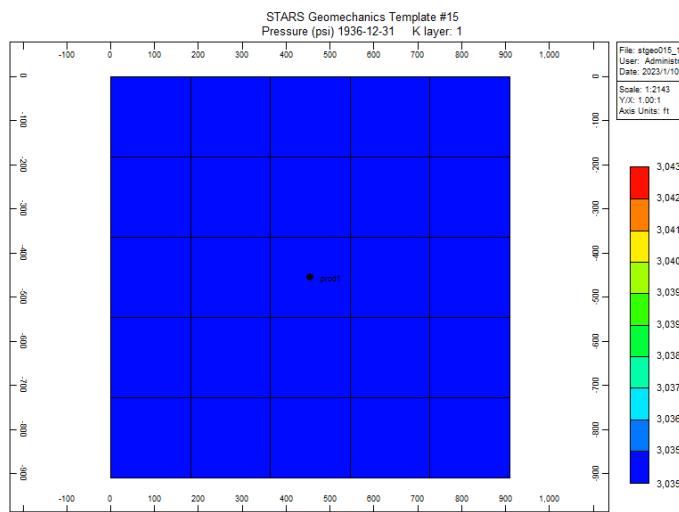
Grid: 26*1*4
 Well: 2
 Year: 2

 FIM
 NR: 207(+2)
 LS: 2755(+36)
 LTime: 0.06 (59%)
 Total: 0.11s

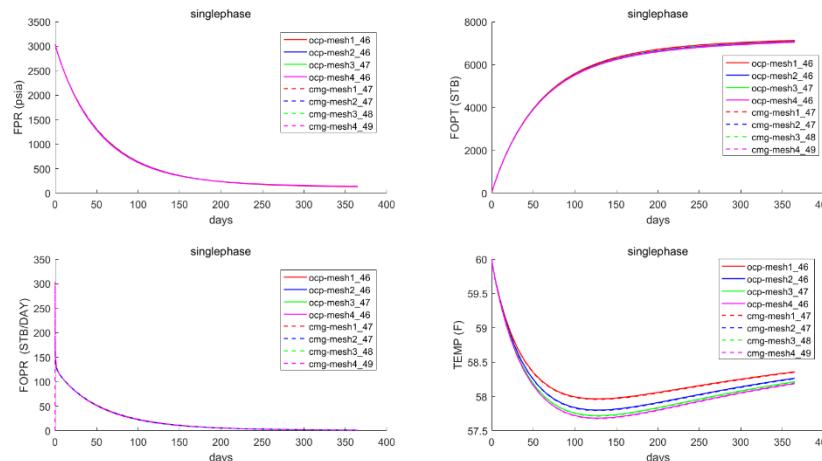




STGEO015加密算例：非等温



网格加密收敛性测试



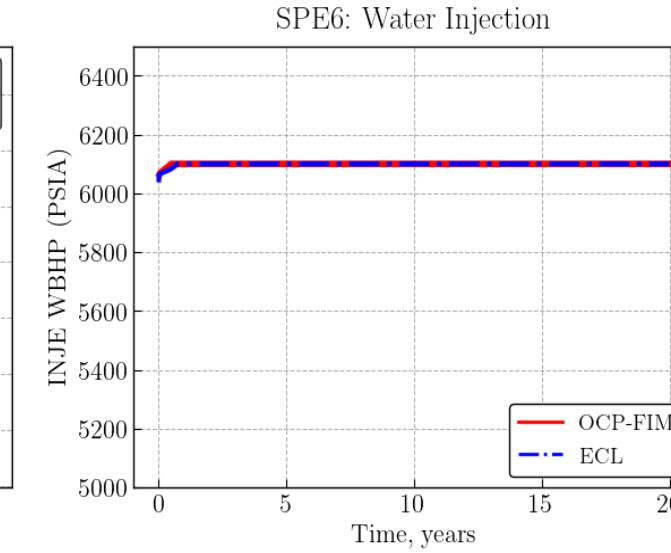
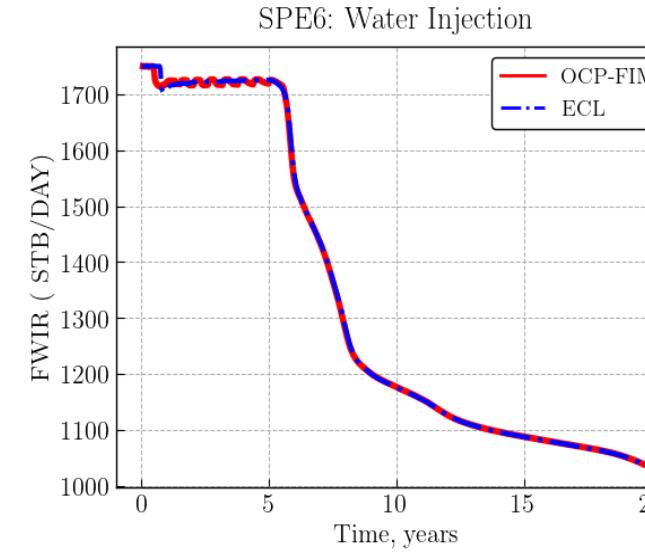
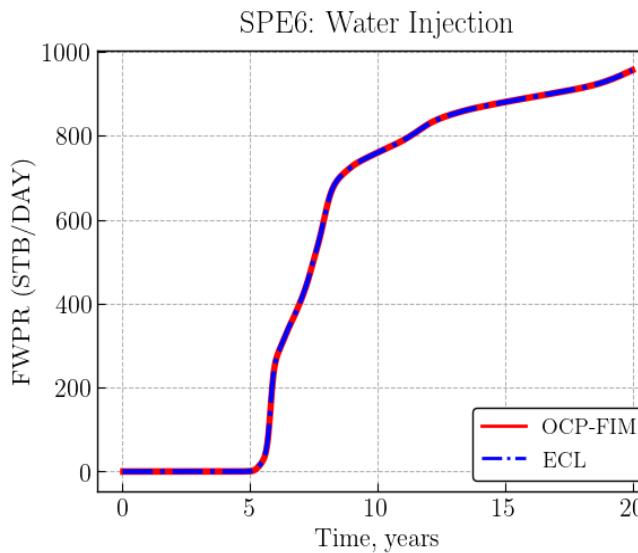
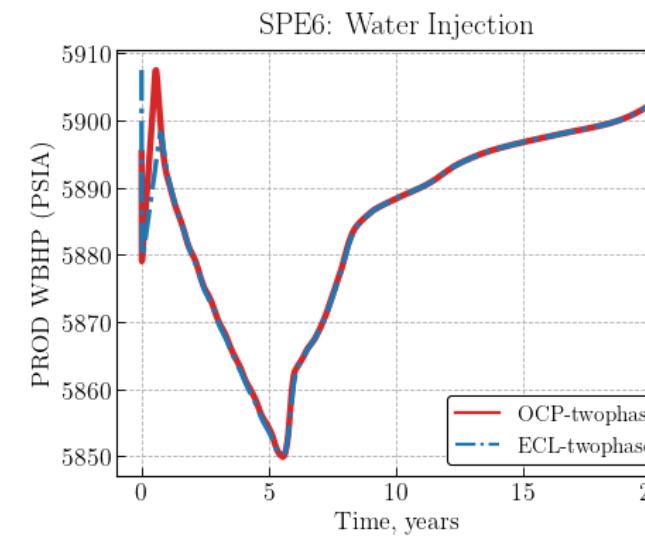
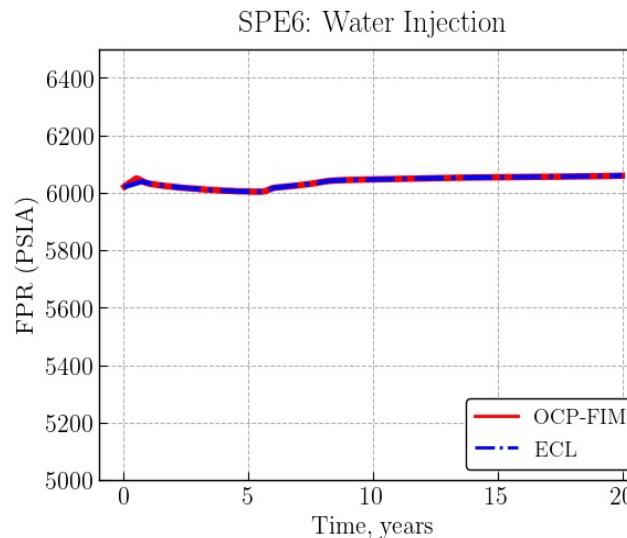
基于CMG-STARS的算例stgeo015构造：油田区域的水平方向为边长909.05ft的正方形，垂向厚度为40ft。初始状态下，参考深度(5010ft)的油压为3035psia，初始油饱和度1，初始水饱和度0。为了对比方便，所有模拟均使用BILU(1)作为预条件方法。

mesh1 : 5×5×2 , mesh2 : 11×11×5 , mesh3 : 23×23×11 , mesh4 : 47×47×23

模拟器	解法器	网格	总时间步数	线性迭代步数	模拟时间(秒)
OCP	vFGMRES	1	46	276	0.103
		2	46	518	0.422
		3	47	907	3.870
		4	46	1626	61.262
	BiCGstab	1	46	179	0.099
		2	46	363	0.397
		3	47	705	4.203
		4	46	1268	68.673
CMG	BiCGstab	1	46	210	11
		2	46	484	10
		3	47	850	14
		4	48	1330	54



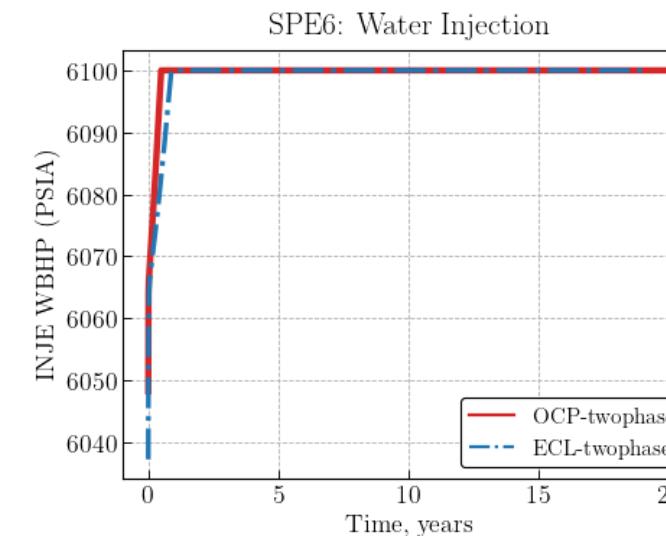
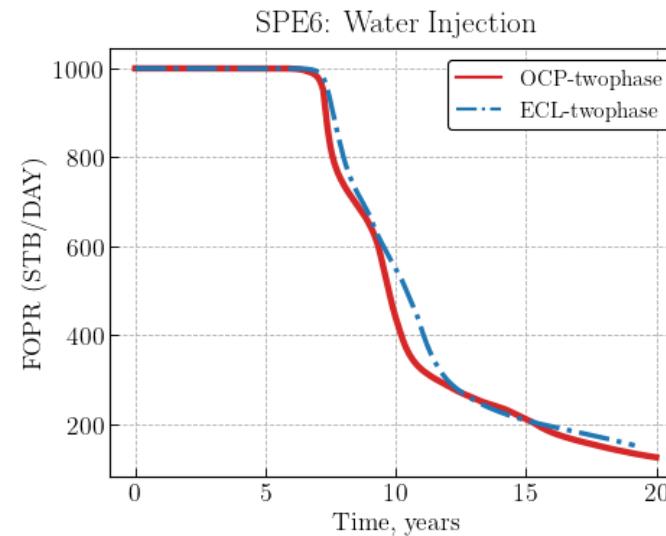
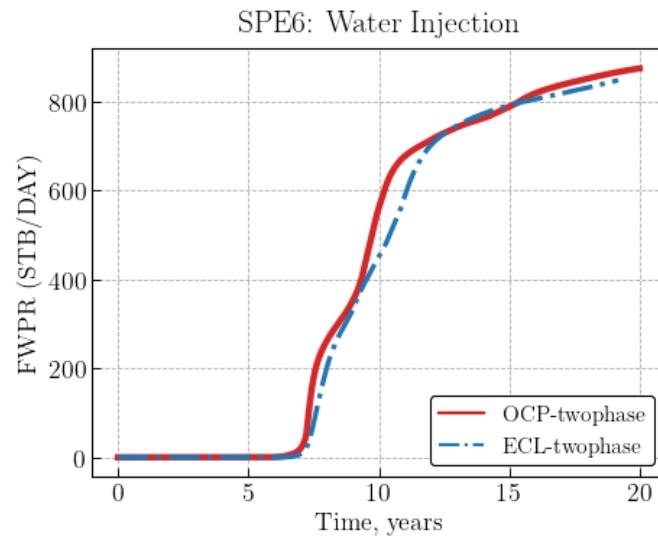
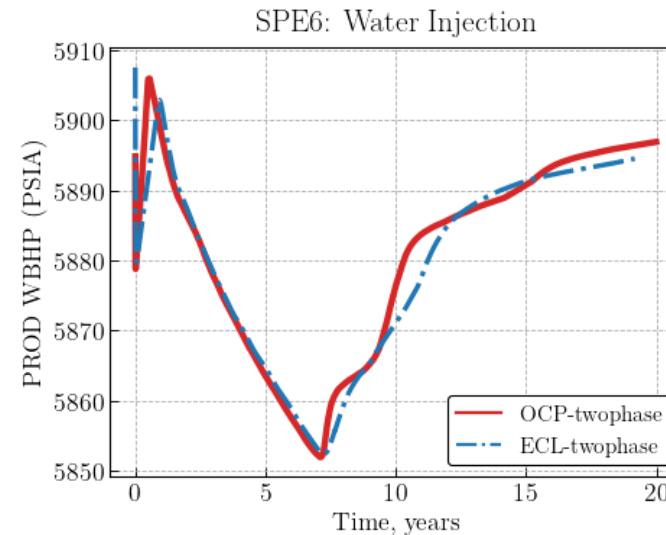
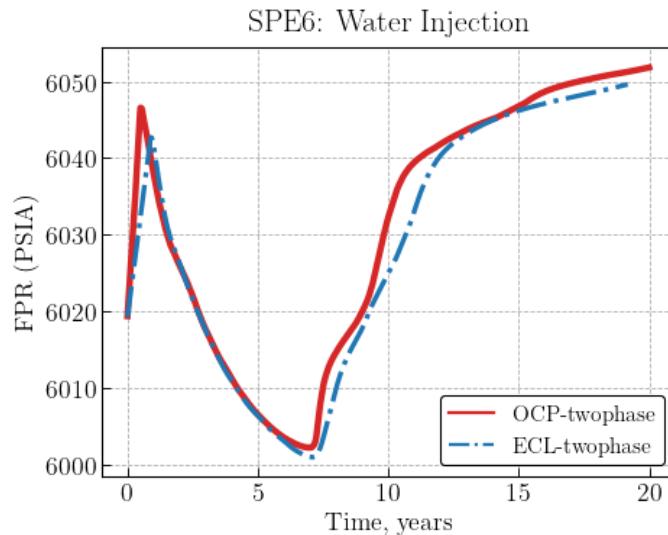
SPE6标准算例：DP模型



Grid: $10 \times 1 \times 5$
Well: 2
Time: 20 Years
FIM
NR: 828 (+2)
LS: 11127 (+42)
LS time: 0.146s (15.8%)
Total time: 0.927s



SPE6标准算例：DP模型、GRAVDR



Grid: 10 × 1 × 5
Well: 2
Time: 20 Years
FIM
NR: 7320 (+2)
LS: 34518 (+42)
LS time: 0.58s (15.8%)
Total time: 6.28s

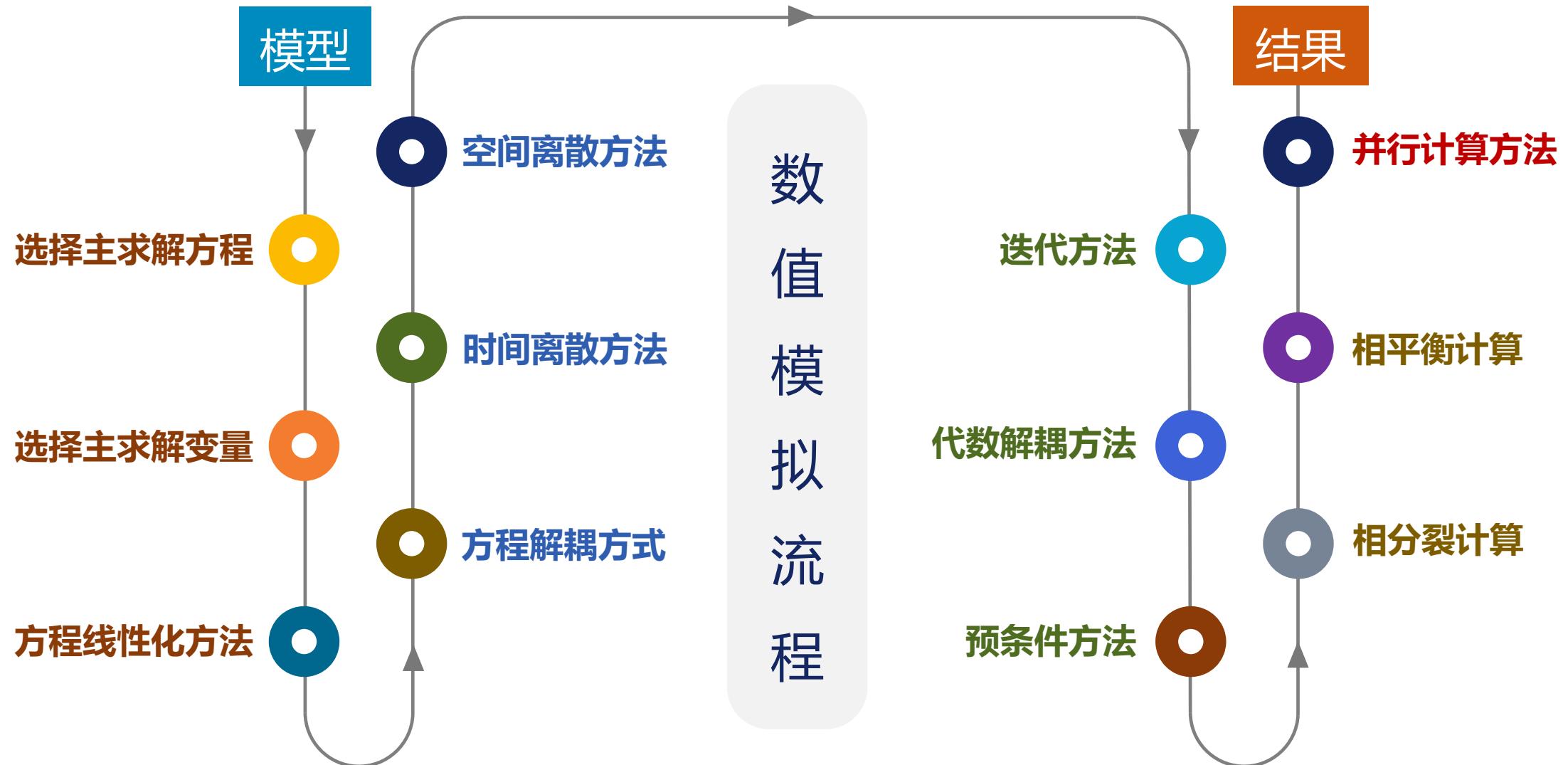
03

数值方法

Numerical methods for porous media flows



数值模拟方法





OpenCAE[®]Poro求解方法的选择

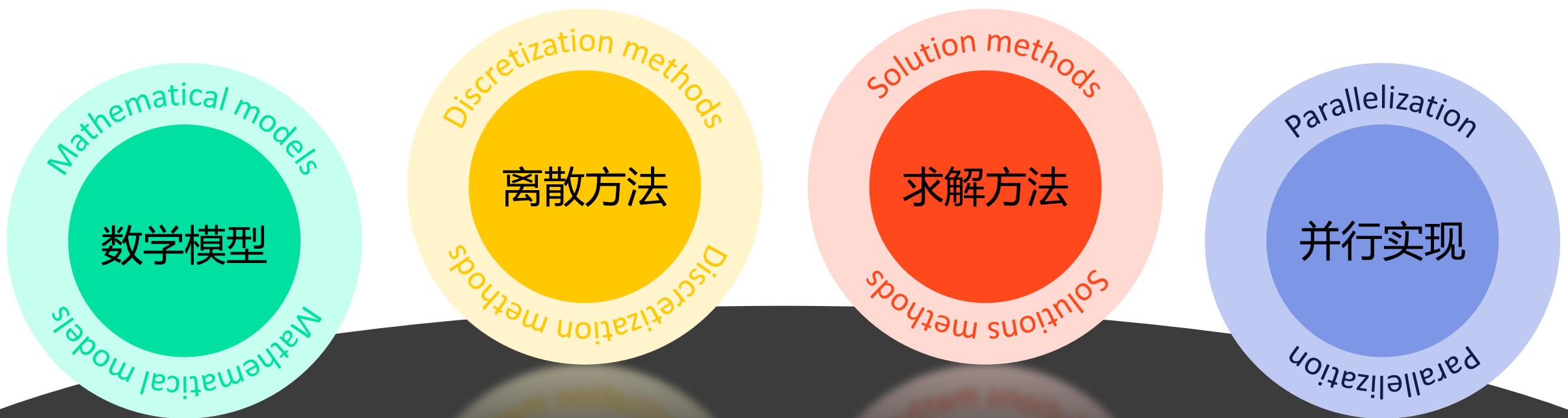


全隐式方法 + 向后Euler时间离散 + 自适应时间步长 + Newton线性化 + 无结构网格

+ TPF有限体积法 + 上游加权 + 拟Newton法 + 半解析解耦方法 + 多阶段预条件 + FGMRES



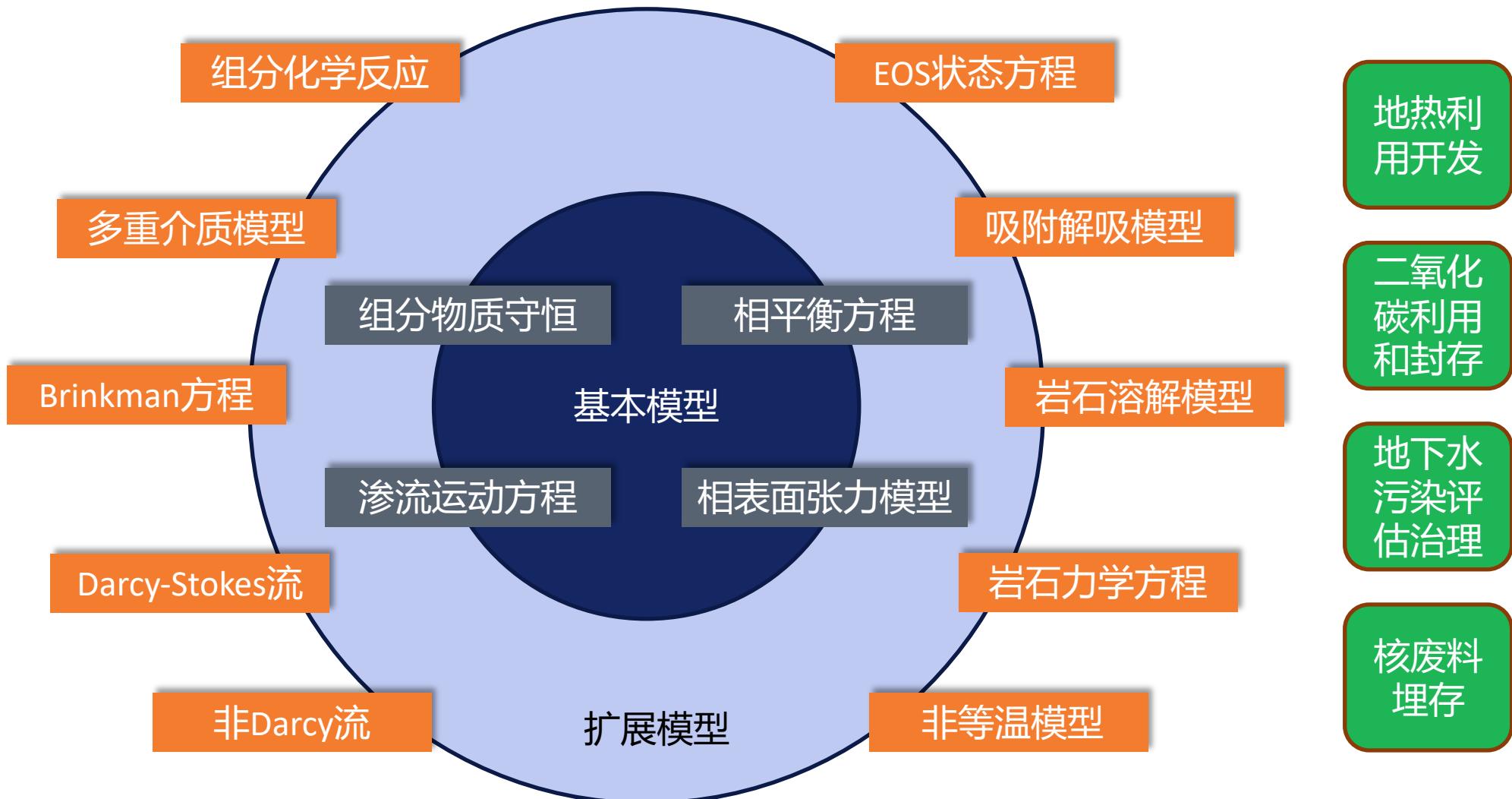
多相多组分渗流求解方法





多相多组分渗流力学方程

传统油气开发
碳酸盐岩油藏
页岩油气开发
凝析气藏开发





等温多组分模型框架



$$\frac{\partial}{\partial t} \left(\phi \sum_{j=1}^{n_p} x_{ij} \xi_j S_j \right) + \nabla \cdot \mathbf{F}_i - \sum_{j=1}^{n_p} S_j r_{ij} = Q_i, \quad i = 1 : n_c \quad \text{物质守恒}$$

$$\mathbf{F}_i = \sum_{j=1}^{n_p} \left(x_{ij} \xi_j \mathbf{u}_j - S_j \mathbf{D}_j \nabla (\xi_j x_{ij}) \right), \quad i = 1 : n_c \quad \text{流量方程}$$

$$\mathbf{u}_j = - \frac{\kappa \kappa_{rj}}{\mu_j} (\nabla P_j - \gamma_j \nabla z), \quad j = 1 : n_p \quad \text{Darcy定律}$$

$$\sum_{j=1}^{n_p} S_j = 1, \quad \text{饱和度关系}$$

$$\sum_{i=1}^{n_c} x_{ij} = 1, \quad j = 1 : n_p \quad \text{组分比例关系}$$

$$P_1 - P_j = P_{c1j}, \quad j = 2 : n_p \quad \text{表面张力}$$

$$f_{ij} = f_{i1}, \quad i = 1 : n_c, \quad j = 2 : n_p \quad \text{相平衡方程}$$

目标：为工程和科学研究提供更丰富、更精确的物理模型选择

多重介质模型

EOS状态方程

Brinkman方程

化学反应方程

Navier-Stokes方程

非等温模型

非Darcy模型

吸附解吸模型

岩石溶解模型

岩石力学方程



简单油水两相模型



物质守恒

$$\frac{\partial}{\partial t} \left(\phi \frac{S_w}{B_w} \right) = -\nabla \cdot \left(\frac{1}{B_w} \mathbf{u}_w \right) + \tilde{q}_W$$

$$\frac{\partial}{\partial t} \left(\phi \frac{S_o}{B_o} \right) = -\nabla \cdot \left(\frac{1}{B_o} \mathbf{u}_o \right) + \tilde{q}_O$$

