数学与系统科学研究院

2022年夏季强化课程

大规模代数系统解法器

中国科学院大学
夏季强化课程
2022

Fast Solvers for Large Algebraic Systems

Brief Introduction on This Course

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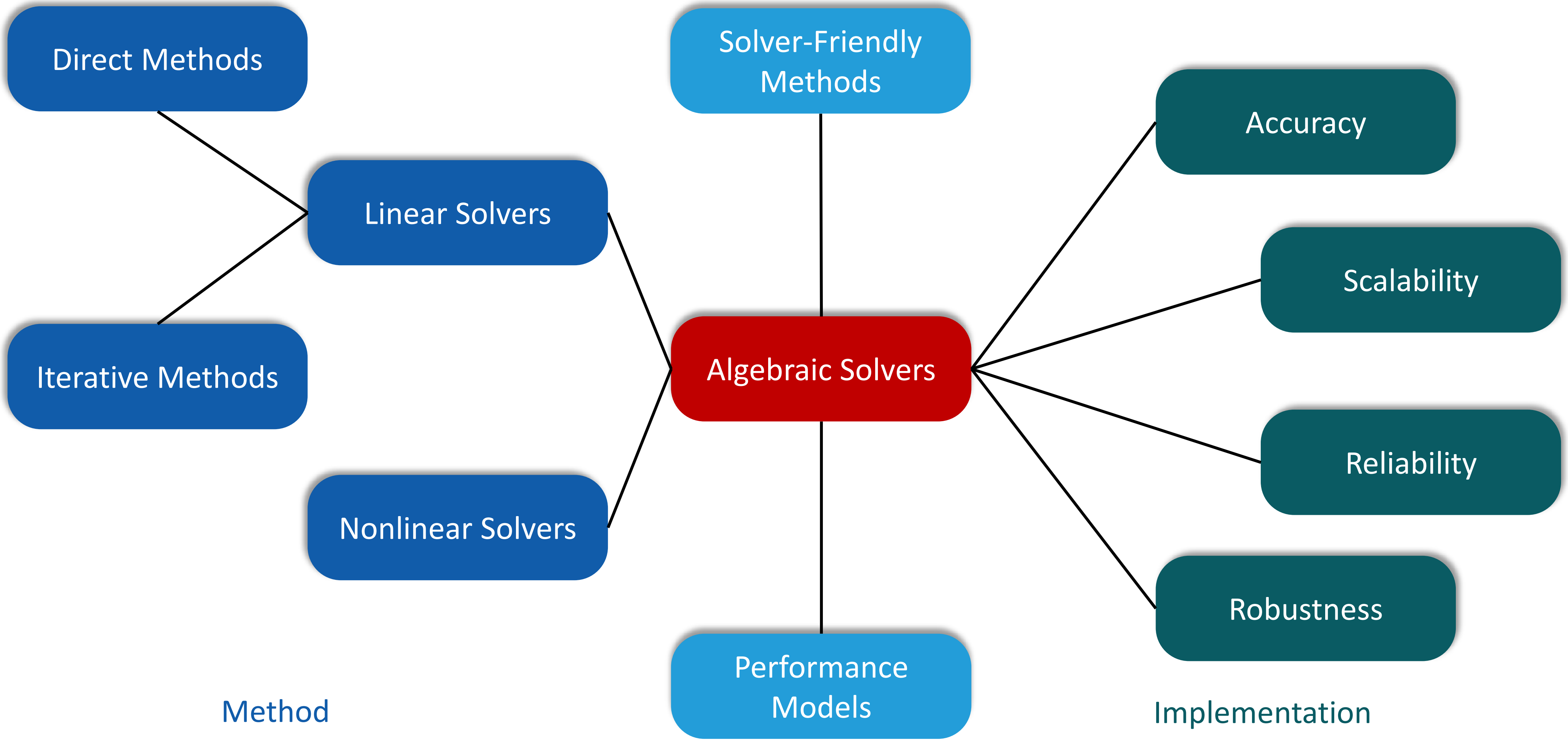
大规模代数系统解法器