Darcy定律

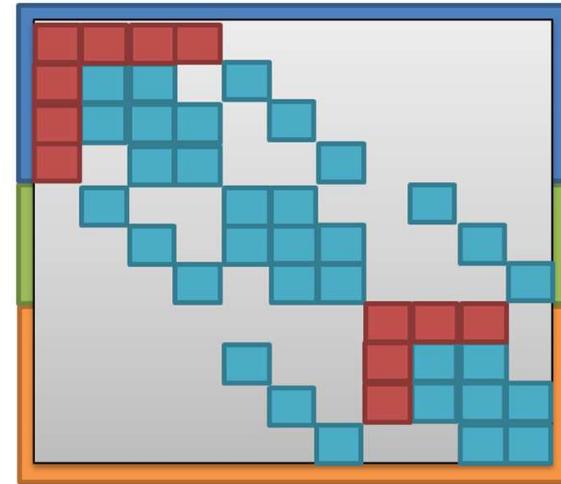
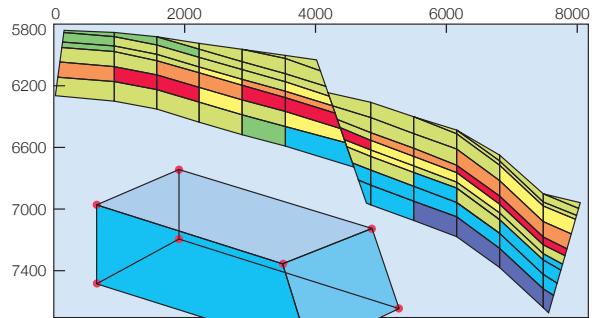
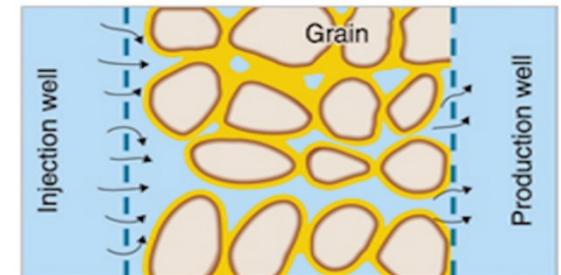
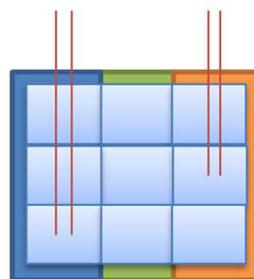
$$\mathbf{u}_j = -\frac{\kappa \kappa_{rj}}{\mu_j} \left(\nabla P_j - \gamma_j \nabla z \right), \quad j = o, w$$

其它关系式

$$S_w + S_o = 1$$

$$P_{cow} = P_o - P_w$$

方程的数学性质 : Trangenstein, Bell SINUM 1989; SISC 1989





经典三相黑油模型



可以利用这些关系式来给出组分模型框架下的黑油模型，并在统一的程序框架内对黑油和组分模型进行模拟！

$$\begin{array}{c}
 \begin{matrix} O & G & W \end{matrix} \\
 \begin{matrix} Ww \\ Oo \\ Gg \\ Go \end{matrix} \left(\begin{array}{ccc} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{array} \right) \quad \begin{matrix} \xi_w = \frac{1}{B_w} \\ \xi_g = \frac{1}{B_g} \\ \xi_o = \frac{1 + R_s}{B_o} \end{matrix}
 \end{array}$$

$$\begin{bmatrix} x_{Oo} & x_{Go} & x_{Wo} \\ x_{Og} & x_{Gg} & x_{Wg} \\ x_{Ow} & x_{Gw} & x_{Ww} \end{bmatrix} = \begin{bmatrix} \frac{1}{1+R_s} & \frac{R_s}{1+R_s} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

物质守恒

$$\frac{\partial}{\partial t} \left(\phi \frac{S_w}{B_w} \right) = -\nabla \cdot \left(\frac{1}{B_w} \mathbf{u}_w \right) + \tilde{q}_w$$

$$\frac{\partial}{\partial t} \left(\phi \frac{S_o}{B_o} \right) = -\nabla \cdot \left(\frac{1}{B_o} \mathbf{u}_o \right) + \tilde{q}_o$$

$$\frac{\partial}{\partial t} \left(\phi \frac{S_g}{B_g} + \phi \frac{R_s S_o}{B_o} \right) = -\nabla \cdot \left(\frac{1}{B_g} \mathbf{u}_g + \frac{R_s}{B_o} \mathbf{u}_o \right) + \tilde{q}_G$$

Darcy定律

$$\mathbf{u}_j = -\frac{\kappa \kappa_{rj}}{\mu_j} (\nabla P_j - \gamma_j \nabla z), \quad j = o, w, g$$

其它关系式

$$S_o + S_g + S_w = 1$$

$$P_{cog} = P_o - P_g$$

$$P_{cow} = P_o - P_w$$



热力学平衡与状态方程



问题：如何确定混合物的物质处于什么相态？存在多少相？是否处于稳定的平衡状态？某一具体的相中包含了多少种物质？以及包含了多少该物质？

Van der Waals / Redlich–Kwong / Redlich–Kwong–Soave EOS:

$$P_j := \frac{RT}{V_j - b_j} - \frac{a_j}{V_j(V_j + b_j)}, \quad j = o, g$$

常用相平衡计算方法

- ✓ 平衡常数法
- ✓ 基于RR方程的闪蒸计算
- ✓ 基于Gibbs自由能最小化

Peng–Robinson EOS: [Peng, Robinson 1976]

$$P_j := \frac{RT}{V_j - b_j} - \frac{a_j}{V_j(V_j + b_j) + b_j(V_j - b_j)}, \quad j = o, g$$

Change of variables:

$$A_j := \frac{a_j P_j}{R^2 T^2}, \quad B_j := \frac{b_j P_j}{R T}, \quad Z_j := \frac{P_j V_j}{R T}$$

$$Z_j^3 - (1 - B_j)Z_j^2 + (A_j - 2B_j - 3B_j^2)Z_j - (A_j B_j - B_j^2 - B_j^3) = 0$$

Fugacity:



$$f_{ij} := P_j x_{ij} \varphi_{ij}, \quad i = 1, \dots, n_c, \quad j = o, g \quad (\varphi_{ij} : \text{fugacity coefficient})$$

无量纲化



非等温模型的能量方程



$$\frac{\partial}{\partial t} \left(\phi \sum_{j=1}^{n_p} \xi_j S_j U_j + (1 - \phi) U_r \right) + \nabla \cdot \sum_{j=1}^{n_p} \xi_j \mathbf{u}_j H_j - \nabla \cdot (\kappa_T \nabla T) = \sum_{j=1}^{n_p} q_{j,well} H_j - Q_{loss}, \quad \text{能量守恒}$$

$$U_j = H_j - P/\xi_j, \quad j = 1 : n_p \quad \text{相内能}$$

$$U_r = C_r(T - T_{ref}), \quad \text{岩石内能}$$

$$\kappa_T = \phi \sum_{j=1}^{n_p} S_j \kappa_j + (1 - \phi) \kappa_r, \quad \text{导热率}$$

计算焓的方法

$$H_{g,i} = \int_{T_{ref}}^T (cp_{g1i} + cp_{g2i}t + cp_{g3i}t^2 + cp_{g4i}t^3 + cp_{g5i}t^4) dt,$$

$$H_{v,i} = \begin{cases} hvr_i(T_{crit,i} - T)^{ev_i}, & T < T_{crit,i} \\ 0, & T \geq T_{crit,i} \end{cases}$$

$$H_l = \sum_{i=1}^{n_c} x_{il}(H_{g,i} - H_{v,i}), \quad H_g = \sum_{i=1}^{n_c} x_{ig} H_{g,i}$$

Gas-based

$$H_{l,i} = \int_{T_{ref}}^T (cpl_{1i} + cpl_{2i}t + cpl_{3i}t^2 + cpl_{4i}t^3 + cpl_{5i}t^4) dt,$$

$$H_l = \sum_{i=1}^{n_c} x_{il} H_{l,i}, \quad H_g = \sum_{i=1}^{n_c} x_{ig} (H_{g,i} + H_{v,i}),$$

Liquid-based

$$H_{l,i} = \int_{T_{ref}}^T (cpl_{1i} + cpl_{2i}t + cpl_{3i}t^2 + cpl_{4i}t^3 + cpl_{5i}t^4) dt,$$

$$H_{g,i} = \int_{T_{ref}}^T (cp_{g1i} + cp_{g2i}t + cp_{g3i}t^2 + cp_{g4i}t^3 + cp_{g5i}t^4) dt,$$

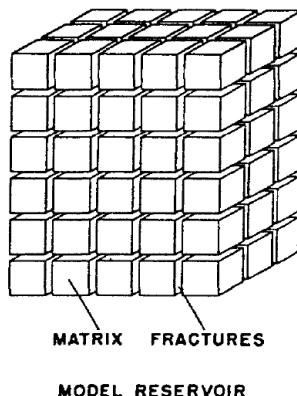
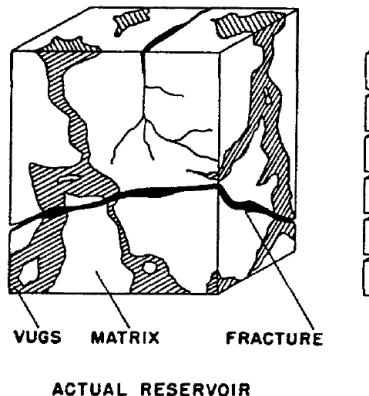
$$H_g = \sum_{i=1}^{n_c} x_{ig} (H_{g,i} + hvapr),$$

$$H_l = \sum_{i=1}^{n_c} x_{il} H_{l,i},$$

Simple Hvap



双重介质的DPDP模型



(单相) DPDP模型 :

$$\phi_m C_{mt} \frac{\partial p_m}{\partial t} - \nabla \cdot \frac{k_m}{\mu} \nabla p_m = -Q$$
$$\phi_f C_{ft} \frac{\partial p_f}{\partial t} - \nabla \cdot \frac{k_f}{\mu} \nabla p_f = Q + q_p$$

ϕ_m/ϕ_f : porosities

C_{mt}/C_{ft} : compressibilities

p_m/p_f : pressures

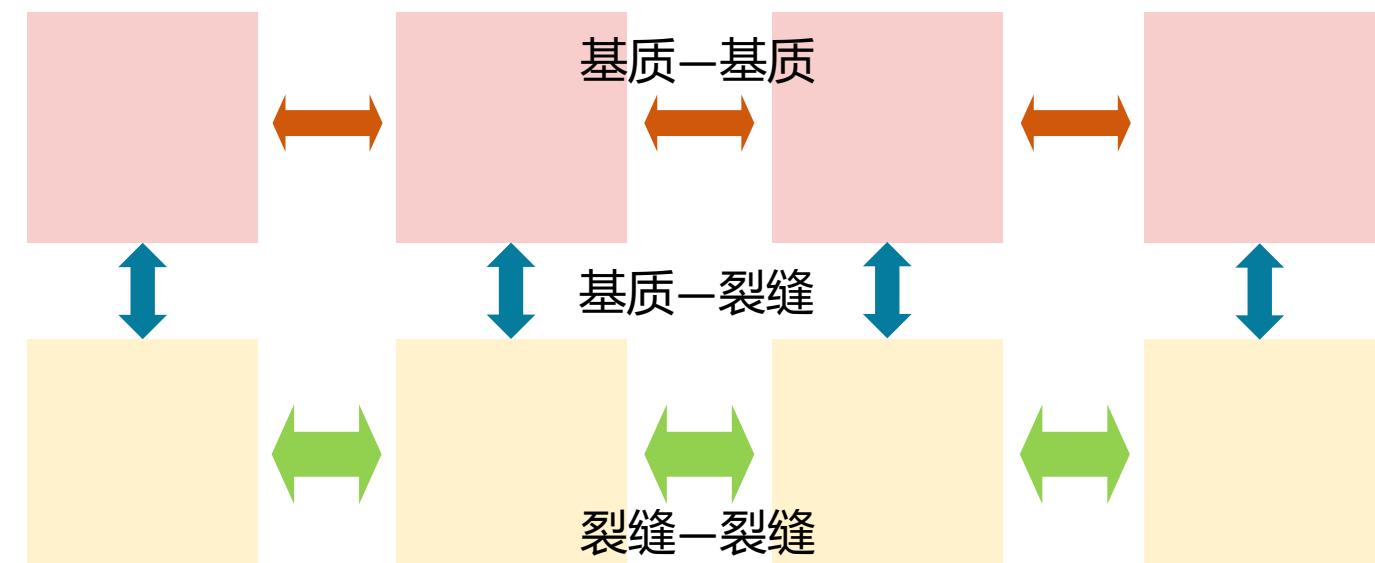
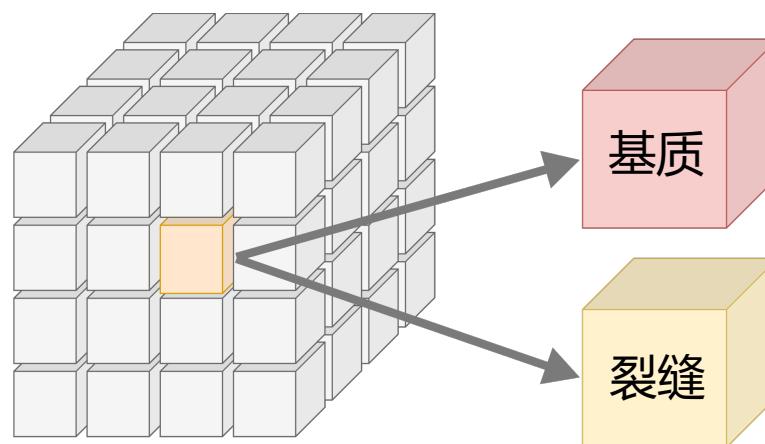
k_m/k_f : permeabilities

μ : dynamic viscosities

q_p : sink/source term

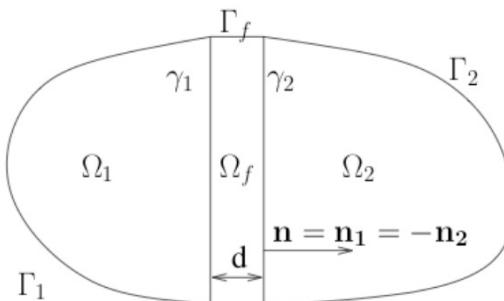
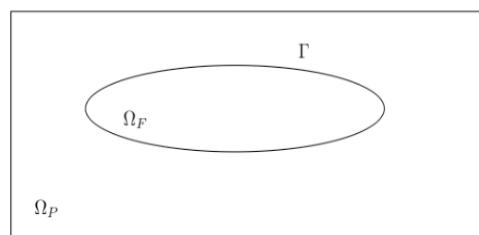
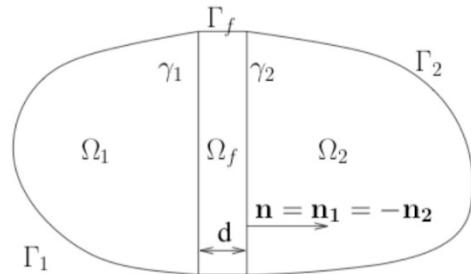
$Q = \frac{\sigma k}{\mu} (p_m - p_f)$: mass exchange

σ : shape factor





裂缝与溶洞等介质的常用模型



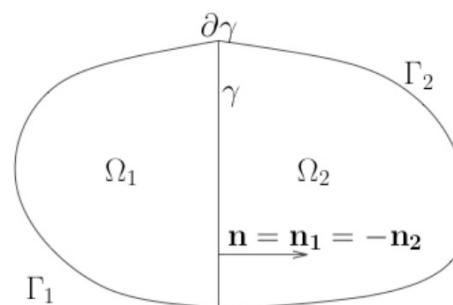
$$\left\{ \begin{array}{ll} \mathbf{u}_i = -\kappa_i \nabla p_i, & \Omega_i, \quad i = 1, 2, f, \\ \nabla \cdot \mathbf{u}_i = f_i, & \Omega_i, \quad i = 1, 2, f, \\ \mathbf{u}_1 \cdot \mathbf{n} = \mathbf{u}_f \cdot \mathbf{n}, & \gamma_i, \quad i = 1, 2, \\ p_i = p_D, & \gamma_i, \quad i = 1, 2, \\ p_i = p_D, & \Gamma_i, \quad i = 1, 2, f. \end{array} \right.$$

$$\left\{ \begin{array}{ll} -\nabla \cdot (\mu(x) \nabla \mathbf{u}) + \kappa^{-1} \mathbf{u} + \nabla p = \mathbf{f}, & \Omega, \\ \nabla \cdot \mathbf{u} = g, & \Omega, \\ \mathbf{u} = \mathbf{0}, & \partial\Omega. \end{array} \right.$$

Darcy-Darcy

Brinkman

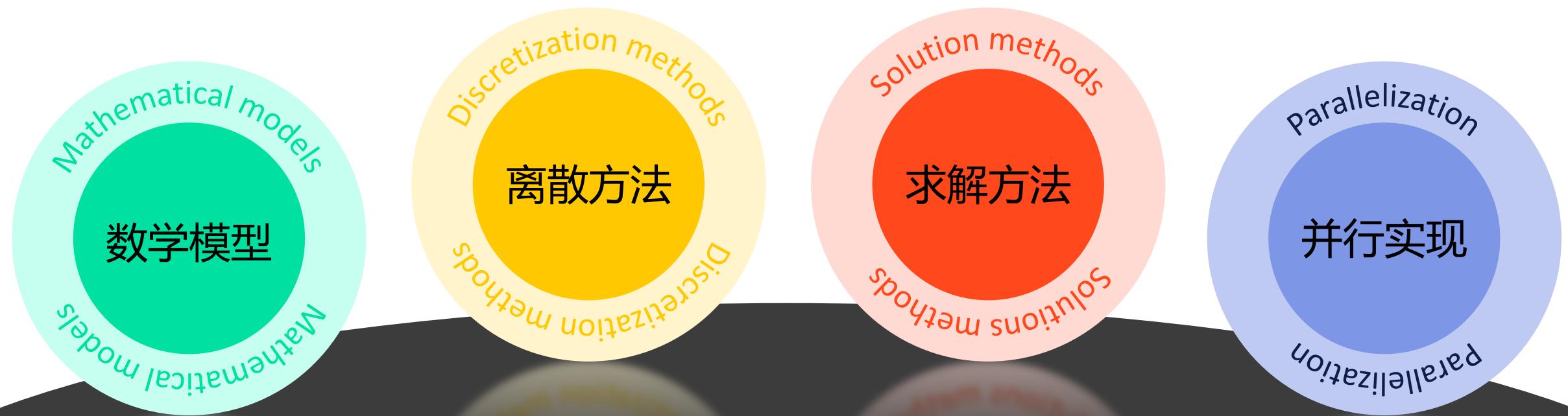
$$\left\{ \begin{array}{ll} \mathbf{u} = -\kappa \nabla p_P, & \Omega_P, \\ -\mu \Delta \mathbf{u} + \nabla p_F = \mathbf{f}, & \Omega_F, \\ \nabla \cdot \mathbf{u} = g, & \Omega, \\ \mathbf{u}_F \cdot \mathbf{n} = \mathbf{u}_P \cdot \mathbf{n}, & \Gamma, \\ p_F - 2\mu(\nabla \mathbf{u}_F \cdot \mathbf{n}) \cdot \mathbf{n} = p_P, & \Gamma, \\ \mathbf{u}_F \cdot \mathbf{t} = -2\beta\mu(\nabla \mathbf{u}_F \cdot \mathbf{n}) \cdot \mathbf{t}, & \Gamma, \\ \mathbf{u} \cdot \mathbf{n} = 0, & \partial\Omega. \end{array} \right.$$



$$\left\{ \begin{array}{ll} \mathbf{u}_i = -\kappa_i \nabla p_i, & \Omega_i, \quad i = 1, 2 \\ \nabla \cdot \mathbf{u}_i = f_i, & \Omega_i, \quad i = 1, 2 \\ \mathbf{u}_f = -\kappa_{f,\tau} d \nabla_\tau p_f, & \gamma, \\ \nabla_\tau \cdot \mathbf{u}_f = f_f + (\mathbf{u}_1 \cdot \mathbf{n}_1 + \mathbf{u}_2 \cdot \mathbf{n}_2)|_\gamma, & \gamma, \\ -\xi \mathbf{u}_1 \cdot \mathbf{n}_1 + \alpha_f p_1 = \alpha_f p_f - (1 - \xi) \mathbf{u}_2 \cdot \mathbf{n}_2, & \gamma, \\ -\xi \mathbf{u}_2 \cdot \mathbf{n}_2 + \alpha_f p_2 = \alpha_f p_f - (1 - \xi) \mathbf{u}_1 \cdot \mathbf{n}_1, & \gamma, \end{array} \right.$$

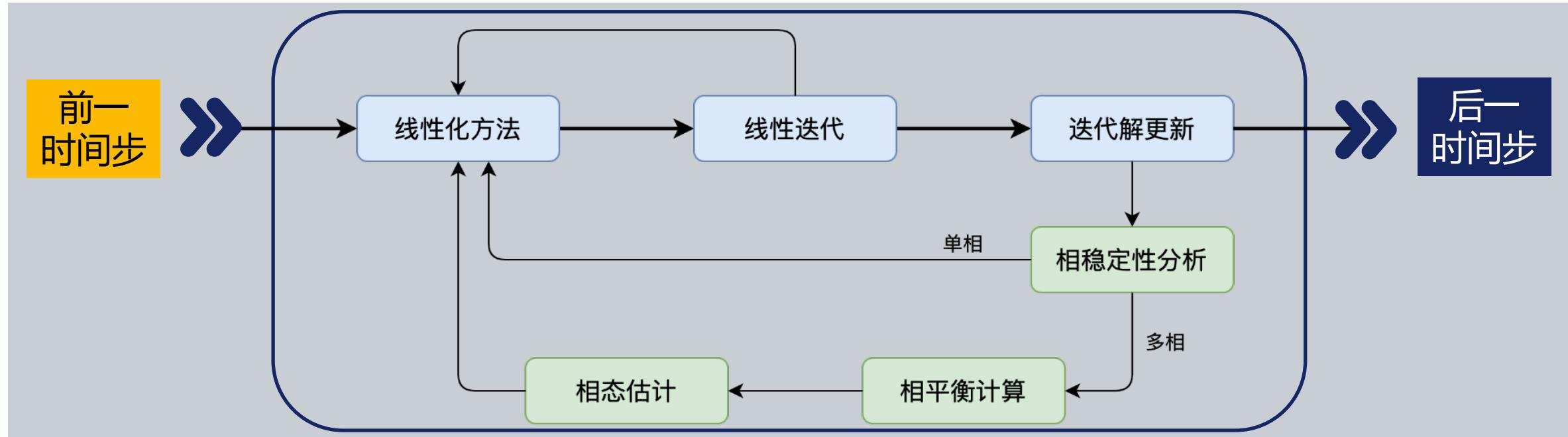


多相多组分渗流求解方法





单时间步算法流程图

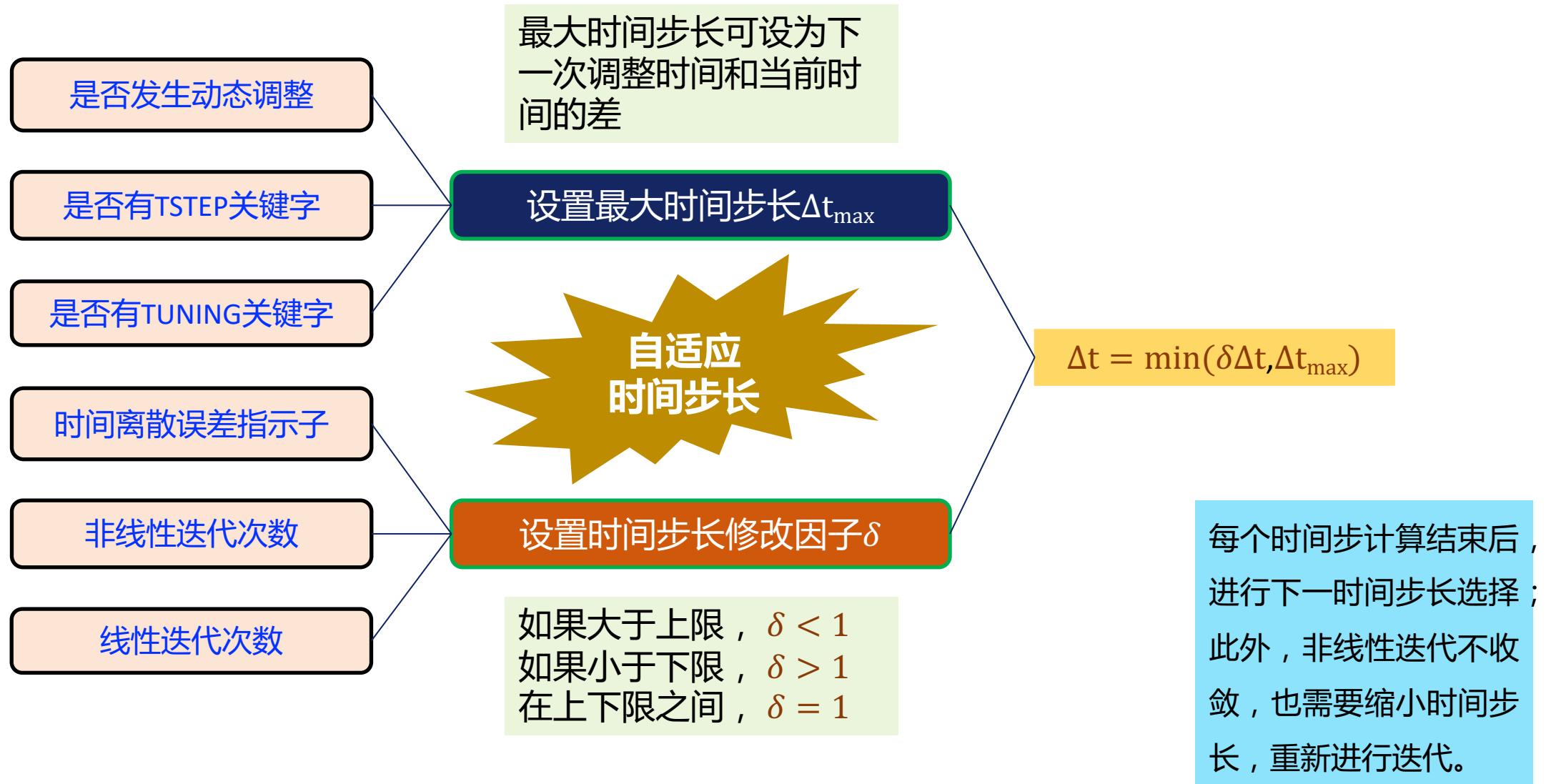


求解非线性方程组，使得耦合的方程组成立，该过程对时间步长和初值非常敏感：

- 计算主变量（非线性方程组）
- 检查混合物相态（单相？两相？多相？稳定？）
- 对多相情况进行闪蒸计算（非线性代数方程）
- 更新变量，自动选择时间步长（根据后验误差、非线性迭代次数、线性迭代次数、……）



时间步长自适应选择方法





离散主变量的选择方法



$$\frac{\partial}{\partial t} N_i + \nabla \cdot F_i - R_i - Q_i = 0, \quad i = 1, \dots, n_c$$

物质守恒方程微分形式

$$\int_{\Omega} \frac{\partial}{\partial t} N_i dV + \int_{\Omega} \nabla \cdot \mathbf{F}_i dV - \int_{\Omega} R_i dV - \int_{\Omega} Q_i dV = 0$$

物质守恒方程积分形式

$$N_i = \phi \sum_{j=1}^{n_p} x_{ij} \xi_j S_j \quad \text{Overall Molar Density}$$

$$F_i = \sum_{j=1}^{n_p} \left[x_{ij} \xi_j \mathbf{u}_j - S_j D_j \nabla (\xi_j x_{ij}) \right] \quad \mathbf{u}_j = -\frac{k k_{rj}}{\mu_j} (\nabla P + \nabla P_{cj} - \gamma_j \nabla z) \quad \text{Pressure}$$

$$R_i = \sum_{j=1}^{n_p} S_j r_{ij}$$

$n_c + 1$ 个主求解变量 \longleftrightarrow $n_c + 1$ 个主方程

$$Q_i = q_i$$

物质守恒 + 流体充满孔隙



有限体积法空间离散

$$\int_{V_k} \frac{\partial}{\partial t} N_i dV + \int_{V_k} \nabla \cdot \mathbf{F}_i dV - \int_{V_k} R_i dV - \int_{V_k} Q_i dV = 0 \quad \text{单元积分形式}$$

↓
Green公式 (散度形式)

$$\frac{\partial}{\partial t} \int_{V_k} N_i dV + \int_{\bar{S}_k} \mathbf{F}_i \cdot \mathbf{n} dS - \int_{V_k} R_i dV - \int_{V_k} Q_i dV = 0 \quad \text{单元守恒形式}$$

↓
按体积元离散

传导率系数 (调和平均)

$$\frac{\partial}{\partial t} N_{i,k} + \sum_{s \in \bar{S}_k} F_{i,s} - R_{i,k} - Q_{i,k} = 0$$

$$T_{c,s} = \frac{2}{\frac{1}{T_{c,k_1}} + \frac{1}{T_{c,k_2}}}.$$

$$F_{i,s} = \left(\frac{Ak}{d} \right)_s \sum_j^{n_p} \left(x_{ij} \xi_j \frac{k_{rj}}{\mu_j} \right)_s \Delta_s (P + P_{cj} - \gamma_j Z)$$

流动性、密度 (上游权)

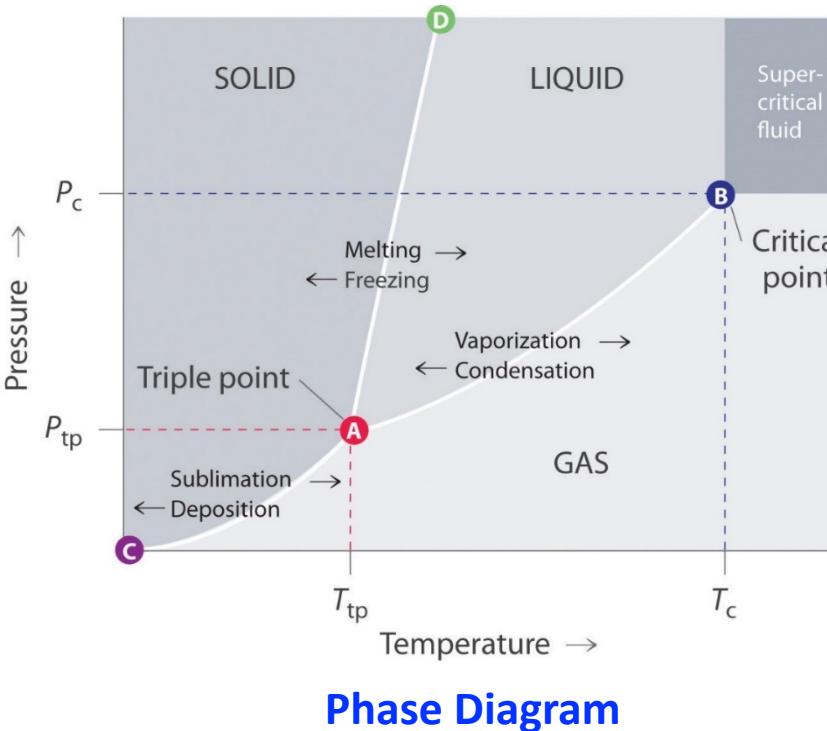
$$= T_{c,s} \sum_j^{n_p} \lambda_{j,s} (x_{ij} \xi_j)_s \Delta_s (P + P_{cj} - \gamma_j Z)$$

$$\lambda_{j,s} = \lambda_{j,up},$$

$$\{x_{ij} \xi_j\}_s = \{x_{ij} \xi_j\}_{up}.$$

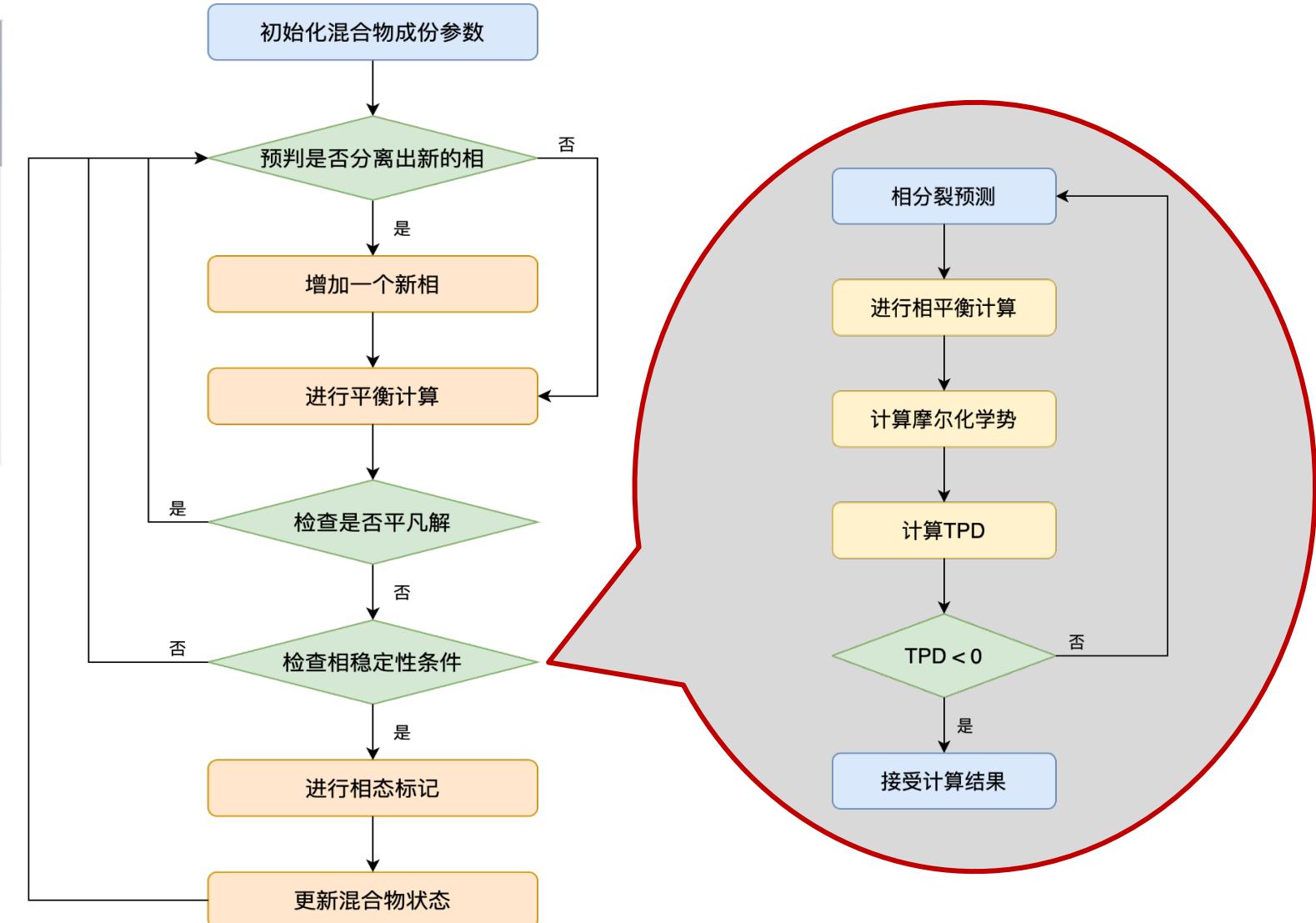


基于RR方程的相平衡计算



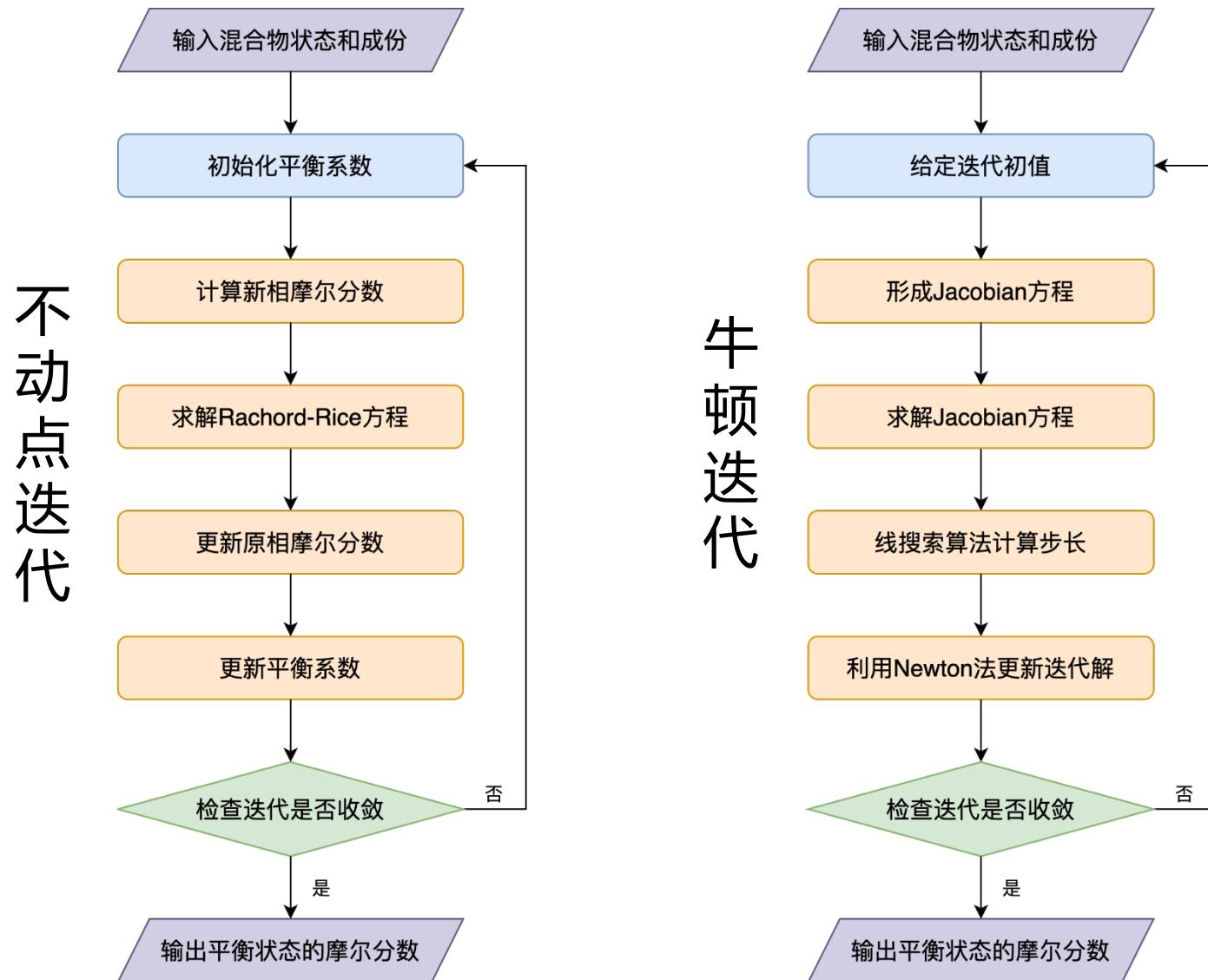
参考文献 : General Chemistry --
Principles, Patterns, and
Applications

http://saylordotorg.github.io/text_general-chemistry-principles-patterns-and-applications-v1.0/index.html





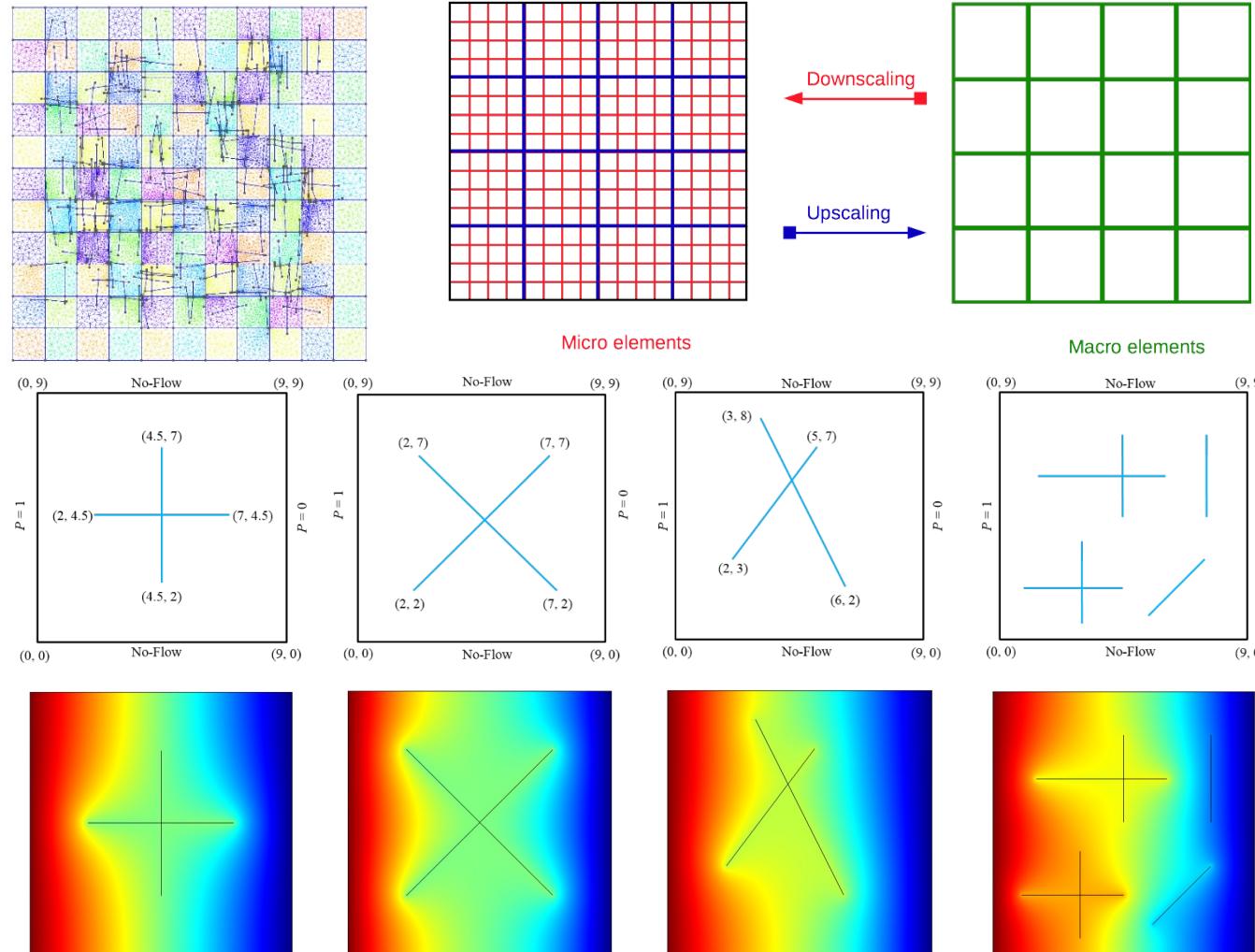
相平衡计算非线性方程求解



可将两种迭代法（不动点迭代与牛顿迭代）结合起来：首先使用SSM方法，收敛到一定程度之后，切换到Newton法，增强迭代法的稳健性



离散裂缝模型的MHDFM方法



合作者 : P. Devloo (Univ of Campinas), 滕文超

- Downscaling: The fine-scale behavior of solution is captured by solving local flow equations at the interior of the macro elements
- Upscaling: The fine-scale properties are transferred to a small global problem associated with the fluxes

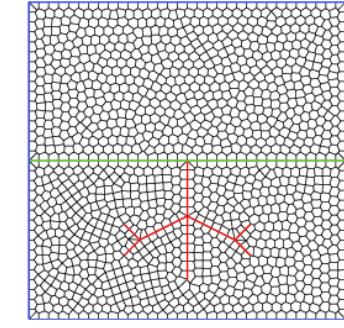
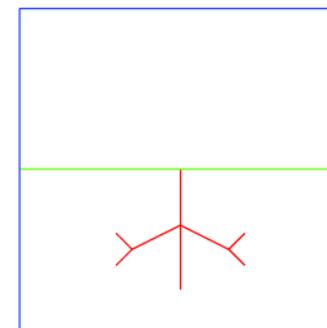
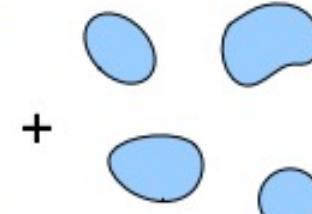
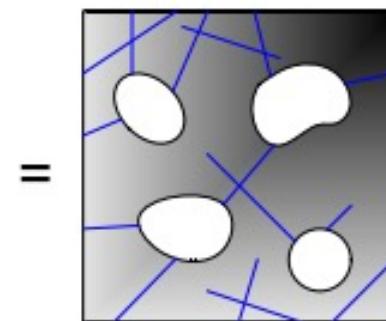
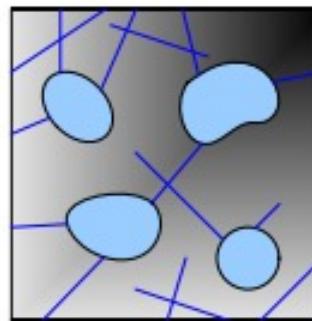
Case	DFM	MHDFM	Diff
1	1.2876	1.2843	2.56e-3
2	1.6122	1.6081	2.54e-3
3	1.2724	1.2661	4.95e-3
4	1.4070	1.3940	9.24e-3