Agenda

- **Lecture 1: Large-scale numerical simulation**
- **Lecture 2: Fast solvers for sparse linear systems**
- **Lecture 3: Methods for non-symmetric problems**
- **Lecture 4: Methods for nonlinear problems**
- **Lecture 5: Mixed-precision methods**
- **Lecture 6: Communication hiding and avoiding**
- **Lecture 7: Fault resilience and reliability**
- **Lecture 8: Robustness and adaptivity**

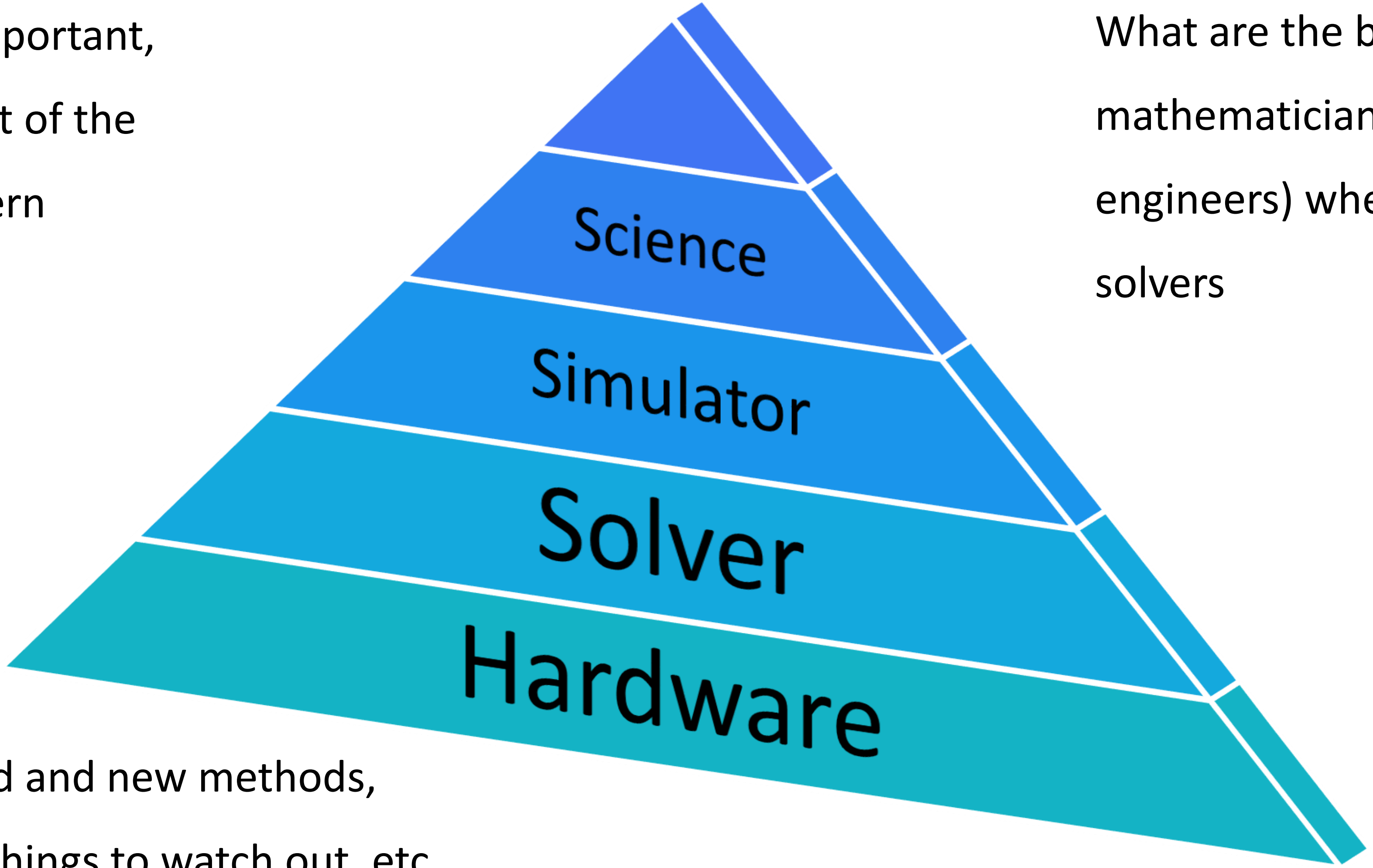
✓ Arnoldi	✓ TG	✓ SD
✓ LU	✓ MG	✓ Newton
✓ CG	✓ AMG	✓ Broyden
✓ GMRES	✓ DDM	✓ TR
✓ PGMRES	✓ MSC	✓ Dogleg
✓ FGMRES	✓ SSC	✓ FP/MP
✓ GMRES-DR	✓ PSC	✓ MatMul
✓ GMRES-IR	✓ RSC	✓ ECC
✓ MP-GMRES	✓ FAS	✓ CP/R
✓ CA-GMRES	✓ ASPIN	⋮
✓ FT-GMRES	✓ MSPIN	