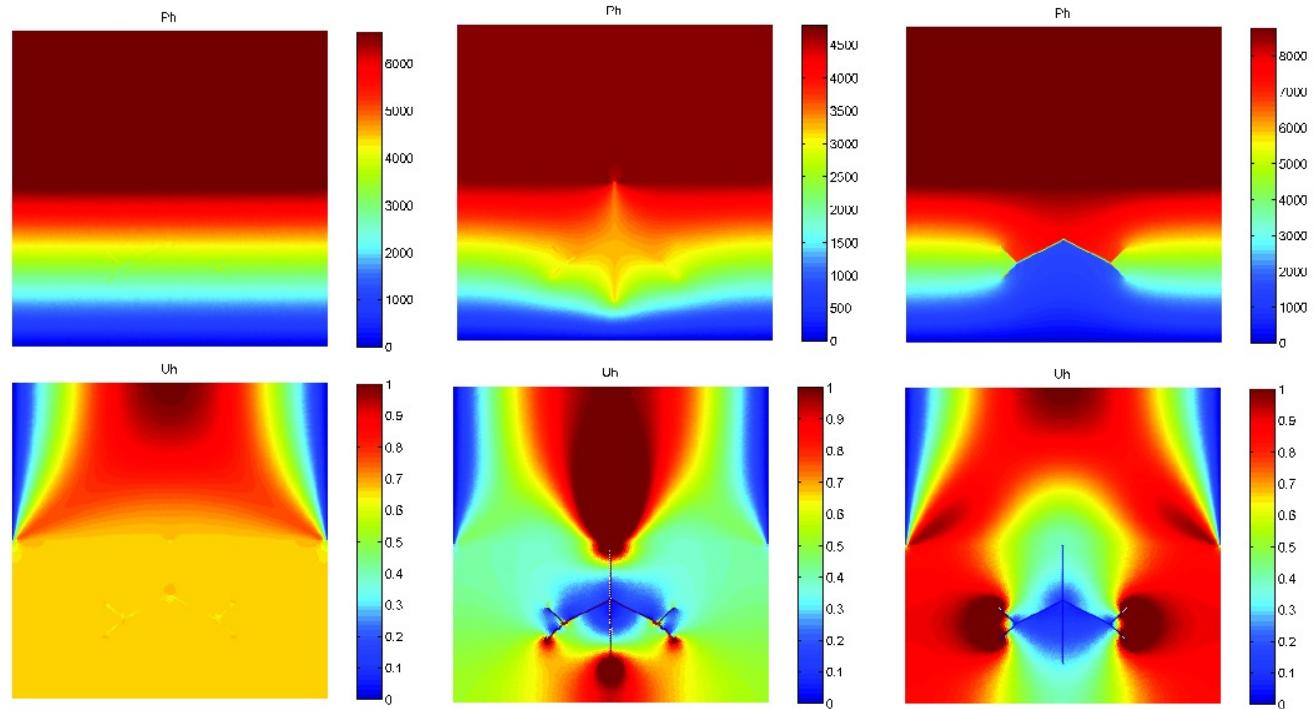
Darcy-Darcy-Stokes模型的DG方法



多孔介质+裂
缝介质+溶洞



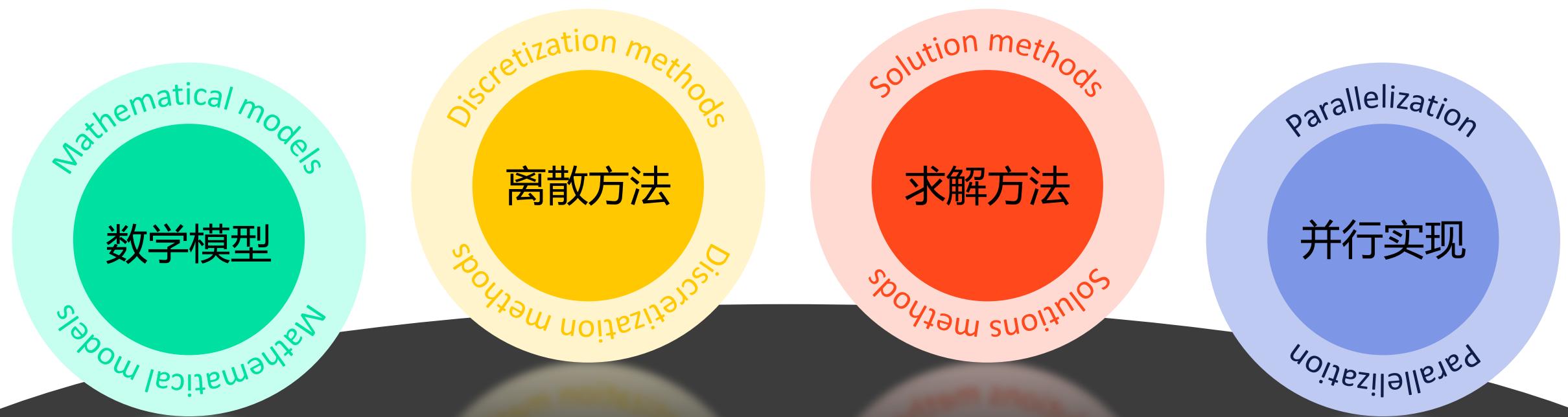
$$\left\{ \begin{array}{ll} -\nabla \cdot (\mu(\nabla \mathbf{u}_F + \nabla^T \mathbf{u}_F) - p_F \mathbf{I}) = \mathbf{f} & \text{in } \Omega_F, \\ \nabla \cdot \mathbf{u}_F = 0 & \text{in } \Omega_F, \\ -\nabla \cdot (\kappa \nabla p_P) = f_P & \text{in } \Omega_P, \\ -\nabla_\tau \cdot (\kappa_{f,\tau} d \nabla_\tau p_f) = f_f + [-\kappa \nabla p_P] \cdot \mathbf{n}_f & \text{in } \gamma, \\ \mathbf{u}_F \cdot \mathbf{n} = \mathbf{u}_P \cdot \mathbf{n} & \text{on } \Gamma, \\ p_F - \mathbf{n} \cdot (\mu(\nabla \mathbf{u}_F + \nabla^T \mathbf{u}_F) \cdot \mathbf{n}) = p_P & \text{on } \Gamma, \\ -\mathbf{t} \cdot (\beta \mu(\nabla \mathbf{u}_F + \nabla^T \mathbf{u}_F) \cdot \mathbf{n}) = \mathbf{t} \cdot \mathbf{u}_F & \text{on } \Gamma, \\ \mathbf{u}_f \cdot \tau_f = \mathbf{u}_F \cdot \mathbf{n} & \text{on } \partial \gamma \in \Gamma, \\ -2\{\kappa \nabla p_P\} \cdot \mathbf{n}_f = \alpha_f [p_P] & \text{on } \gamma, \\ -[\kappa \nabla p_P] \cdot \mathbf{n}_f = \frac{2\alpha_f}{2\xi-1} (\{p_P\} - p_f) & \text{on } \gamma. \end{array} \right.$$



合作者：李瑞、高娅莉、陈掌星

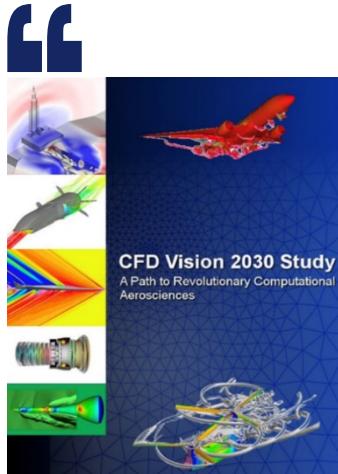


多相多组分渗流求解方法

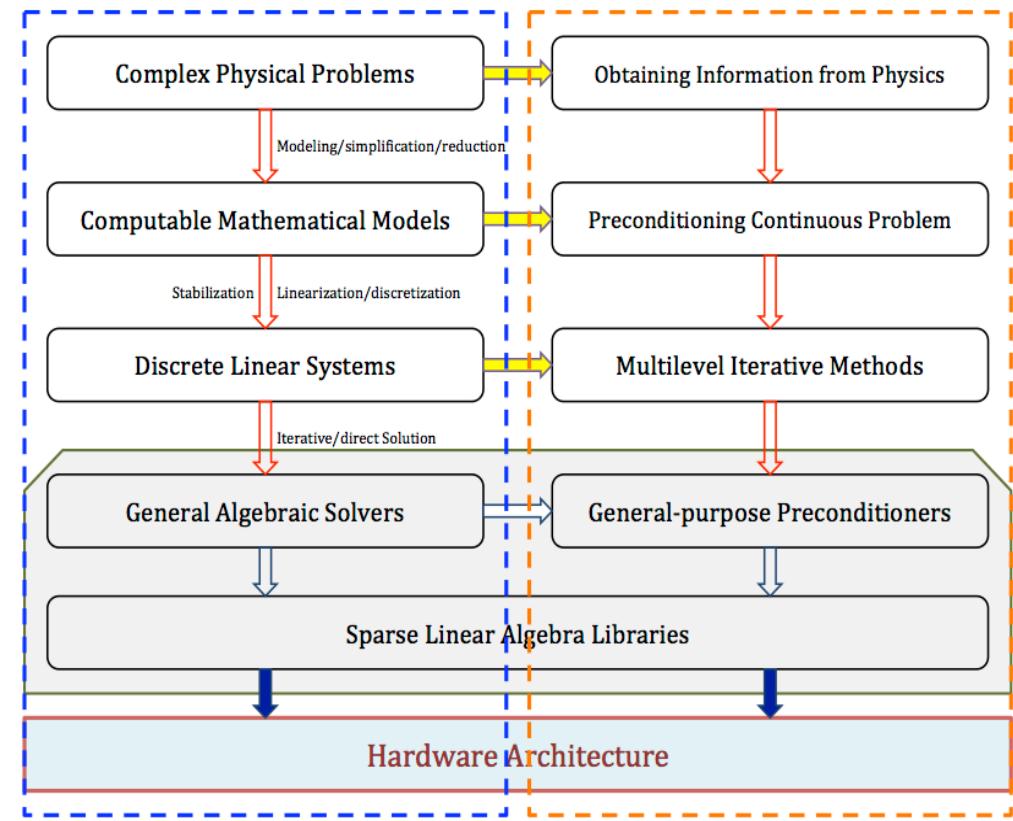
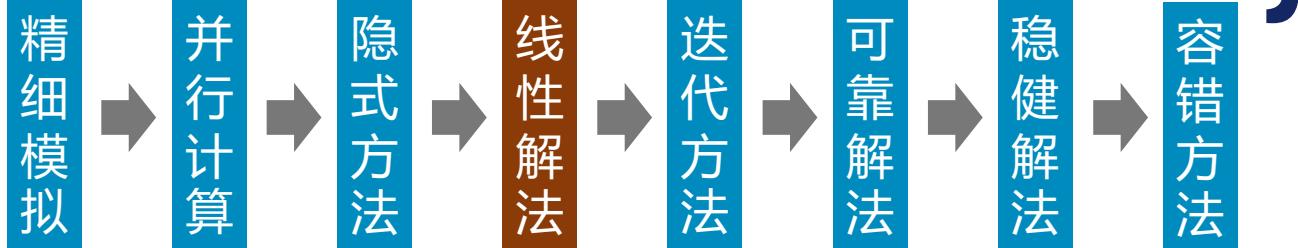




大规模数值模拟中的线性解法器



- 大规模高精度的模拟需要变革性的算法支撑
- 大规模网格并行生成和自适应仍是主要技术瓶颈
- 分析和优化过程需要稳健的自动化的求解器技术
- 精细模拟带来大量的数据需要存储、处理和传输
- HPC硬件发展迅速，其发展趋势难以预测



- 快速线性解法器同时是大规模计算中的主要瓶颈，形成**高效、通用、可扩展**的线性解法器软件是一个难题
- 快速线性解法器是大规模数值模拟的重要组件，在一些应用问题的数值模拟中占用了80%以上的时间
- 对超算硬件的性能排名（如HPC TOP500）常采用线性解法器作为Benchmark（如HPL、HPCG等）



线性解法器最优算法的重要性

- 对超算硬件的性能排名（如HPC TOP500）就常采用线性解法器的性能作为标准（如HPL、HPCG等）
- 线性解法器是大规模数值模拟的重要部分，在很多全隐式油藏数值模拟问题中占用了80%以上的时间
- 同时，线性解法器也是并行计算中的主要瓶颈，形成高效、通用、可扩展的线性解法器软件是一个公认的难题

问题规模	网格剖分	64x64x64			128x128x128	256x256x256	512x512x512
	变量个数	274,625			2,146,689	16,974,593	135,005,697
稀疏直接法软件 Intel MKL Pardiso 北京超级云超算	计算核数	8x1	16x1	32x1	16x8	16x64	16x512
	求解时间	5.38s	3.86s	3.26s	59.78s	999.46s	内存不足
几何多重网格法 FASP解法器软件 个人笔记本电脑	计算核数	1x1			1x1	1x1	1x1
	求解时间	0.030s			0.303s	2.815s	23.54s

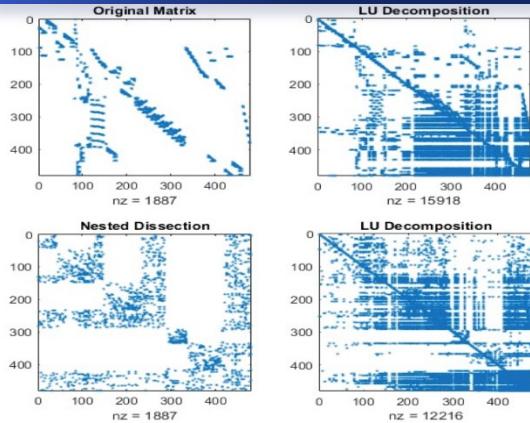
三维Poisson方程（均匀网格七点差分格式）的线性解法器对比，稀疏直接法Pardiso（北京超级云超算）和几何多重网格法FASP（笔记本电脑）：线程数×进程数。2020年，北京超级云计算中心A分区以Linpack测试性能3.74PFlops，获中国HPC TOP100榜单第三名及通用CPU算力第一名。单节点配两块AMD EPYC7452共64核心256GB内存。



科学/工程计算中的预条件方法



基于代数的方法

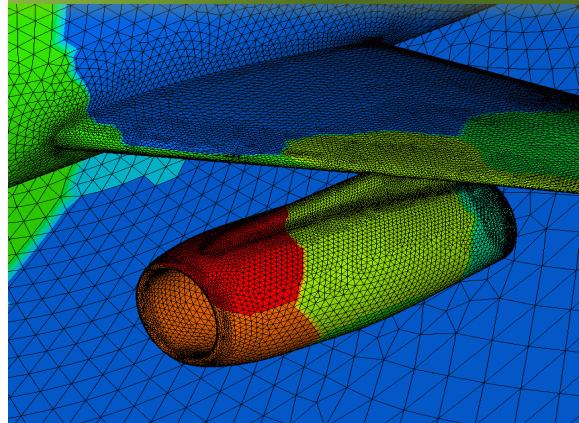


01.

LU, ILU, SAI, ...

纯代数，通用性强，稳健性高，用户友好；效率一般不高，并行可扩展性较差。

基于区域分解的方法

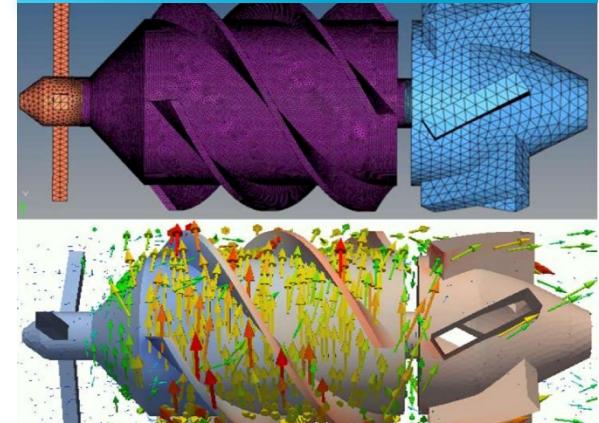


02.

DDM, RAS, FETI-DP, ...

可以基于网格进行，效率高，通用性较强，可扩展性较强；难以兼顾通用性与最优化。

基于物理的方法



03.

Block Preconditioners

算法灵活，基于成熟算法开发，效率高，可扩展性强；通用性弱，用户友好度差。



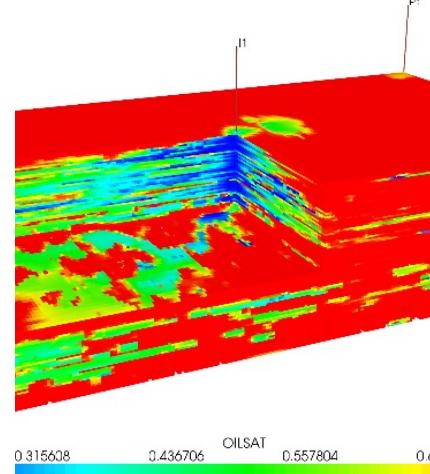
求解全隐式离散方程中的困难



- 全隐式模拟中，线性方程组求解时间常常超过80%！
- 全隐式模拟方法稳健、可用较大的时间步长，但会给线性代数方程求解带来很多困难

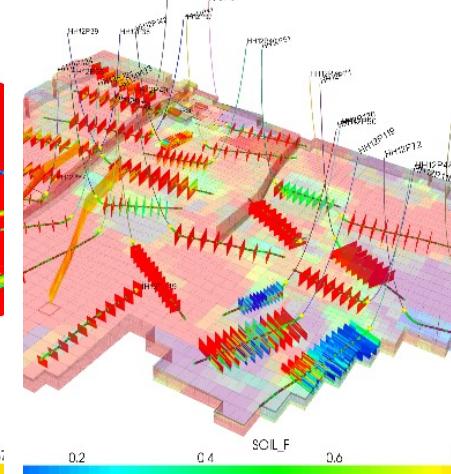
性质不同的耦合方程

$$\begin{aligned}\frac{\partial}{\partial t} \left(\phi \sum_{j=1}^{n_p} x_{ij} \xi_j S_j \right) + \nabla \cdot \mathbf{F}_i - \sum_{j=1}^{n_p} S_j r_{ij} &= Q_i, \\ \mathbf{F}_i &= \sum_{j=1}^{n_p} \left(x_{ij} \xi_j \mathbf{u}_j - S_j \mathbf{D}_j \nabla (\xi_j x_{ij}) \right), \\ \mathbf{u}_j &= -\frac{\kappa \mathbf{K}_{rj}}{\mu_j} (\nabla P_j - \gamma_j \nabla z), \\ f_{ij} &= f_{i1}, \quad i = 1 : n_c \\ \sum_{j=1}^{n_p} S_j &= 1, \\ \sum_{i=1}^{n_c} x_{ij} &= 1, \\ P_1 - P_j &= P_{c1j},\end{aligned}$$

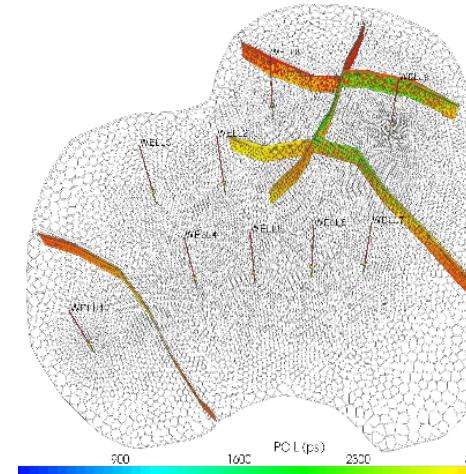


系数的强非均质性

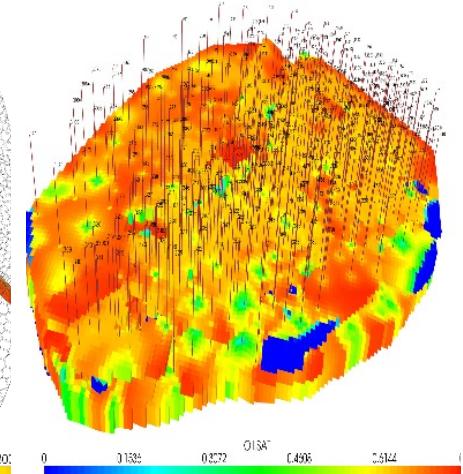
井方程的复杂变化



网格复杂和退化



有效节点数量巨大



设计与预条件方法配合的高效解耦方法，在代数层面处理耦合性

在预条件方法中使用低复杂度代数多重网格法，提升算法稳健性

在预条件方法中使用纯代数方法来处理井方程，提升算法稳健性

采用无结构的矩阵存储格式BSR，用统一的存储结构处理各种情况

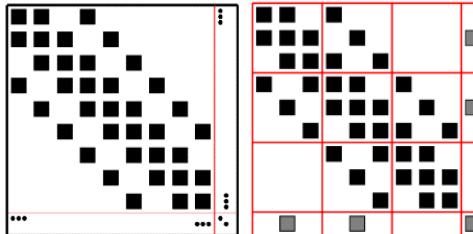
设计最优预条件方法，并结合大规模并行计算技术提高计算效率



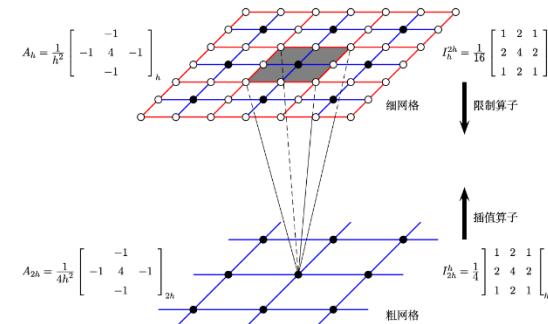
线性解法器：多阶段预条件



- 方便求解多种不同模型
- 提高内存数据访问效率



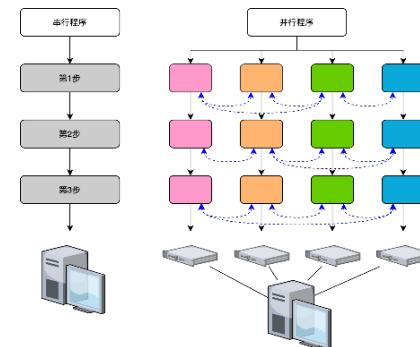
统一矩阵结构



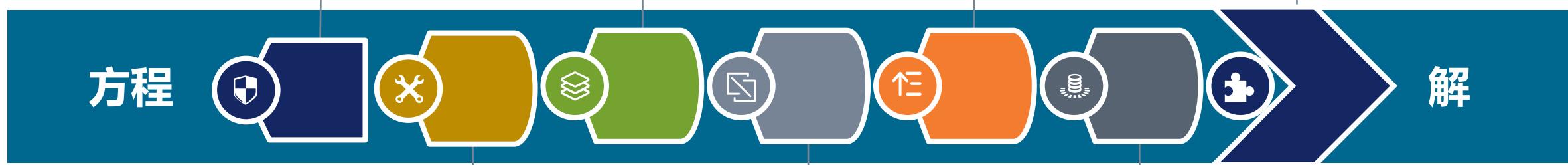
AMG方法



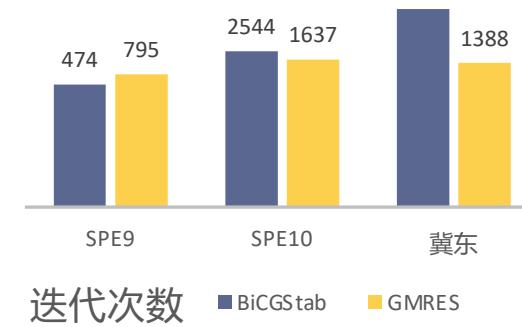
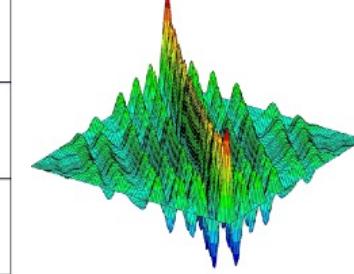
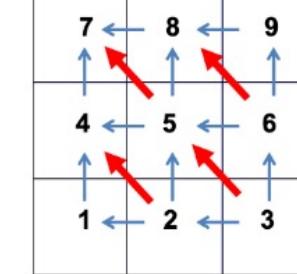
ILU方法



矩阵并行划分

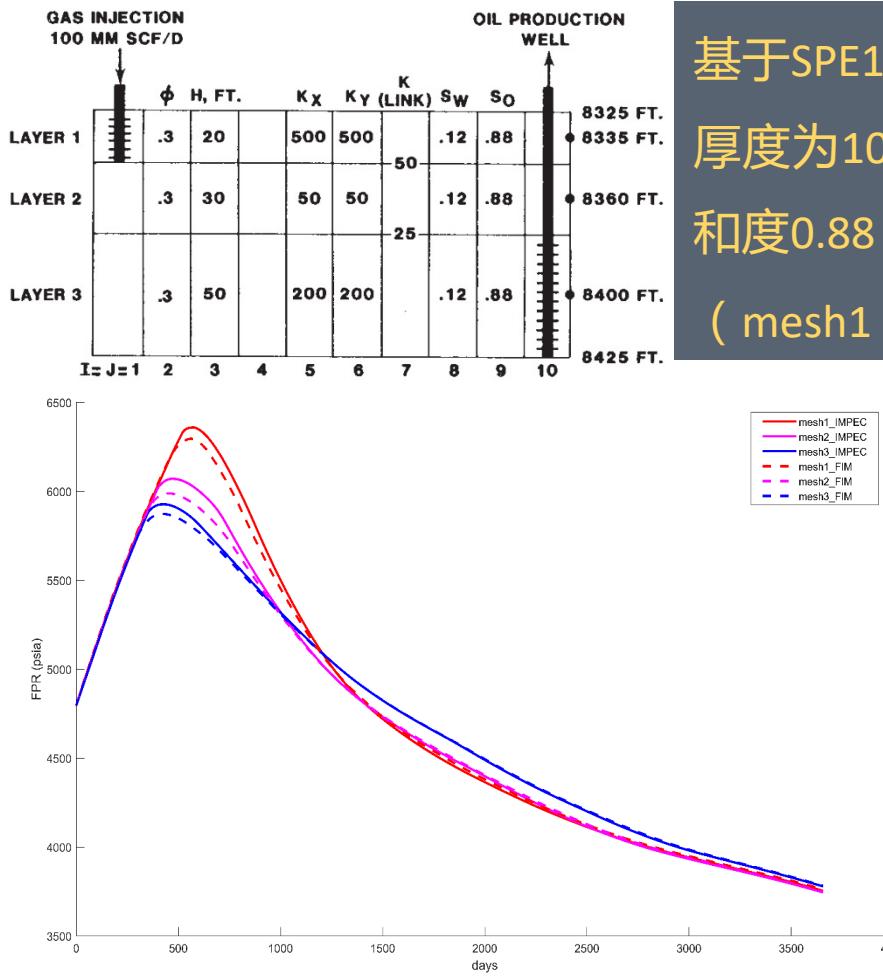


合作者：吴淑红、
王宝华（中石油
勘探院）、许进
超（PSU）等





网格与线性解法器收敛性



基于SPE1A标准算例构造：油田区域的水平方向为边长1000ft的正方形，垂向厚度为100ft。初始状态下，参考深度(8400ft)的油压为4800psia，初始油饱和度0.88，初始水饱和度0.12；平衡状态油水界面为8500ft，油气界面为7000ft
(mesh1 : 20×20×10 , mesh2 : 40×40×20 , mesh3 : 80×80×40)

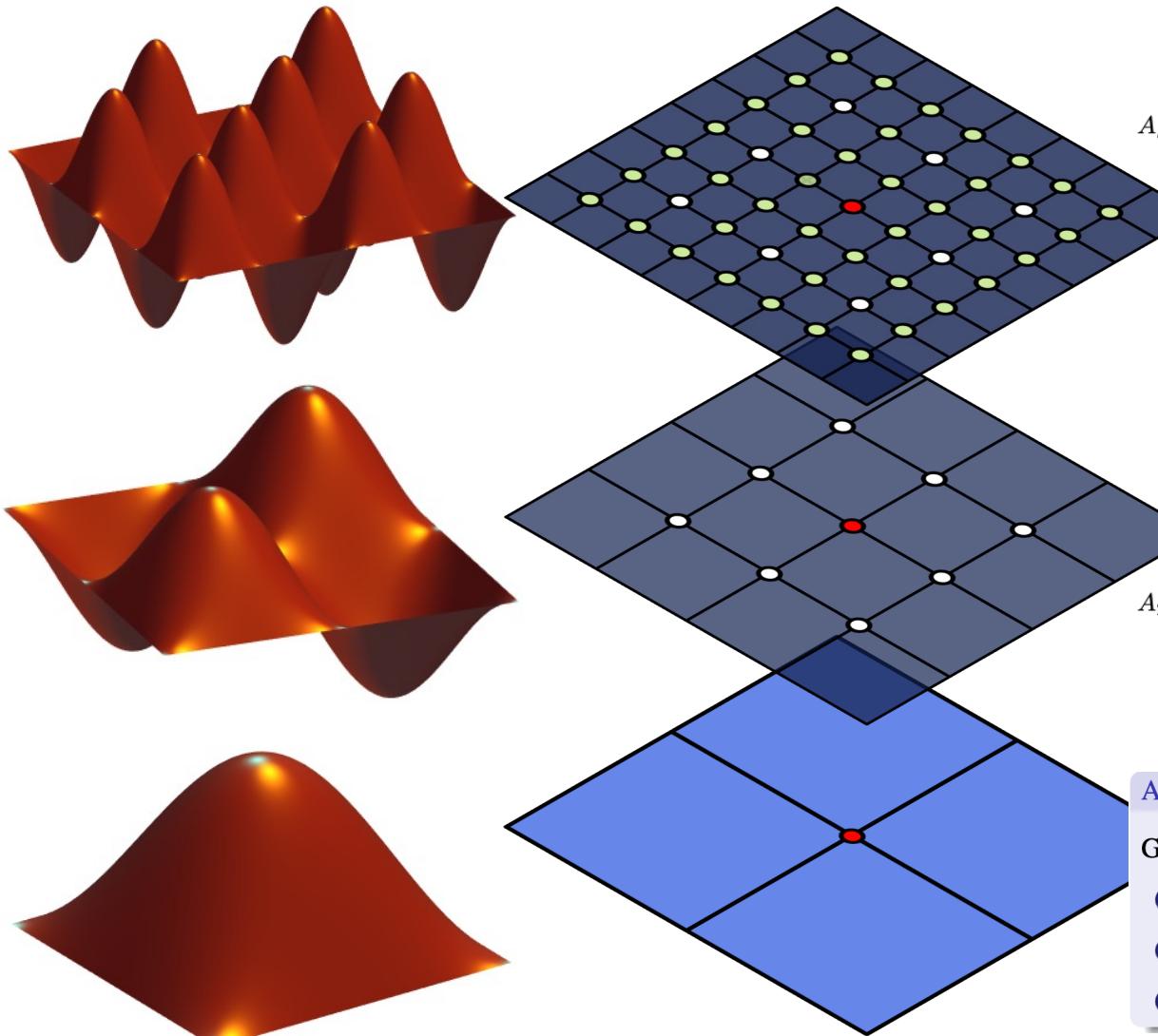
求解器	网格	总时间步数	总线性迭代数	线性求解时间 (秒)	模拟时间 (秒)
BILU(0)	1	145 (356)	16100 (45.2)	18.801 (87%)	21.543
	2	173 (629)	50406 (80.1)	652.123 (94%)	693.709
	3	272 (1227)	141763 (115.5)	14799.249 (96%)	15360.906
MSP	1	143 (337)	1781 (5.3)	9.681 (81%)	11.956
	2	167 (547)	3098 (5.7)	141.640 (80%)	178.143
	3	275 (1244)	7239 (5.8)	2788.746 (83%)	3344.826

预条件	网格	无解耦	ANL 解耦	ABF 解耦	SEM 解耦
CPR	1	16781 (609 秒)	2327 (6.232 秒)	2343 (7.846 秒)	2326 (6.229 秒)
	2	×	5466 (144.1 秒)	4807 (121.6 秒)	5666 (137.3 秒)
	3	×	13747 (2722 秒)	13834 (2694 秒)	13642 (2726 秒)
MSP	1	×	×	1781 (9.681 秒)	1404 (7.259 秒)
	2	×	×	3098 (138.0 秒)	2798 (140.0 秒)
	3	×	×	7239 (2789 秒)	7049 (3007 秒)

张晨松，油藏数值模拟中的线性解法器
数值计算与计算机应用, 2022, 43(1): 1-26.

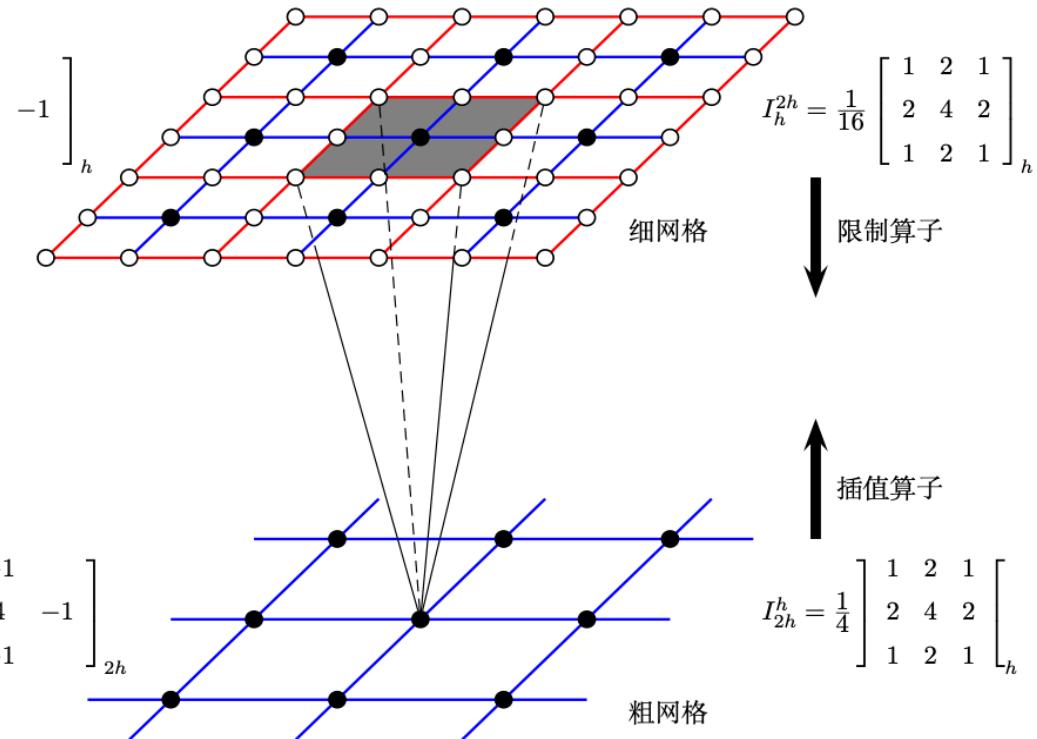


几何多重网格法



$$A_h = \frac{1}{h^2} \begin{bmatrix} -1 & & \\ & 4 & -1 \\ & -1 & \end{bmatrix}_h$$

$$A_{2h} = \frac{1}{4h^2} \begin{bmatrix} -1 & & \\ & 4 & -1 \\ & -1 & \end{bmatrix}_{2h}$$



Algorithm (Twogrid method in operator form)

Given an initial guess $u^{(0)} \in V$.

- ① Pre-smoothing: $u^{(1)} = u^{(0)} + \mathcal{S}(f - \mathcal{A}u^{(0)})$;
- ② Coarse-grid Correction: $u^{(2)} = u^{(1)} + (\mathcal{I}_c \mathcal{B}_c \mathcal{I}_c^T)(f - \mathcal{A}u^{(1)})$;
- ③ Post-smoothing: $u^{(3)} = u^{(2)} + \mathcal{S}^T(f - \mathcal{A}u^{(2)})$.



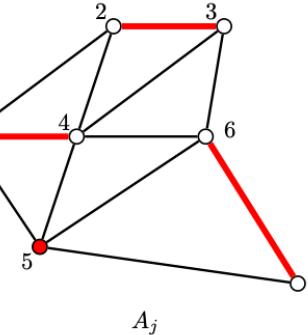
代数多重网格法



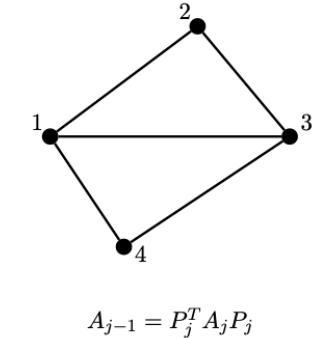
- 代数多重网格法通过系数矩阵构造限制和提升算子，从而得到不同“网格层”之间的信息传递方式和粗网格问题
- 粗网格自由度：C/F分裂、聚集法
- 插值和限制算子：
 - 确定插值局部区域 – 稀疏模式
 - 确定插值权系数 – 获得 P (and R)
- 粗空间解法器：
 - 确定粗水平上的求解问题
 - 多层迭代: V, W, AMLI, K, ...
- 磨光算子：降低误差的光滑部分
 - 简单通用的光滑子
 - 依赖问题的光滑子

聚集法：

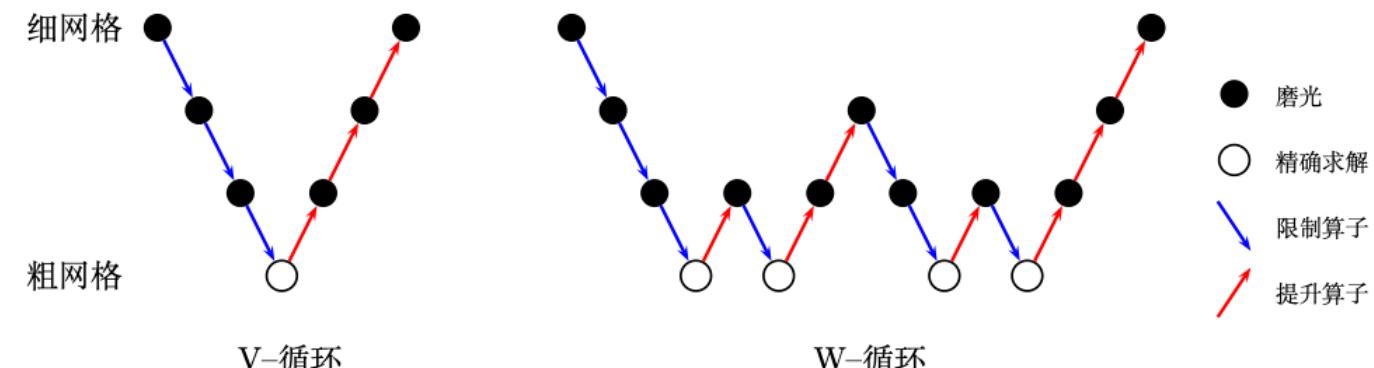
$$P_{ij} = \begin{cases} 1, & \text{if } i \in A_j, \\ 0, & \text{if } i \notin A_j. \end{cases}$$



$$P_j = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

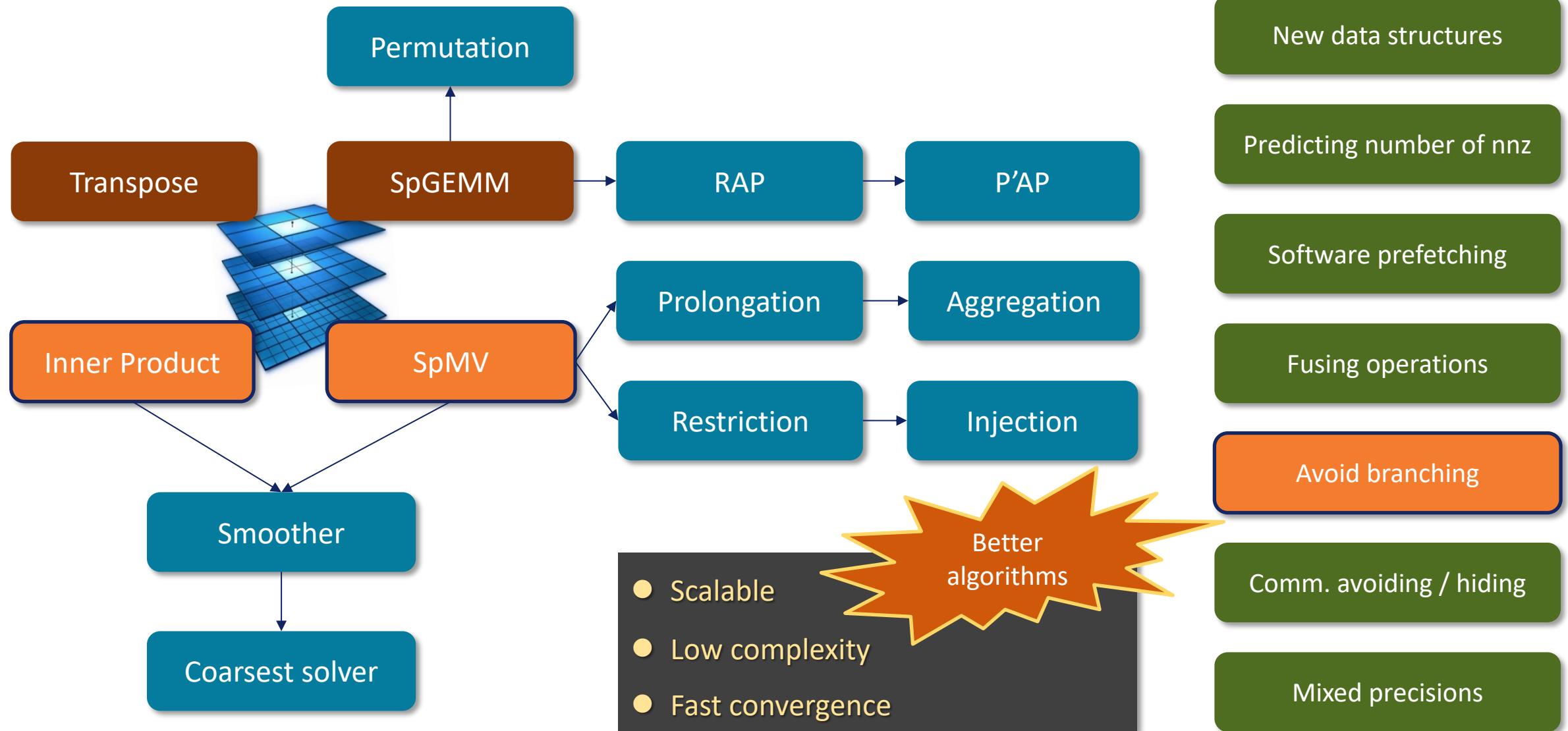


- 非光滑聚集法的插值算子简单，基于聚集法的AMG方法过程更简单，更容易并行！
- 光滑聚集法AMG的插值算子是在非光滑聚集法AMG的插值算子的基础上左乘一个磨光算子



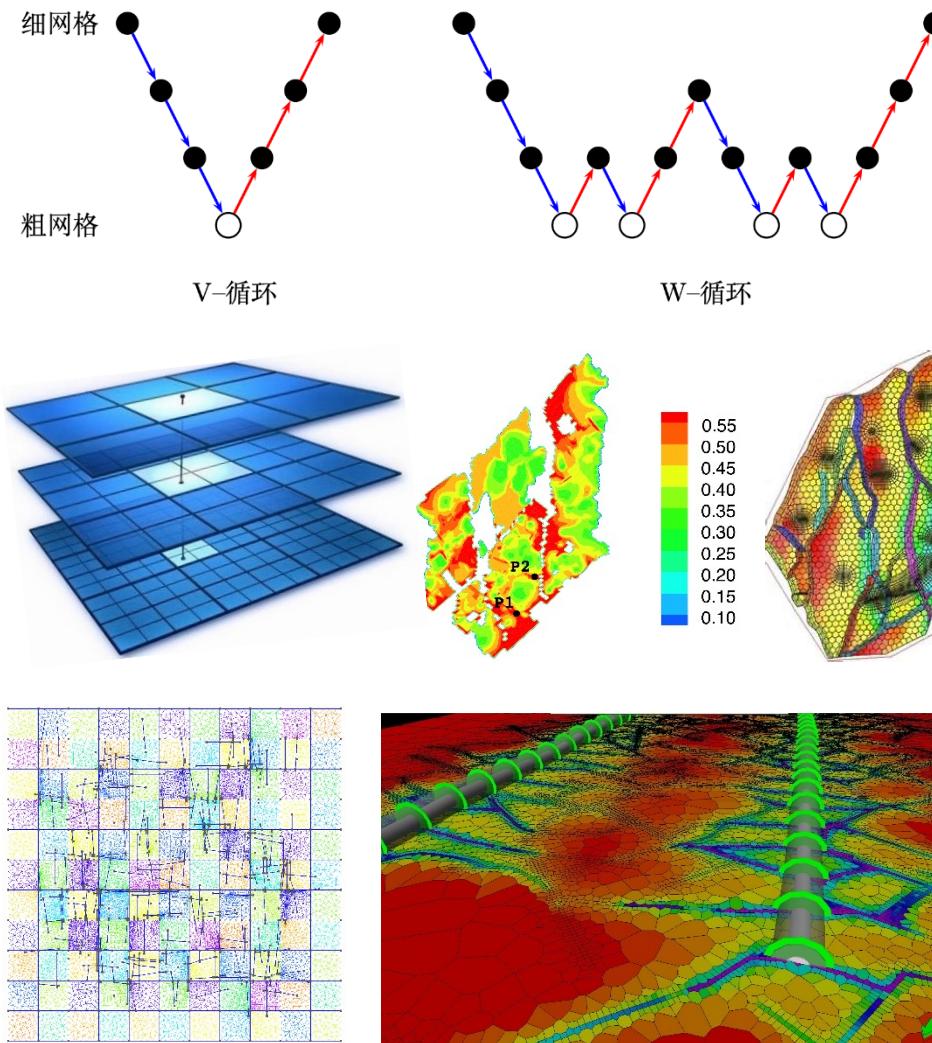


多重网格法中的基本操作





两层网格法的收敛性分析



- 多层迭代法是高效解法，如GMG, HB, BPX, AMG等
- 几何多层迭代法的收敛性分析相对比较成熟
 - J. Xu & L. Zikatanov, *Acta Numerica*, 2017: “*a rigorous multilevel convergence theory for AMG without using geometric information is still very much an open problem ...*”
- 从**最优(Optimal)**插值算子到**理想(Ideal)**插值算子
 - X. Xu & Z., *SINUM*, 2018. Math Review: “*This interesting and clearly written paper establishes new characterizations* (including a sufficient condition, a necessary condition, and an equivalent condition) *of the so-called ideal interpolation operator ...*”
 - 徐雪枫获2018年北京计算数学学会优秀青年论文一等奖
- **非精确两层网格收敛性分析**：给出量化上下界估计
 - Y. Notay, *SINUM*, 2007
 - X. Xu & Z., *SINUM*, accept; *SIMAX* accept



解耦方法与预条件方法



压力	耦合项
耦合项	饱和度等

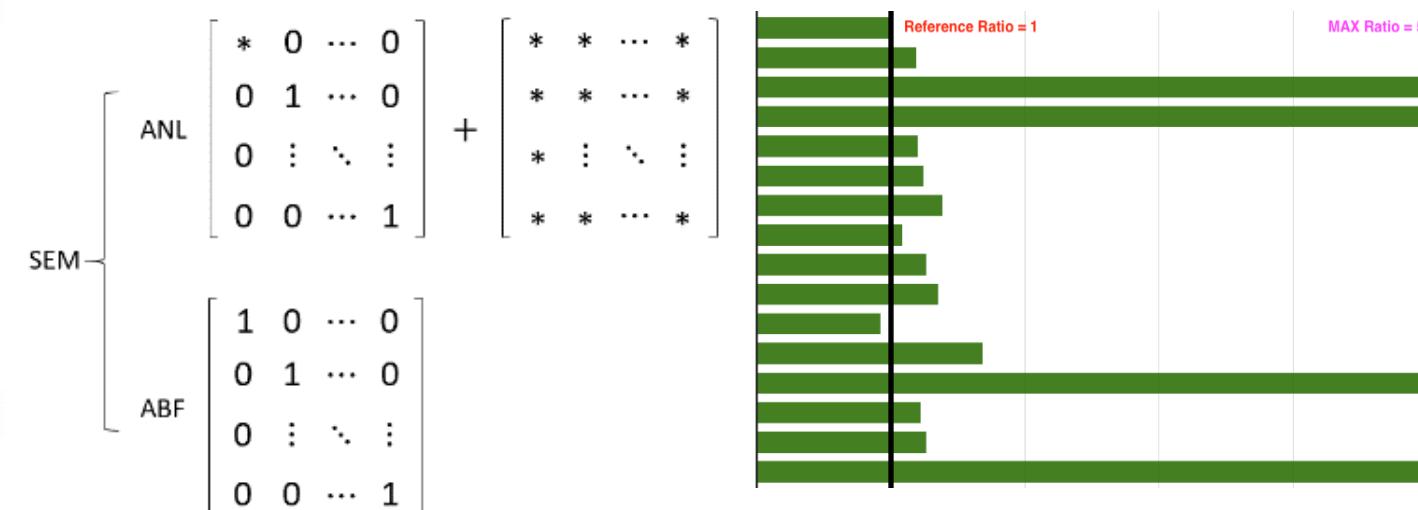
↓ 部分解耦方法

压力	0
耦合项	饱和度等

↓ 完全解耦方法

压力	0
0	饱和度等

$$\begin{array}{c} \text{Accumulation} \\ \text{Term} \\ \left[\begin{array}{cccc} * & * & \cdots & * \\ 0 & 1 & \cdots & 0 \\ 0 & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{array} \right] + \left[\begin{array}{ccccc} 0 & 0 & \cdots & 0 \\ * & * & \cdots & * \\ * & \vdots & \ddots & \vdots \\ * & * & \cdots & * \end{array} \right] \end{array}$$



- 解耦方法简单，复杂度低，本身不需要收敛
- 解耦后的问题，需要适用于整体多阶段预条件方法
- 解耦后的问题，每个子问题都“易于求解”

Qiao, Wu, Xu, Zhang. JCP2017

ABF方法的解耦效果强，但是会使得压力方程更难求解，需要对其进行特殊处理才能获得较高的整体性能

迭代次数

Method	Time Steps	Nonlinear Iterations	Linear Iterations	AMG Iterations	Linear Solver Time (s)
ABF	60	352	2505	37235	7756
Analytical	57	332	2209	16212	3149
Semi-analytical	56	320	1338	13813	2464

79

31

21



油藏模拟解法器代码优化



中国石油大学（华东）油藏工程系：SimFast模拟器的解法器优化

- 继承了石油部引进的黑油模拟器代码，进行二次开发
- 增加前后处理、各种现场应用功能和实用模型等，……，已经花费了近30年时间

中国石油勘探开发研究院：个性化井网设计软件求解性能测试与优化

- 通过斯坦福大学的Industrial Consortium获得油藏模拟器全套代码
- 18万行代码，消化这些代码比较困难，更重要的是：没有人愿意去读
- 一些算例不能算，一些算法不能算；或者跑一段时间死机，或者跑得很慢……

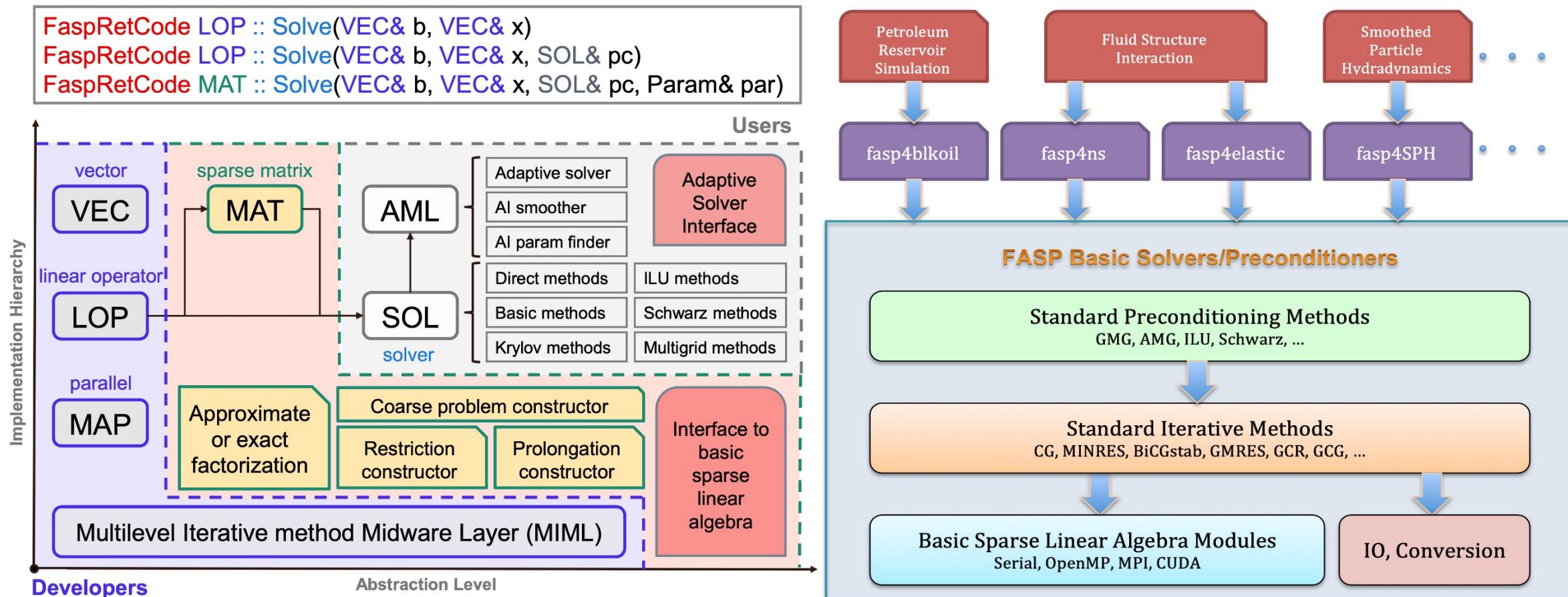


AMG求解时间	算例A			算例B		
	耗时(秒)	调用次数	加速比	耗时(秒)	调用次数	加速比
修改前	1705.188	192	---	2034.765	107	---
修改后	7.815	72	219倍	94.475	37	22倍