Topics


Direct Methods
Linear Solvers
Iterative Methods
Nonlinear Solvers
Solver-Friendly Methods
Algebraic Solvers
Performance Models
Accuracy
Scalability
Reliability
Robustness
Method
Implementation

Goals

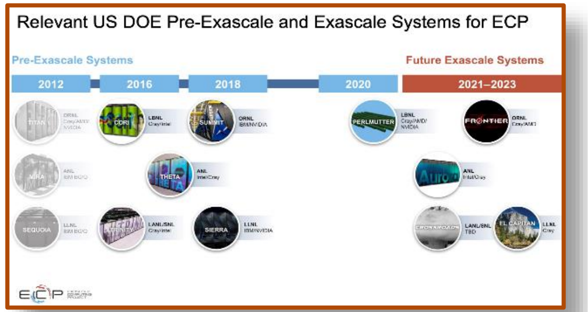
Complexity is important, but it is only part of the picture on modern computers

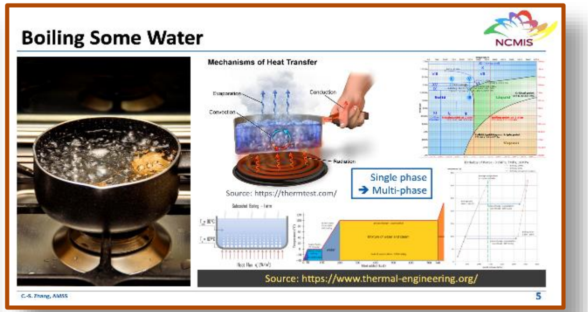


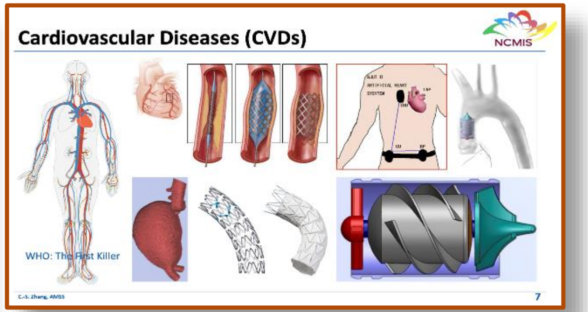
What are the blind spots for mathematicians (or software engineers) when they design solvers

Discuss some old and new methods, available tools, things to watch out, etc

Styles





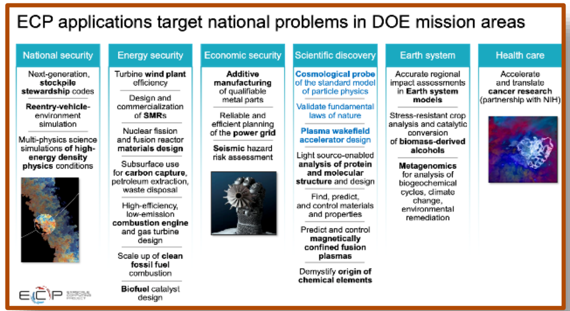


Theorem (Leray 1932-34)

For every $T>0$ there exists a weak solution (in the sense of distribution) of the Navier-stokes equations, which also satisfies

$$\vec{u} \in C_w([0,T], L^2(\Omega)) \cap L^2([0,T], H^1(\Omega))$$

The uniqueness of weak solutions in the three dimensional Navier-Stokes equations case is still an open question.