预条件方法代码修改（其中一行）前后计算速度对比



FASP线性解法器软件介绍



FASP开源项目网址

<http://www.multigrid.org/fasp>
<https://github.com/FaspDevTeam/faspolver>
<https://github.com/FaspDevTeam/faspXX>



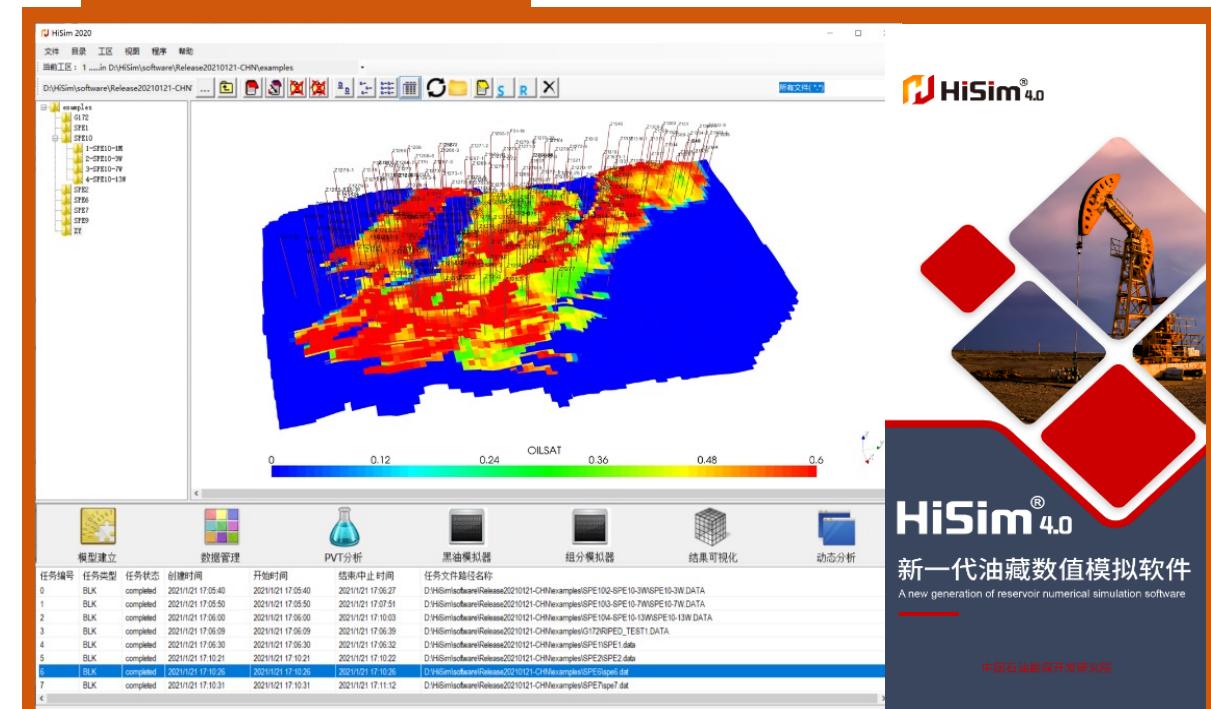
解法器在油藏模拟中的应用



国内外油藏模拟软件

- Monix Energy : Blackoil, Volatile, DPDP (8 tests)
- SOCF, CNOOC : Blackoil, Polymer Flooding (10 tests)
- Simfast, CUP Qingdao : Blackoil (16 tests)
- KarstSim, Sinopec : Carbonate (5 tests)
- Ennosoft : Blackoil, DFN, DPDP (5 tests)
- XXSim, PEClouds : Blackoil, Thermal, Vapor (70 tests)
- PennSim : Compositional (10 tests)
- OpenCAEPoro : Compositional (10 tests)
- HiSim, PetroChina : Blackoil, Compositional (40 tests)

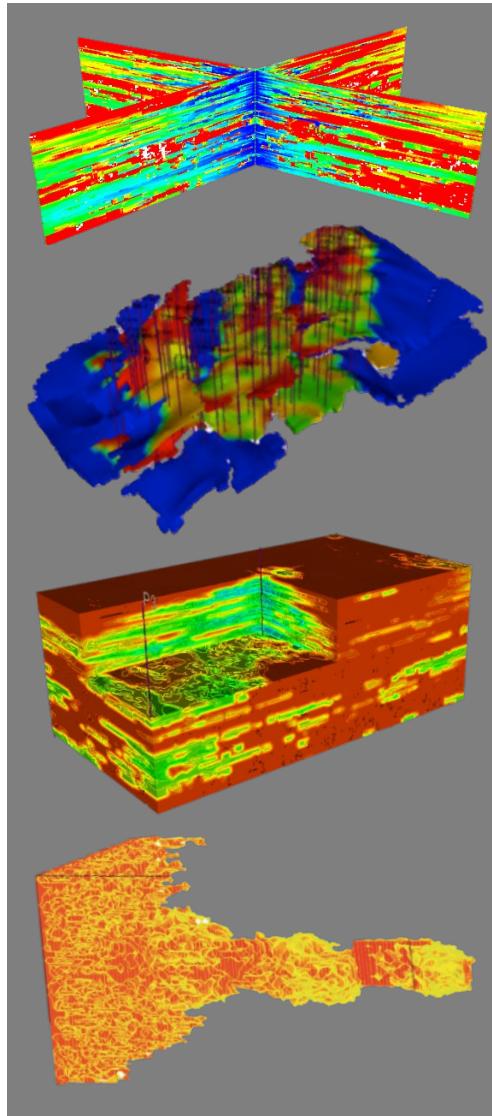
中石油HiSim模拟器



具备地质建模、黑油模拟、组分模拟、裂缝模拟、化学驱模拟等十大功能模块，已在国内外百余个油藏区块中得到应用，节省软件购置费用超3亿元。2017年，国资委刊文《打破国外垄断，中国石油新一代油藏数值模拟软件研制成功》！



一些模拟软件中的测试结果



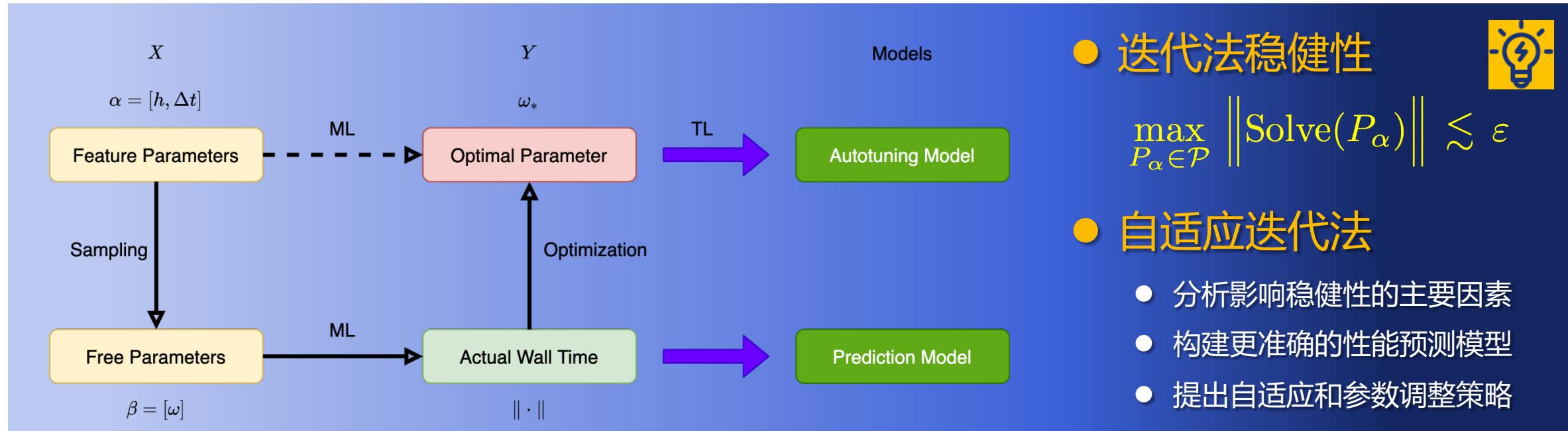
No	Name	Properties				Ecl100		HiSim	
		Model	# Total Cells	# Active Cells	Peroid (day)	Newton	Time (min)	Newton	Time (min)
1	SPE10-2	Two-phase	1122000	1094422	2000	—	—	295	41.82
2	SPE9-9k	Black-oil	9000	9000	900	339	0.12	269	0.20
3	SPE1	CO2 flooding	300	300	3656	536	0.04	445	0.08
4	SPE2	Three-phase coning	150	150	900	209	0.01	538	0.14
5	SPE10-3	Black-oil	1122000	1094422	2000	—	—	1462	354.12
6	SPE6	Dual porosity	100	100	7300	306	0.01	322	0.02
7	DPSP	Dual porosity	60984	40294	360	545	2.64	116	0.81
8	SPE7	Horizontal wells	488	488	1500	120	0.01	75	0.02
9	Volatile	Extended black-oil	2100	2100	0.694	—	—	67	0.03
10	Zaoyuan	Field test (black-oil)	417480	143786	10653	3302	105.49	5204	66.20
11	Jidong	Field test (black-oil)	335664	154598	10587	1091	139.69	161	4.41
12	Chengbei	Field test (black-oil)	1646500	585123	2191	1971	155.57	420	28.47
13	Daqing1	Field test (black-oil)	1453248	466913	15616	—	—	5227	338.00
14	Daqing2	Field test (black-oil)	847895	241474	15096	8562	92.46	3072	88.05
15	SPE10-10M	Two-phase (large-scale)	11220000	10944220	2000	—	—	592	962.12
16	SPE9-9M	Black-oil (large-scale)	9000000	9000000	900	—	—	2460	10932.81

应用单位	模型	有效网格	使用FASP解法器	未使用FASP解法器
北京软能创	页岩气	762万	61小时	245/小时
PEClouds	SPE10	109万	0.8小时	5.5小时
PEClouds	黑油实例	14万	0.28小时	0.78小时

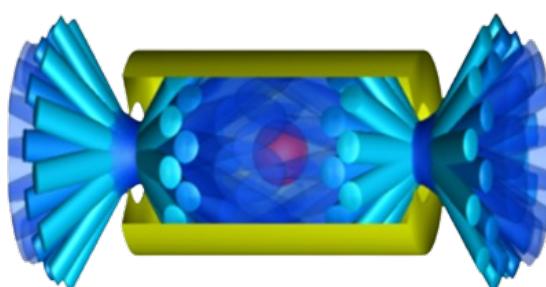
合作者：李想（软能创）、Eamon Zhang（PEClouds）等



自适应线性解法器



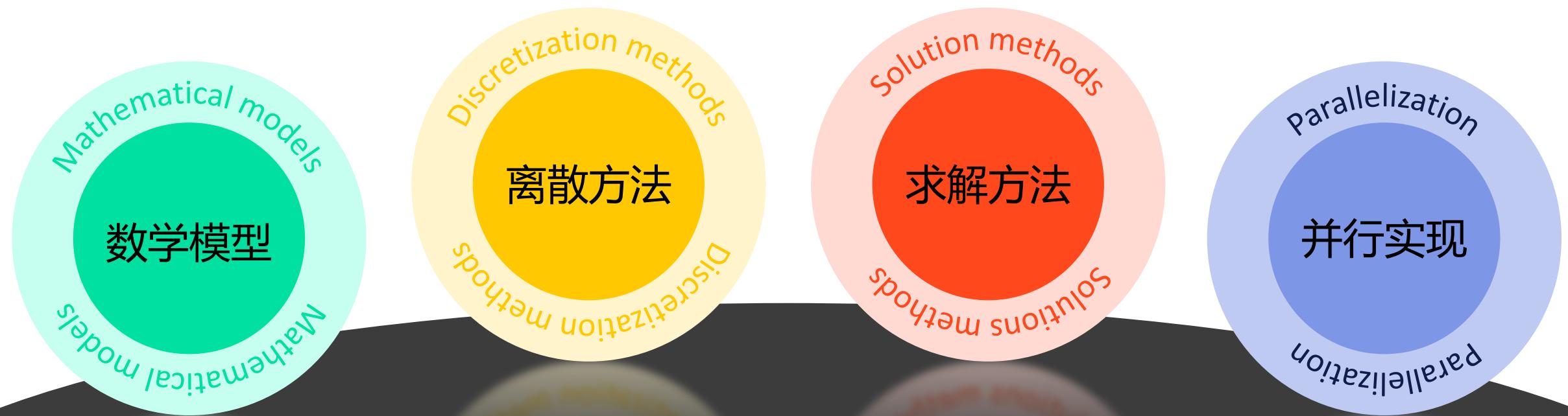
三维ICF算例 (2020年国防科工局科学挑战专题，合作者：邹海峰、徐小文、莫则尧)



自由度个数		平均迭代次数			
Graph	Subgraph	$\theta = 0.25$	$\theta = 0.5$	Optimal	AutoAMG
6.29M	4.91M	51.3	466.6	23.1	27.7



多相多组分渗流求解方法





提高日常工作的效率

百万规模黑油问题，夕发朝至，甚至朝发夕至

——曾经是油藏工程师的梦想

过去需要大规模集群，现在只用笔记本电脑

过去需要几天至几周，现在已在分、秒量级

满足高含水、
高采出程度
的双高油田
的开发需求

使用化学驱
替剂，如聚
合物、表面
活性剂等

多种流体物
质组分之间，
及流体与岩
石间的反应

地层中存在
裂缝、溶洞、
断层、尖灭、
高低渗透带

深层及超深
层储层，需
要考虑地层
骨架变形

储层地质情
况越发复杂，
非均质性强，
不确定性强

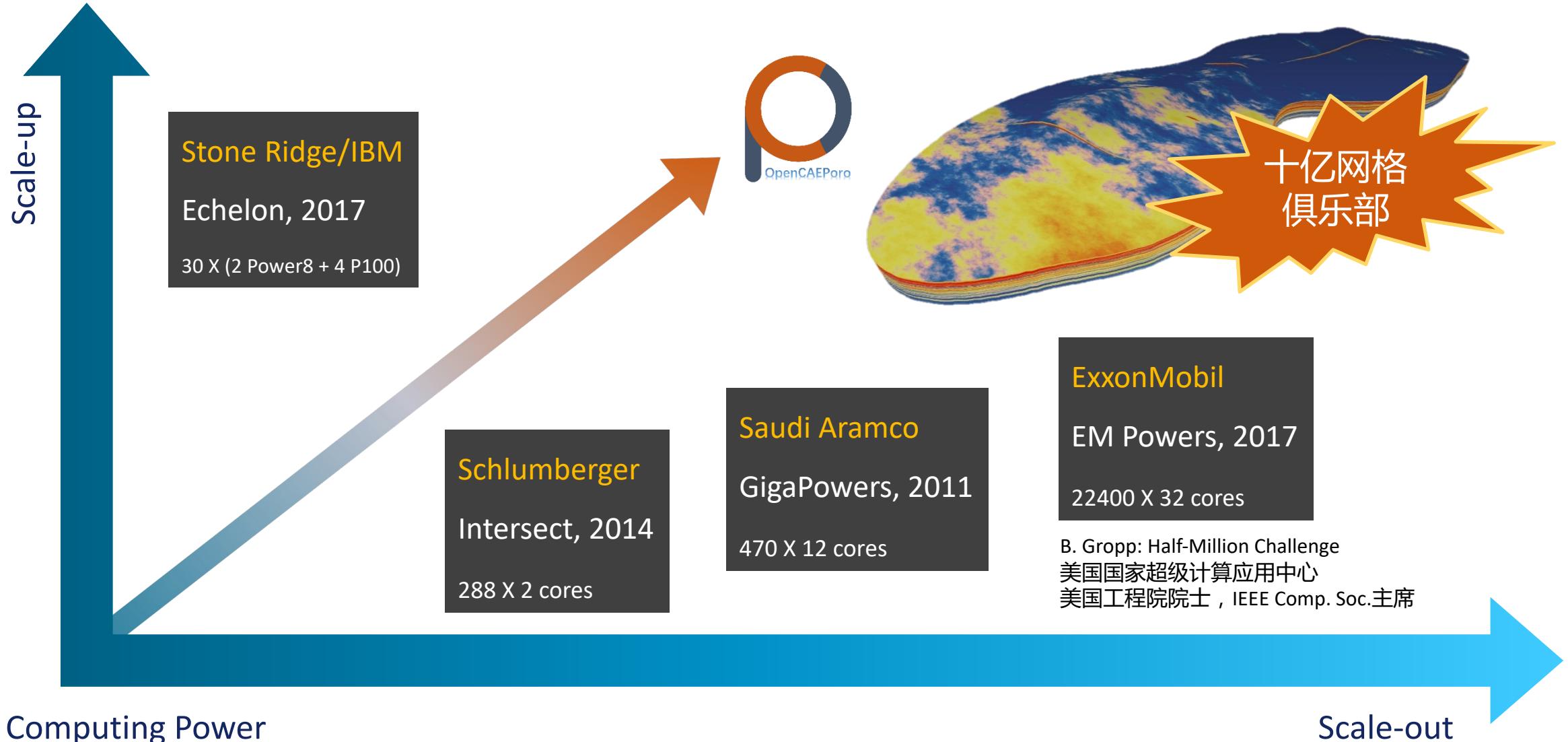
油气开发越
发趋向于强
耦合的复杂
多物理过程



- 数万至数百万量级自由度的问题仍是目前工程中最常用需要求解的规模（中小规模）
- 传统的简化模型和算法已不能满足工程师的需要
- 更精细的模型、更复杂的物理、更快速地求解
- 更复杂的计算硬件环境（CPU、GPU、DCU）

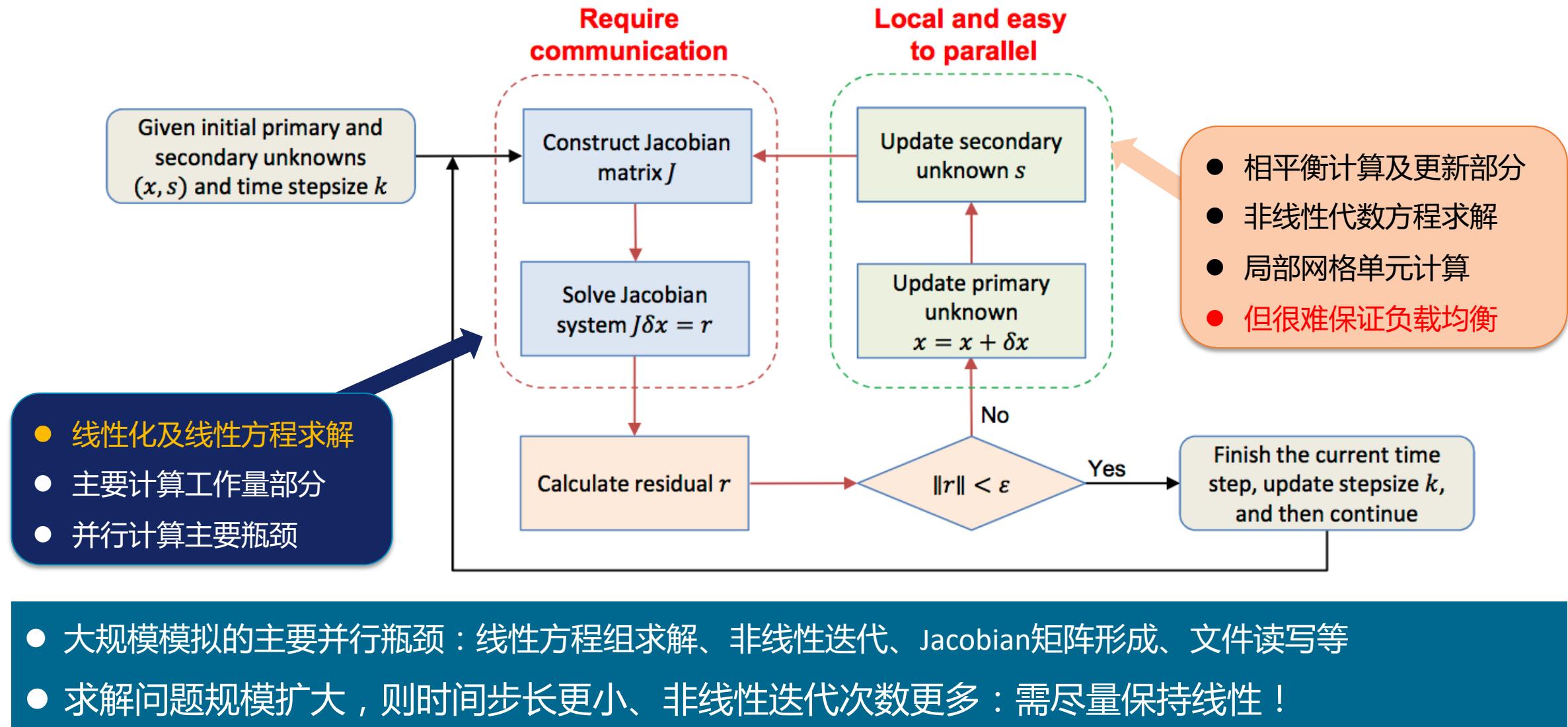


超大规模并行油藏模拟





并行油藏模拟的性能瓶颈





并行计算效率与最优算法



Amdahl's Law 1967

”

如果串行部分占总时间的10%，那并行加速比不可能超过10倍

对于大规模系统来说，很多应用程序的强可扩展性是很难实现的！

Gustafson-Barsis's Law 1988

”

对于很多应用来说，更需要的是计算越来越大规模的问题！需要是弱可扩展性，而不是强可扩展性

当问题规模与计算资源同比例增大 s 倍时，加速比最高就可达 $0.9s+0.1$

Gabriel Wittum: HPC Paradox

”