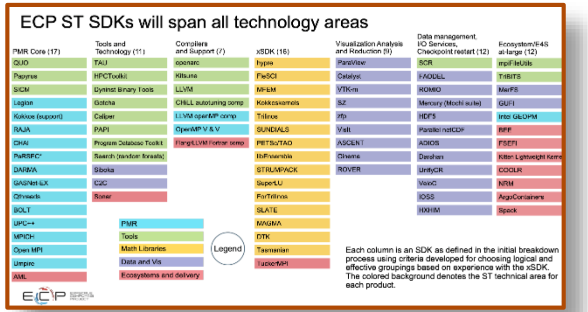


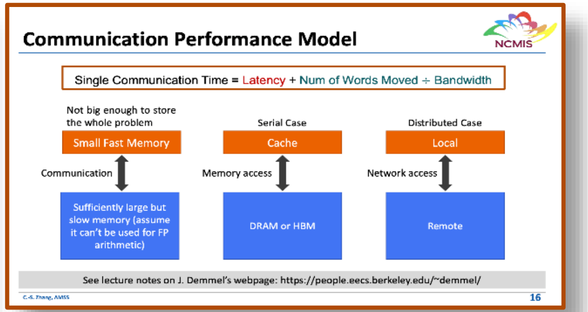
To Impress ➡ To Interest ⬅ To Inform

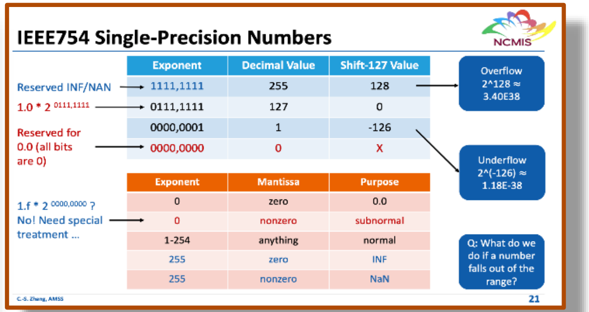
Results

- Chongsheng Cao and E.S.T. (2003)

* the uniqueness of weak solutions
* the global existence of the strong solutions for any initial data in H^1
* existence of the global attractor.
* upper bounds for the dimension of the global attractor.







Bénard Convection Porous Medium

$$\gamma \frac{\partial}{\partial t}\vec{u} + \vec{u} + \nabla p - RT\vec{k} = 0$$
$$\nabla \cdot \vec{u} = 0$$
$$\frac{\partial}{\partial t}T - \kappa\Delta T + (\vec{u}\cdot\vec{\nabla})T = 0$$

Subject to certain physical boundary conditions.

- P. Fabrie [1986] Global Existence & Uniqueness
- H.V. Ly E.S.T. [1999] $(\gamma = 0)$
  Same result based on Galerkin numerical procedure.
  This gived leads to Spatial Analyticity, and exponential rate of convergence of the Galerkin procedure.
- M. Oliver and E.S.T. $(\gamma > 0)$
  Spatial analyticity of the attractor.

Left-outs

Method

Now we consider a descent direction method with search direction $p^{(m)}$, i.e.

$$u^{(m+1)} = u^{(m)} + \alpha_m p^{(m)}. \tag{2.22}$$

In this case, the "optimal" stepsize from the exact line-search is

$$\alpha_m := \frac{\left(r^{(m)}, p^{(m)}\right)}{\left(p^{(m)}, p^{(m)}\right)_{\mathcal{A}}}. \tag{2.23}$$

We notice that the residual after one iteration is

$$r^{(m+1)} = r^{(m)} - \alpha_m \mathcal{A} p^{(m)}.$$

In order to keep the iteration going, we wish to construct a new search direction which is orthogonal to the previous search directions. This motives us to define

$$p^{(m+1)} := r^{(m+1)} + \beta_m p^{(m)}, \quad \text{such that} \quad \left(p^{(m)}, p^{(m+1)}\right)_{\mathcal{A}} = 0.$$

By simple calculations, we get the weight

$$\beta_m := -\frac{\left(\mathcal{A} r^{(m+1)}, p^{(m)}\right)}{\left(\mathcal{A} p^{(m)}, p^{(m)}\right)}. \tag{2.24}$$

This is basically the so-called conjugate gradient (CG) method.