当购买了大10倍的硬件系统，希望能更快地求解大10倍的问题；但现实很残酷，必须有最优算法才可以！

最优算法对于充分发挥HPC效率及实现弱可扩展性至关重要！

硬件投资



并行效率



最优算法



软件投资



并行效率的衡量方法

● 强可扩展性

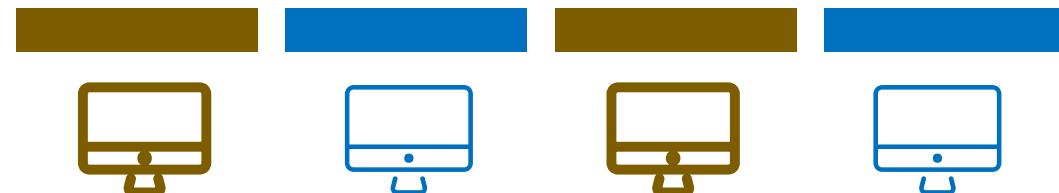


$$\frac{W_1}{kp_1} \quad S = \frac{T_1}{T_p} \approx k?$$

需要解决一个大任务，把计算资源扩大到原来的 k 倍，是否能加速 k 倍？

定义**并行效率** $E = S/k$ ，我们希望是100%！

● 弱可扩展性



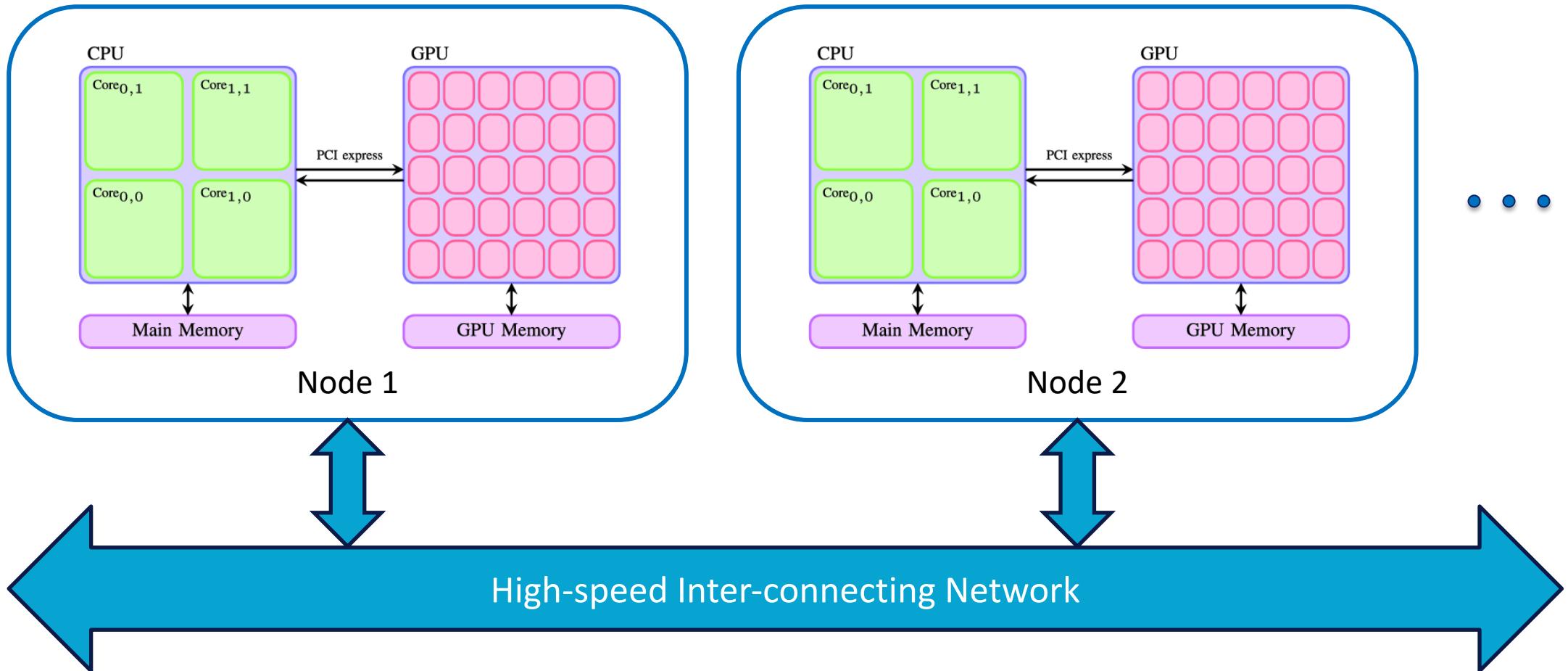
$$\frac{W_k}{kp_1}$$

需要把任务扩大 k 倍，若计算资源同比例增多，是否能保持相同速度？

为了**效率**保持不变，需要多大的问题规模？



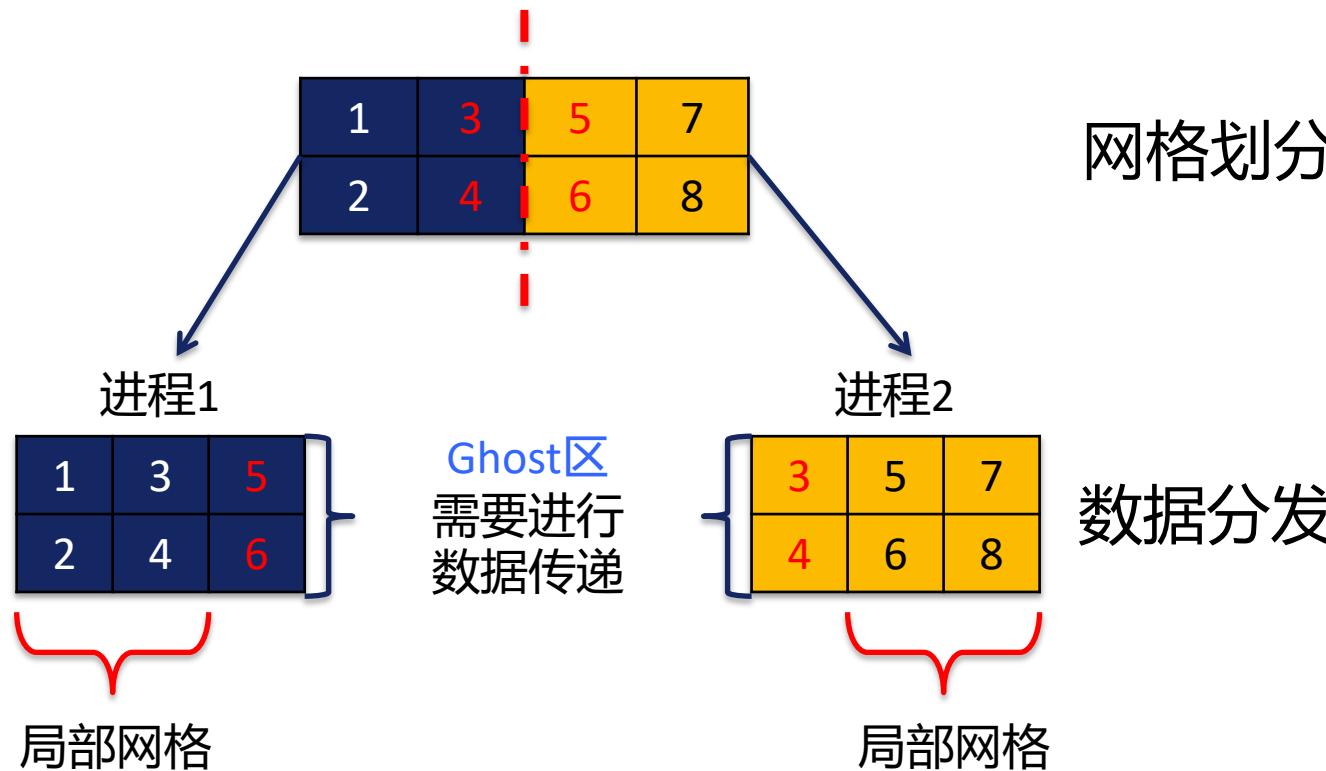
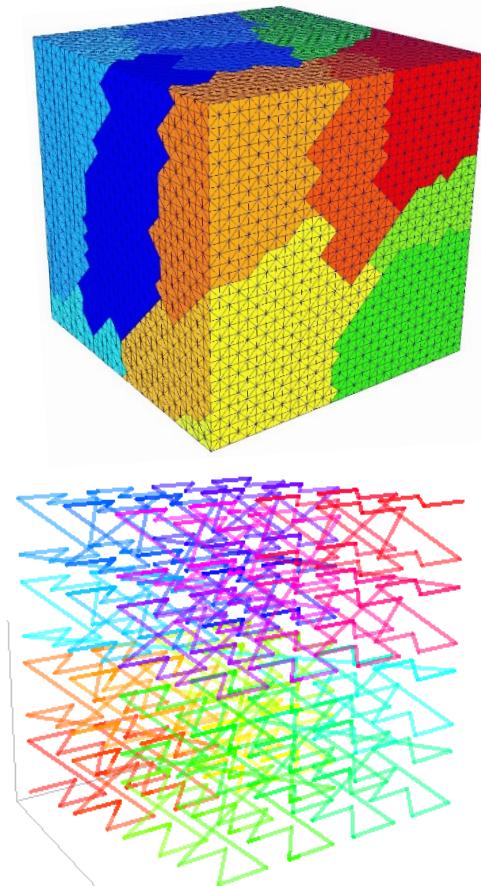
大规模集群的典型体系结构



算法的复杂度和可扩展性、对多核CPU的利用率、对众核加速卡的利用率、数据传输时间.....



并行网格划分与数据分发



多目标优化问题：每个部分的工作量的变化极小，界面面积极小，裂缝和井等特征不跨区域.....



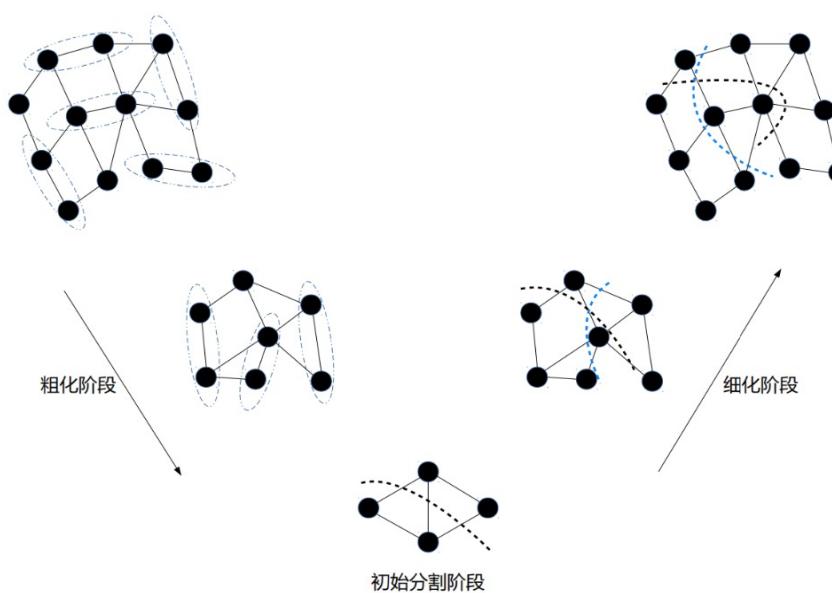
划分油藏网格的图分割方法



图分割一般有两个主要目标：

- 负载均衡 Load Balancing (减少存储代价)
- 最小化切割边或点的数目 Minimum Cuts (减少通讯代价)

要同时优化这两个目标是平衡图分割 (Balanced Graph Partitioning) 问题，是并行计算的基础问题和热点问题，但这是NP难问题！



多层分割算法 (Multi-level Partitioning) 核心思想是：

- 1) 对原图结构进行稀疏化 (如随机匹配、重边匹配算法等)，降低原图的大小
- 2) 达到一定节点数量后对缩减后的图结构进行分割 (如经典图增长、贪婪图增长算法等)
- 3) 将分割后的小图还原成原始结构保证每份子图的均衡性

合作者：刘伟峰团队（中国石油大学，北京）

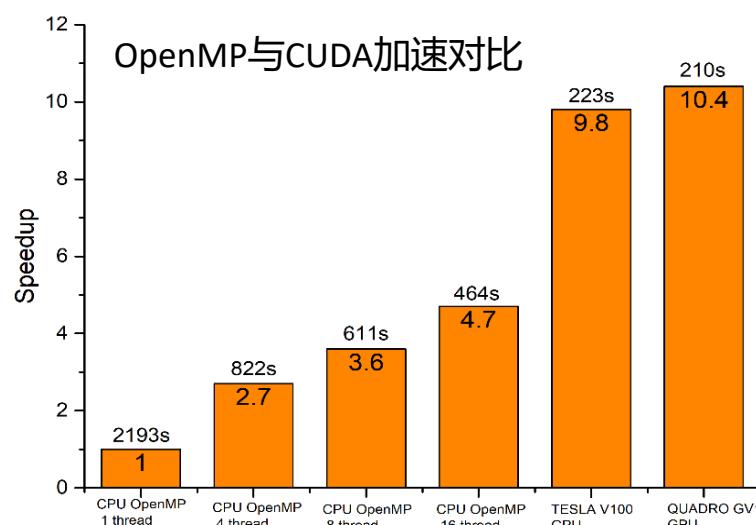




解法器节点内多线/进程并行测试



- 基于一般组分模型框架，实现黑油与组分模型的统一处理，完成了组分模型多相平衡计算的测试，非线性方程组解法器的稳健性得到验证
- 多阶段线性解法器在组分模型框架下的适用性和正确性得到初步验证
- 完成几种并行计算平台的测试

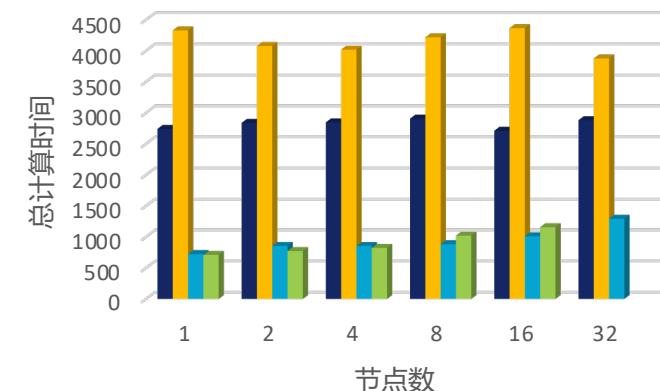
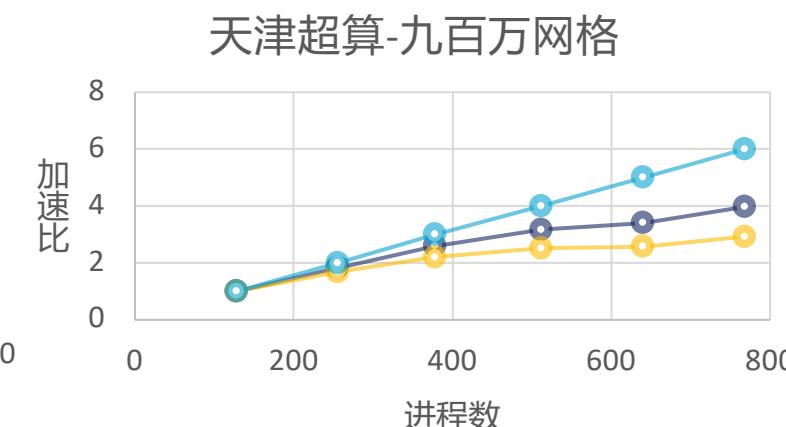
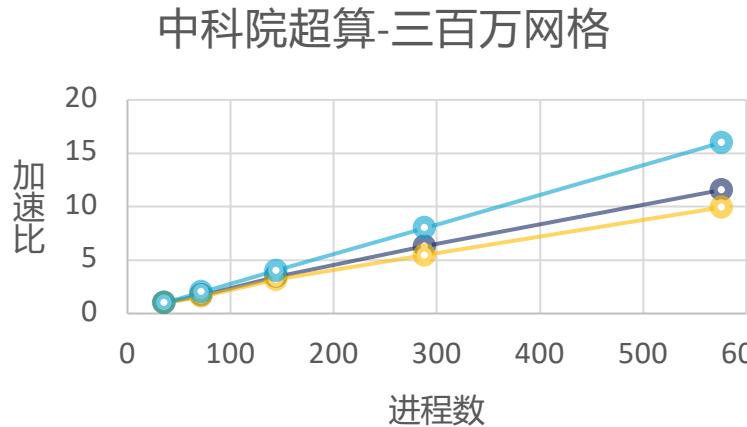


节点内MPI多进程并行测试（计算数学所LSSC-IV机器）						
进程数	1	2	4	8	16	32
Newton步数	165	165	166	166	167	162
解法器步数	905	912	926	927	940	911
解法器时间 (秒)	9992.0	5259.5	2686.1	1377.7	947.9	360.0
总计算时间 (秒)	21023.4	10285.1	5179.1	2661.1	1616.9	717.3
并行效率 (%)	100	100	101	98.8	81.3	91.6

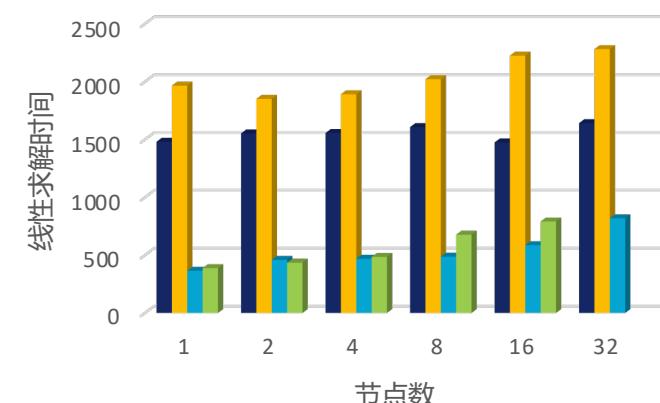
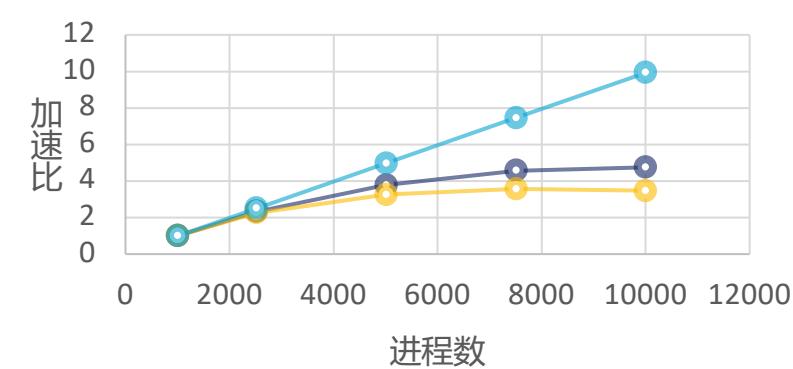
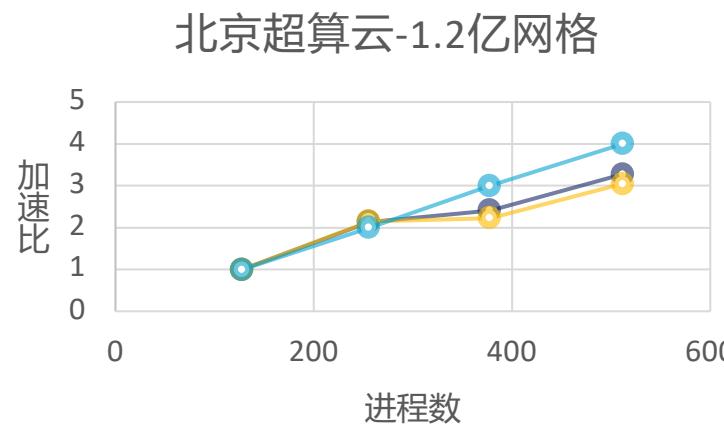
CPU-GPU/DCU异构并行测试（成都超算、网络中心419机器）				
计算硬件	CPU	V100	成都超算	网络中心
初次调用求解时间 (秒)	10.97	0.97	4.41	7.37
加速比 (初次调用)	—	11.3	2.5	1.5
再次调用求解时间 (秒)	10.34	0.36	0.84	1.33
加速比 (再次调用)	—	28.5	12.4	7.8



解法器节点间多进程并行测试



■ 广州超算-3M/24核 ■ 天津超算-2.4M/24核
■ 中科院超算-1.5M/36核 ■ 北京超算云-1.5M/32核



■ 广州超算-3M/24核 ■ 天津超算-2.4M/24核
■ 中科院超算-1.5M/36核 ■ 北京超算云-1.5M/32核



合作者：许进超（PSU）、关文超、张永东、许跃生等（中山大学）



模拟器节点内多进程并行测试



SPE10 (60x220x85=1.122M , 两相)							SPE1改 (384X320X64=7.864M , 三相)						
进程数	牛顿迭代	线性迭代	网格更新(s)	矩阵组装(s)	线性求解(s)	总时间(s)	进程数	牛顿迭代	线性迭代	网格更新(s)	矩阵组装(s)	线性求解(s)	总时间(s)
1	226	2087	101.8 (1)	786.3 (1)	2837.2 (1)	3849.6 (1)	1	28	104	1066.7 (1)	4528.4 (1)	2701.1 (1)	10694.7 (1)
2	233	2229	52.9 (1.92)	399.7 (1.97)	1795.9 (1.58)	2321.1 (1.66)	2	28	103	532.9 (2.00)	2217.1 (2.04)	1518.1 (1.78)	5612.0 (1.91)
4	242	2329	27.6 (3.69)	224.2 (3.51)	1111.5 (2.55)	1412.7 (2.73)	4	28	103	269.8 (3.95)	1090.9 (4.15)	913.9 (2.96)	2980.8 (3.59)
8	238	2647	13.8 (7.38)	109.9 (7.15)	643.2 (4.41)	797.0 (4.83)	8	28	103	140.0 (7.62)	530.7 (8.53)	427.6 (6.32)	1456.4 (7.34)
16	245	2528	7.5 (13.57)	57.8 (13.60)	364.0 (7.79)	449.2 (8.57)	16	28	104	71.4 (14.94)	266.2 (17.01)	250.7 (10.77)	791.0 (13.52)
32	241	2782	4.0 (25.45)	29.7 (26.47)	253.6 (11.19)	301.3 (12.78)	32	29	119	37.0 (28.83)	138.4 (32.72)	163.5 (16.52)	474.0 (22.56)
64	237	3120	5.1 (19.96)	25.1 (31.33)	294.0 (9.65)	344.4 (11.18)	64	27	124	30.0 (35.56)	90.2 (50.20)	145.2 (18.60)	421.1 (25.40)

北京超算云23区(64核)



模拟器节点内多进程并行测试



SPE5million (400x400x6=0.96M , 8组分)							SPE5改 (767X767X6=3.530M , 7组分)						
进程数	牛顿迭代	线性迭代	网格更新(s)	矩阵组装(s)	线性求解(s)	总时间(s)	进程数	牛顿迭代	线性迭代	网格更新(s)	矩阵组装(s)	线性求解(s)	总时间(s)
1	34	138	144.8 (1)	312.9 (1)	1648.9 (1)	2313.1 (1)	1	40	187	8900.0 (1)	6412.9 (1)	5636.4 (1)	25346.1 (1)
2	34	140	71.6 (2.02)	149.5 (2.09)	1157.8 (1.42)	1478.1 (1.56)	2	40	193	4427.0 (2.01)	3126.7 (2.05)	3432.4 (1.64)	13326.7 (1.90)
4	32	139	32.7 (4.43)	71.9 (4.35)	539.6 (3.06)	695.1 (3.33)	4	39	189	2153.1 (4.13)	1490.1 (4.30)	1856.3 (3.04)	6693.0 (3.79)
8	32	130	16.7 (8.67)	34.9 (8.97)	275.6 (5.98)	354.3 (6.53)	8	39	190	1070.0 (8.32)	728.2 (8.81)	911.6 (6.18)	3283.7 (7.72)
16	33	145	8.6 (16.83)	17.9 (17.48)	153.9 (10.71)	194.5 (11.89)	16	39	190	536.1 (16.60)	362.7 (17.68)	497.3 (11.33)	1711.7 (14.81)
32	34	140	4.5 (32.18)	9.3 (33.65)	95.7 (17.23)	118.3 (19.55)	32	39	192	271.0 (32.84)	180.5 (35.53)	321.0 (17.56)	928.0 (27.31)
64	32	129	3.4 (42.59)	6.6 (47.41)	82.3 (20.04)	101.6 (22.77)	64	39	192	198.9 (44.75)	123.5 (51.93)	320.4 (17.60)	812.1 (31.21)

北京超算云23区(64核)



预条件方法的自适应初始化

- 相对于商业软件（如tNavigator等）所使用的求解方法，我们的方法仍过于复杂
- 虽然迭代次数少，对大规模问题有一定的性能优势，但是并行效率提升难度大（ILU和AMG初始化、GS磨光、稀疏三角解、……）

减少Setup次数



降低Setup代价

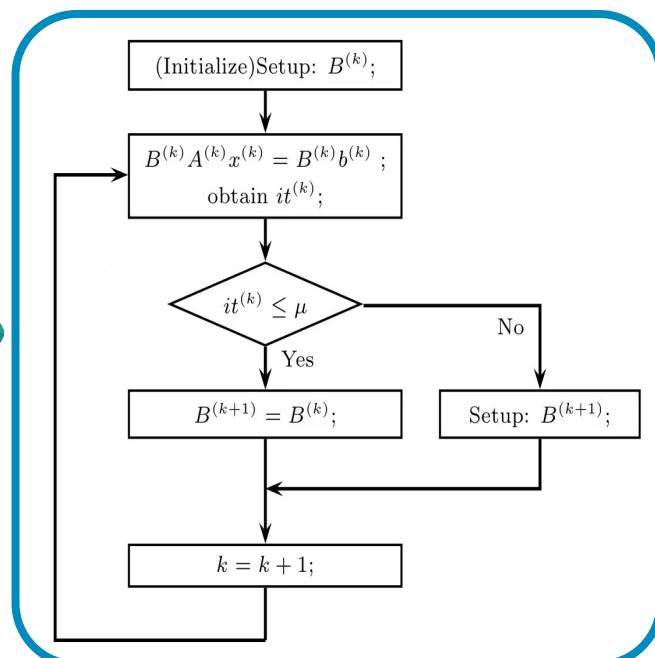


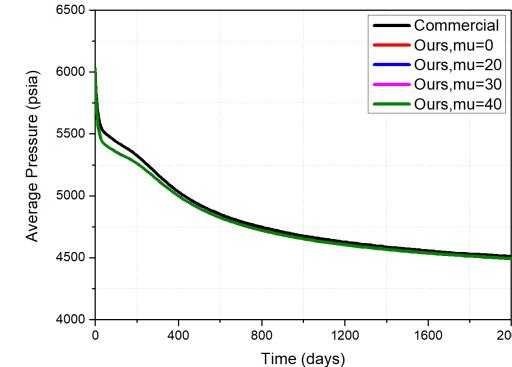
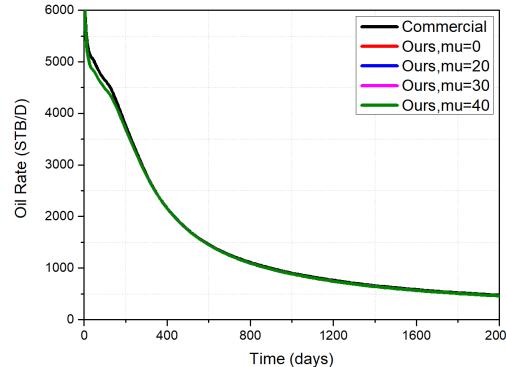
Table 2

SetupCalls, SetupRatio, Iter, Time (s), Speedup*, and Speedup for the two-phase SPE10 problem.

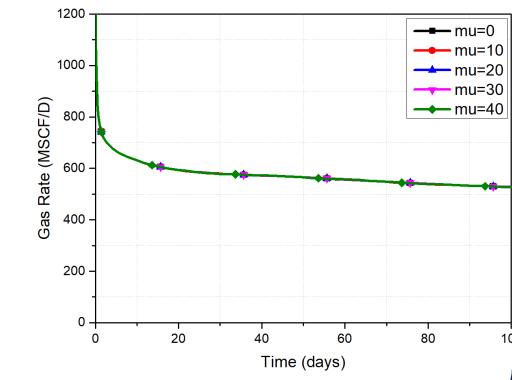
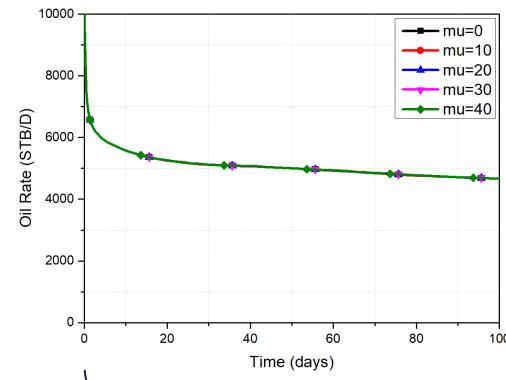
	μ	1	2	4	8	16
SetupCalls	0	239	239	239	239	239
	20	188	188	188	188	188
	30	58	58	58	58	58
	40	33	33	33	33	33
SetupRatio	0	11.08%	14.59%	20.63%	29.34%	41.38%
	20	9.45%	12.46%	17.55%	25.45%	38.14%
	30	5.19%	6.52%	9.20%	14.05%	26.09%
	40	4.05%	4.99%	6.62%	11.03%	21.83%
Iter	0	5823	5822	5818	5822	5827
	20	5855	5854	5853	5855	5857
	30	6309	6308	6315	6317	6319
	40	7033	7034	7037	7041	7044
Time	0	4753.00	2593.07	1491.97	970.26	829.24
	20	4821.98	2606.18	1488.95	949.98	804.56
	30	4919.81	2617.66	1444.92	877.85	718.13
	40	5475.72	2880.97	1570.72	946.35	769.34
Speedup*	0	1.00	1.83	3.19	4.90	5.73
	20	0.99	1.82	3.19	5.00	5.91
	30	0.97	1.82	3.29	5.41	6.62
	40	0.87	1.65	3.03	5.02	6.18
Speedup	0	1.00	1.83	3.19	4.90	5.73
	20	1.00	1.85	3.24	5.08	5.99
	30	1.00	1.88	3.40	5.60	6.81
	40	1.00	1.90	3.49	5.79	7.12



自适应初始化对结果的影响



两相结果



三相结果

Table 4

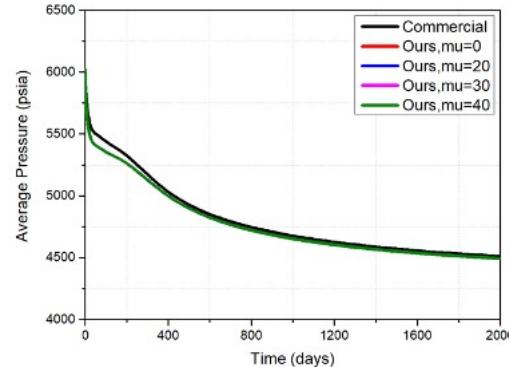
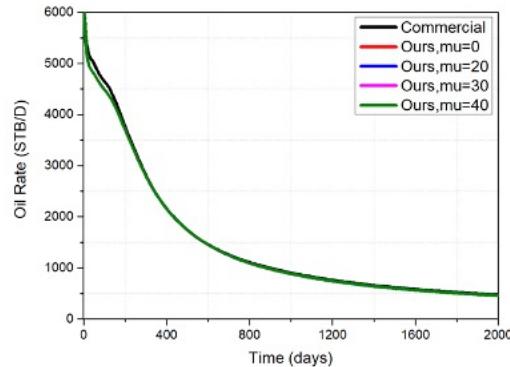
NumTSteps, NumNSteps, Iter, AvgIter, Time (h), and Speedup comparisons of the OpenMP version of commercial and our simulators for the two-phase SPE10 problem.

Simulators	μ	NT	1	2	4	8	16
Commercial	—	<i>NumTSteps</i>	671	785	891	1031	1100
		<i>NumNSteps</i>	1115	1244	1328	1458	1515
		<i>Iter</i>	150152	160254	161432	167757	175452
		<i>AvgIter</i>	134.7	128.8	121.6	115.1	115.8
		<i>Time</i>	14.62	8.45	4.71	2.72	1.54
		<i>Speedup</i>	1.00	1.73	3.10	5.37	9.49
0	0	<i>NumTSteps</i>	164	164	164	164	164
		<i>NumNSteps</i>	239	239	239	239	239
		<i>Iter</i>	5823	5822	5818	5822	5827
		<i>AvgIter</i>	24.4	24.4	24.3	24.4	24.4
		<i>Time</i>	1.48	0.88	0.57	0.43	0.39
		<i>Speedup</i>	1.00	1.68	2.60	3.44	3.79
20	20	<i>NumTSteps</i>	164	164	164	164	164
		<i>NumNSteps</i>	239	239	239	239	239
		<i>Iter</i>	5855	5854	5853	5855	5857
		<i>AvgIter</i>	24.5	24.5	24.5	24.5	24.5
		<i>Time</i>	1.50	0.88	0.57	0.42	0.38
		<i>Speedup</i>	1.00	1.70	2.63	3.57	3.95
30	30	<i>NumTSteps</i>	164	164	164	164	164
		<i>NumNSteps</i>	239	239	239	239	239
		<i>Iter</i>	6309	6308	6315	6317	6319
		<i>AvgIter</i>	26.4	26.4	26.4	26.4	26.4
		<i>Time</i>	1.52	0.88	0.56	0.40	0.36
		<i>Speedup</i>	1.00	1.73	2.71	3.80	4.22
40	40	<i>NumTSteps</i>	164	164	164	164	165
		<i>NumNSteps</i>	246	246	246	246	247
		<i>Iter</i>	7033	7034	7037	7041	7064
		<i>AvgIter</i>	28.6	28.6	28.6	28.6	28.6
		<i>Time</i>	1.68	0.96	0.60	0.42	0.36
		<i>Speedup</i>	1.00	1.75	2.80	4.00	4.50

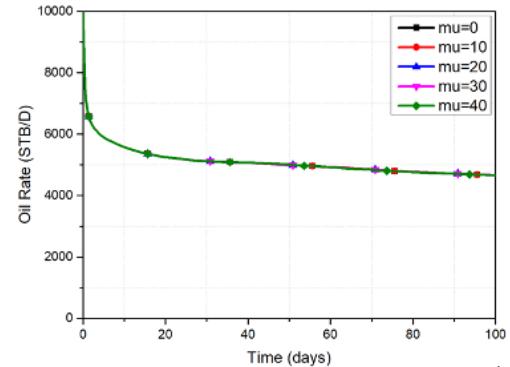
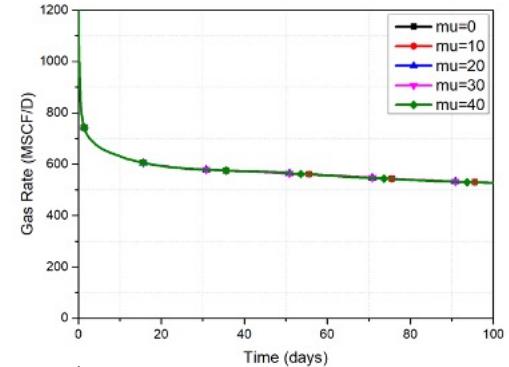




GPU版自适应初始化：黑油模型



两相结果



三相结果

Table 5

NumTSteps, NumNSteps, Iter, AvgIter, Time (h), and Speedup (compared with the commercial simulator)
comparisons of the GPU version of commercial and our simulators for the two-phase SPE10 problem.

Simulators	μ	NumTSteps	NumNSteps	Iter	AvgIter	Time	Speedup
Commercial	-	1004	1431	170276	119.0	3.070	-
Ours	0	164	239	5525	23.1	0.387	7.93
	20	164	240	5659	23.6	0.358	8.57
	30	165	240	6182	25.8	0.280	10.97
	40	167	244	6740	27.6	0.278	11.05

Ref: Li Zhao, Chunsheng Feng, Chen-Song Zhang, Shi Shu, "Parallel multi-stage preconditioners with adaptive setup for the black oil model", Computers & Geosciences, 168, 2022.





GPU版自适应初始化：组分模型

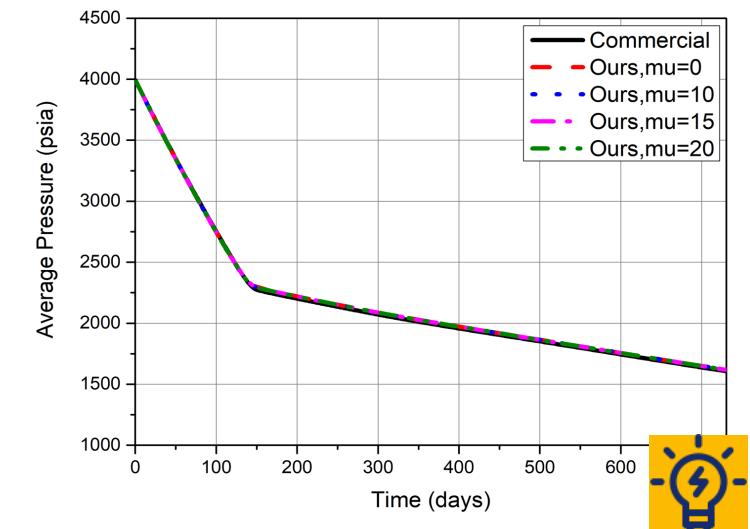
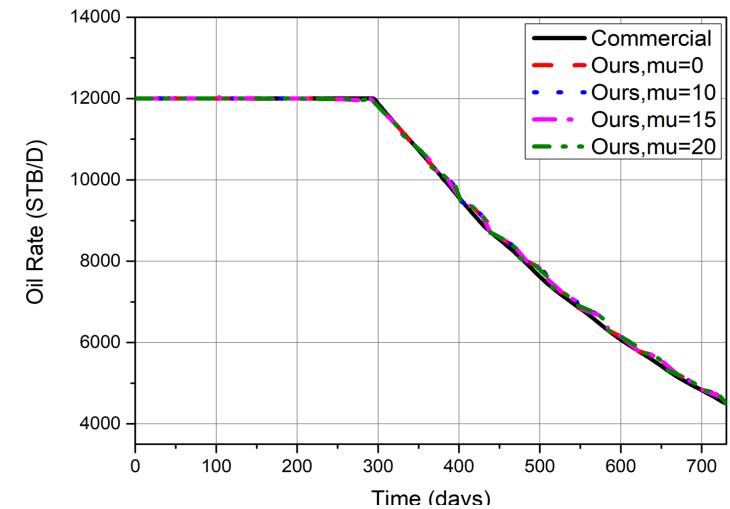


Table 7 SetupCalls, SetupRatio, Iter, Time (s), and Speedup of the different μ for the SPE5 problem.

Solvers	μ	SetupCalls	SetupRatio	Iter	Time	Speedup
ASMSP-GMRES-SEQ	0	389	16.30%	3747	2601.11	—
ASMSP-GMRES-CUDA	0	389	51.43%	3969	341.25	7.62
	10	186	34.59%	4064	324.76	8.01
	15	44	21.72%	4508	313.23	8.30
	20	12	18.01%	4747	314.50	8.27

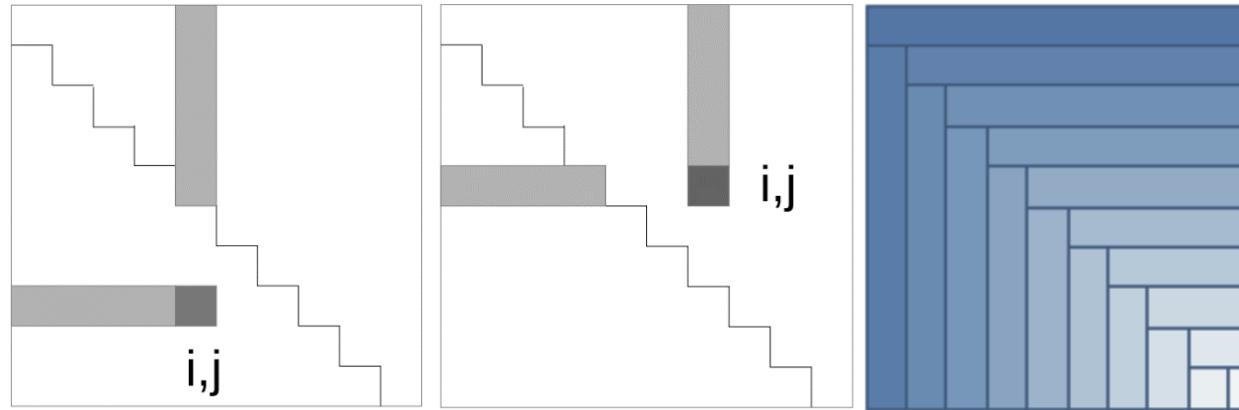
Table 8 NumTSteps, NumNSteps, Iter, AvgIter, Time (s), and Speedup comparisons of the commercial and our simulators for the SPE5 problem.

Simulators	μ	NumTSteps	NumNSteps	Iter	AvgIter	Time	Speedup
Commercial	—	382	748	47027	62.9	2339.00	—
Ours	0	147	389	3969	10.2	2178.78	1.07
	10	147	389	4064	10.4	2159.22	1.08
	15	147	389	4508	11.6	2142.22	1.09
	20	147	389	4747	12.2	2143.47	1.09





ILU方法的多线程并行



Algorithm 2: Fine-Grained Parallel Incomplete Factorization

```

1 Set unknowns  $l_{ij}$  and  $u_{ij}$  to initial values
2 for  $sweep = 1, 2, \dots$  until convergence do
3   parallel for  $(i, j) \in S$  do
4     if  $i > j$  then
5       
$$l_{ij} = \left( a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right) / u_{jj}$$

6     else
7       
$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

8     end
9   end
10 end

```

Ref: Edmond Chow and Aftab Patel. 2015. Fine-Grained Parallel Incomplete LU Factorization. SIAM J. Sci. Comput. 37, 2 (2015), C169–C193.

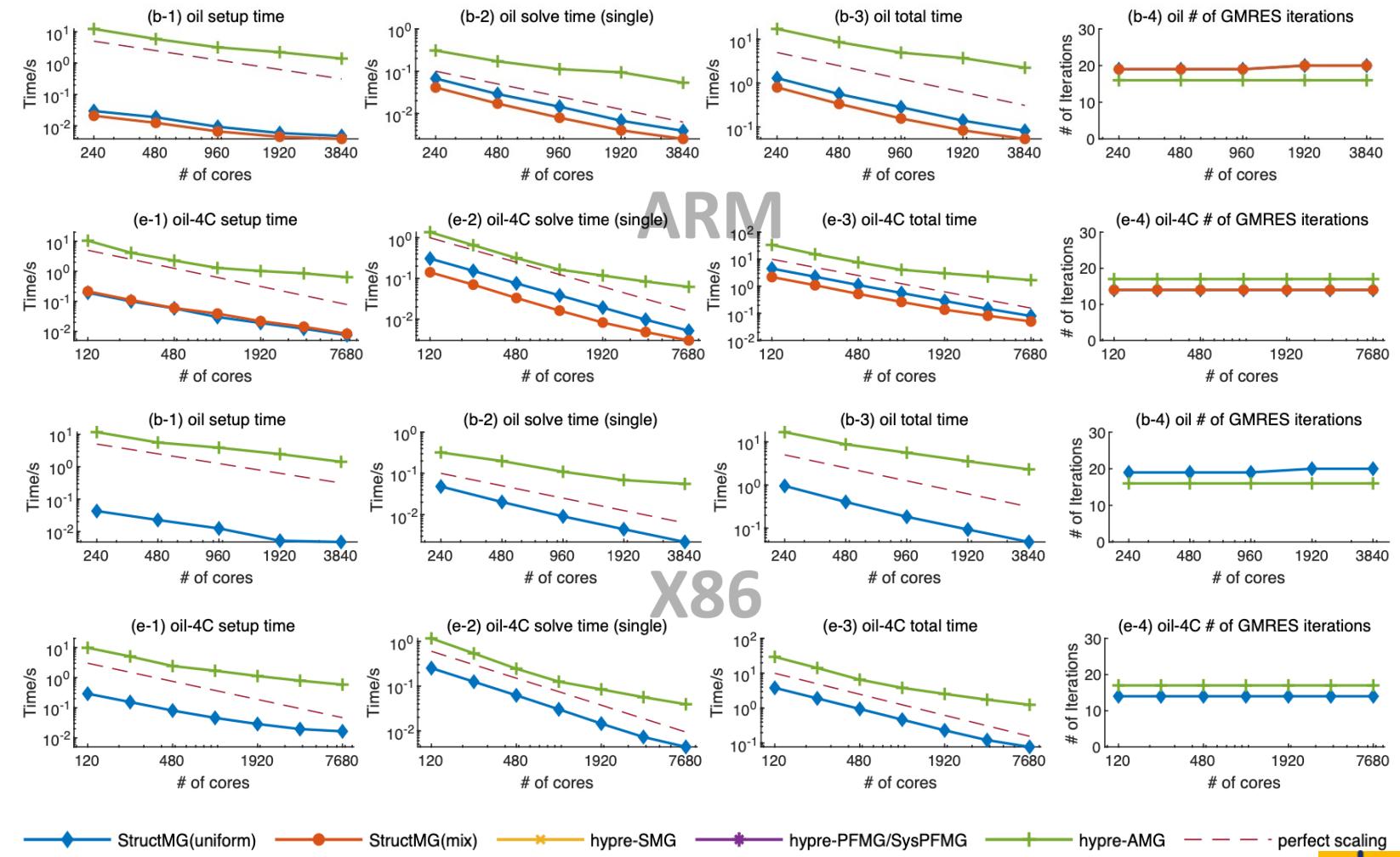
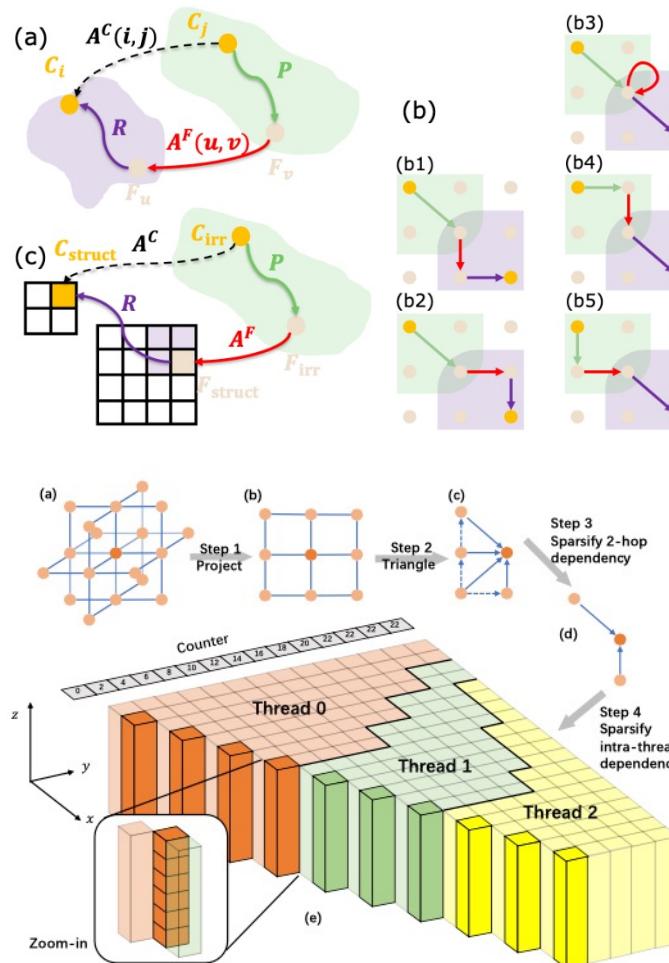


spe10矩阵sweep10次 (北京超算云BSCC-T6)

线程数	迭代步数	相对残量	setup时间 (秒)	solve时间 (秒)	总时间 (秒)	加速比
1	7	9.27E-04	5.2847	3.7803	9.0650	--
2	7	9.27E-04	2.6924	2.9536	5.6460	1.61
4	7	9.27E-04	1.6642	1.5923	3.2565	2.78
8	7	9.27E-04	0.9427	0.9902	1.9329	4.69
16	7	9.27E-04	0.7441	0.5898	1.3339	6.80
32	7	9.27E-04	0.6717	0.4421	1.1138	8.14
48	7	9.27E-04	0.6498	0.4246	1.0744	8.44
64	7	9.27E-04	0.7738	0.5747	1.3485	6.72
96	7	9.27E-04	2.6111	1.1632	3.7743	2.40



基于拓扑结构化网格的多重网格法



合作者：宗毅、薛巍等（清华）

强可扩展性测试（有效网格数约3千万）

04

发展规划

Development plans and conclusion remarks



OpenCAEPoro软件功能开发进度



输入输出	简单输入输出格式	兼容商业软件格式		可视化软件格式
并行支撑	并行区域划分	并行通信	加速卡并行优化	节点内并行优化 节点间并行优化
耦合处理	全隐式方法	半隐式方法	迭代半隐式方法	自适应显隐方法 耦合处理方法优化
初始化	单介质模型初始化	用户指定初始状态	多重介质模型初始化	离散裂缝模型初始化
空间离散	TPF有限体积法	离散裂缝方法	多重介质有限体积法	离散裂缝混合元
时间离散	向后Euler时间离散	时间步长自适应	初值获取技术	优化时间步长选择 时间并行算法
非线性求解	Newton线性化	线搜索方法		拟Newton法
线性求解	解耦方法	多阶段预条件方法	Krylov子空间方法	最优求解参数选择 AIM离散的解法
平衡计算	平衡方程闪蒸计算	稳健的相平衡判断	非等温问题求解	化学反应方程求解

多相多组分渗流问题大规模数值模拟关键技术





OpenCAEPoro软件开发规划





大规模并行技术路线



已有研究基础

共享内存OpenMP并行测试

GPU/DCU并行测试

通用CPU万核并行测试

模型问题时间并行测试

线性解法器适应性测试

非线性解法器稳健性测试

模型问题容错解法器测试

后续重点工作

进一步优化数据结构

减少冗余数据移动

优化主-从核异构并行算法

使用时间-空间并行算法

优化线性解法器效率

使用混合精度算法

结合通信避免和通信隐藏

Nonhydrostatic Atmospheric DyCore,
Summit, 4600节点 (27600 V100GPU)

根据前期数值算法研究（解耦方法、多阶段预条件方法、多层迭代法、稀疏矩阵运算方法等）、在广州超算的万核扩展性实验、国际同行在数万加速器上的测试数据，我们有信心达成项目目标！

最大程度地保持应用目标和最优解法，而不是基于简化的算法



数模云平台建设



- 远程桌面，方便远程使用，数模软件的适应性和性能
- 构建高速网络，提高访问速度，保护数据安全
- 实现前端、平台、数模无缝衔接，实现跨平台可移植
- 助力“东数西算”战略

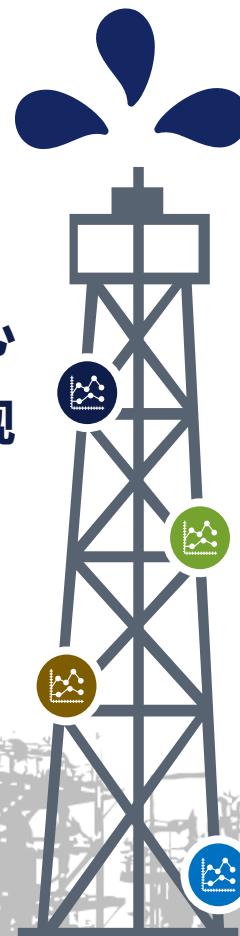




总结



谢谢！



超算能力是一个国家核心
科技竞争力的集中体现

异构并行环境给软件开发
带来重大机遇和巨大挑战

适应硬件体系结构的软件和
算法是发挥硬件性能的推动力

并行工业软件开发需要
长期和坚定不移的努力



主要参考文献

1. Linear solvers for petroleum reservoir simulation, C.-S. Zhang, **Journal on Numerical Methods and Computer Applications**, 43, 1–26 (03/2022), in Chinese.
2. Convergence analysis of inexact two-grid methods: A theoretical framework, X. Xu and C.-S. Zhang, **SIAM Journal on Numerical Analysis**, 60, 133–156 (01/2022)
3. Multiscale hybrid-mixed finite element method for flow simulation in fractured porous media, P. Devloo, W. Teng, and C.-S. Zhang, **Computer Modeling in Engineering and Sciences**, 119, 145–163 (04/2019)
4. On the ideal interpolation operator in algebraic multigrid methods, X. Xu and C.-S. Zhang, **SIAM Journal on Numerical Analysis**, 56, 1693–1710 (06/2018).
5. Analytical decoupling techniques for fully implicit reservoir simulation, C. Qiao, S. Wu, J. Xu, and C.-S. Zhang, **Journal of Computational Physics**, 336, 664–681 (05/2017)
6. On Robust and Efficient Parallel Reservoir Simulation on Tianhe-2, W. Guan, C. Qiao, H. Zhang, C.-S. Zhang, et al., **SPE Reservoir Characterization and Simulation Conference and Exhibition**, SPE-175602 (08/2015)
7. A multilevel preconditioner and its shared memory implementation for a new generation reservoir simulator, S. Wu, J. Xu, C. Feng, C.-S. Zhang, et al., **Petroleum Science**, 11, 540–549 (10/2014)
8. Numerical study of geometric multigrid on CPU–GPU heterogenous computers, C. Feng, S. Shu, J. Xu, and C.-S. Zhang, **Advances in Applied Mathematics and Mechanics**, 6, 1–23 (01/2014)
9. Application of auxiliary space preconditioning in field-scale reservoir simulations, X. Hu, J. Xu, and C.-S. Zhang, **Science China Mathematics**, 56, 2737–2751 (12/2013)
10. Combined preconditioning with applications in reservoir simulation, X. Hu, S. Wu, X.-H. Wu, J. Xu, C.-S. Zhang, S. Zhang, and L. Zikatanov, **Multiscale Modeling and Simulation**, 11, 507–521 (08/2013)