Algorithm

```
%% Given an initial guess u and a tolerance ε;
r ← f − Au,  p ← r;
while ‖r‖ > ε
    α ← (r,r)/(Ap,p);
    ũ ← u + α p;
    r̃ ← r − αAp;
    β ← (r̃,r̃)/(r,r);
    p̃ ← r̃ + β p;
    Update:  u ← ũ,  r ← r̃,  p ← p̃;
end
```

Implementation

```
++numIter; // iteration count

A->Apply(pk, ax); // ax = A * p_k, main computational work

// alpha_k = (z_{k-1}, r_{k-1})/(A*p_{k-1},p_{k-1})
tmpb = ax.Dot(pk);
if (fabs(tmpb) > CLOSE_ZERO * CLOSE_ZERO)
    alpha = tmpa / tmpb;
else {
    // Update solution and residual
    x.AXPY(alpha, pk);   // x_k = x_{k-1} + alpha_k*p_{k-1}
    rk.AXPY(-alpha, ax); // r_k = r_{k-1} - alpha_k*A*p_{k-1}
    // Check residual for convergence
    resAbs = rk.Norm2();
    resRel = resAbs / denAbs;
    if (resRel > params.relTol && resAbs > params.absTol) {
        FASPXX_WARNING("Divided by zero!");
        errorCode = FaspRetCode::ERROR_DIVIDE_ZERO;
    } // otherwise converged to zero solution
    break;
}

// Update solution and residual
x.AXPY(alpha, pk);   // x_k = x_{k-1} + alpha_k*p_{k-1}
rk.AXPY(-alpha, ax); // r_k = r_{k-1} - alpha_k*A*p_{k-1}
```

- Convergence analysis
- Specific hardware architectures
- Writing a solver code
- Practical usages of numerical packages

→

- Numerical Analysis, Numerical Linear Algebra, …
- Computer Architectures, Parallel Computing, …
- Data Structures, Software Engineering, MPI, …
- User Manuals, Technical Descriptions, …

Final Project

- At the end of each lecture, you will be given some papers to read.
- There will be some questions related to the papers.
- All the questions are simple but open-ended (do not expect uniform answers).
- You can read at least three papers (you are welcome to extend your reading).
- You can answer some of the questions or you can raise more questions to yourselves.
- You will need to attend all lectures and hand in a final report (in the format of article/essay).
- Write your own understandings, not what papers told you.
- For extra credit, answer questions online and catch bugs/typos offline.

Schedule

06/18 (Sat), 06/19 (Sun), 06/25 (Sat), 06/26 (Sun),

07/02 (Sat), and 07/03 (Sun)

13:30—17:00, 20 hours in total

Lecture 1

会议时间：2022/06/18 13:30-17:30 (GMT+08:00) 北京时间

https://meeting.tencent.com/dw/yJOTfCfgHeaO

腾讯会议：580-936-725, 会议密码：1234

Lecture 2

会议时间：2022/06/19 13:30-17:30 (GMT+08:00)北京时间

https://meeting.tencent.com/dw/QlpW4J4H0npS

腾讯会议：169-573-566, 会议密码：1234

腾讯网络研讨会

功能介绍

- 网络研讨会(Webinar)是腾讯会议推出的一款面向沙龙、圆桌会议、行业峰会等场景的公开会议产品；
- 具有更低的延时，支持人数更多，同时在会中能够赋予观众与嘉宾更多的互动可能性；
- 相比常规会议，网络研讨会更强调公开和广泛推广，更强调可管、可控。具体包括：
  - 会前：品牌展示，会议详情介绍，嘉宾邀请，观众报名；
  - 会中：会议秩序管理，举手互动，问答互动；
  - 会后：回放、历史会议沉淀；
- 商业版、企业版最高支持2万名观众同时参会；
- 网络研讨会现已支持客户端，小程序和电话入会，暂不支持web观看。

使用条件

- 创建网络研讨会：
  - 腾讯会议官网(https://meeting.tencent.com/user-center)；
  - Windows/macOS 电脑端腾讯会议App；
  - iOS/Android 手机端 2.20 以上版本的腾讯会议App（需 Android4. 系统）；
- 加入网络研讨会：
  - Windows/macOS 电脑端腾讯会议 App；
  - iOS/Android 手机端 2.14 以上版本的腾讯会议 App (
  - 腾讯会议微信小程序。

Contact Me

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